Front. Optoelectron. 2012, 5(3): 341–344
DOI 10.1007/s12200-012-0271-0

RESEARCH ARTICLE

Local density of states in photonic crystal cavity

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Abstract Local radiative density of optical states (LDOS) offers a tool to control the radiative rate of spontaneous emission from molecules, atoms, and quantum dots, which is proportional to LDOS. This paper presents that LDOS how to make the population of excited-state decay exponentially in time, and how these dynamics can be affected. By adopting the plane-wave expansion method, properties of an inverse-opal photonic crystal are studied with the help of photonic dispersion relations. Results in this paper show that the LDOS is radically modified in photonic crystal, and the rate of spontaneous emission can be described by the functions of position in the crystal and orientation of transition dipole moment.

Keywords spontaneous emission, local radiative density of optical states (LDOS), photonic crystal, plane-wave method

1 Introduction

The radiative rate of spontaneous emission of elementary light source (atoms, molecules or quantum dots) is proportional to local radiative density of optical states (LDOS), and sources with certain orientations of transition dipole moments couple to LDOS [1]. This projected LDOS represents the number of electromagnetic states at a given frequency, location and orientation of the transition dipole. Therefore, based on the frequency and position dependence of the LDOS, a tool is offered to control the radiative rate of spontaneous emission from molecules, atoms, and quantum dots [2].

Photonic crystal is optical structure, it contains a periodic modulation of their refractive index and form band gaps, which can prevent electromagnetic from propagation in the plane of the crystal. Photonic crystal with defects ruin the translational symmetry of crystal lattice, form a cavity surrounding the defect, and introduce an increased LDOS within the band gap [1]. In this paper, plane-wave expansion method was adopted to calculate the LDOS in photonic crystal cavity, and the effects of photonic crystal cavity on LDOS and radiative rate of spontaneous emission were investigated.

Received May 9, 2012; accepted June 12, 2012

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2 Local density of states

Spontaneous emission of light is called a transition of an emitter (atom, molecule or quantum dot) from its excited state to its lower energy state by emitting one or more photons. In the case of a two-level atom, ε_a and ε_b are the energies of the excited state a and ground state b respectively. And the interaction between the two-level atom in its excited state a with vacuum-field modes with frequency ω_k leads to a transition to the atomic ground state b via emission of a photon with energy $\hbar\omega_k = \varepsilon_a - \varepsilon_b$, as shown in Fig. 1.

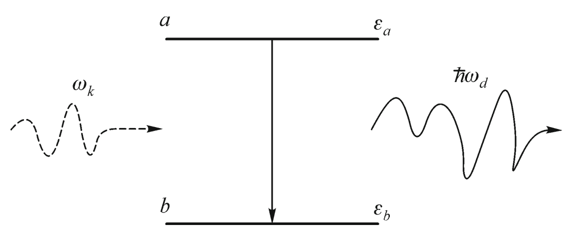

Fig. 1 Scheme of interaction of two-level atom with vacuum-field mode

The Schrodinger equation of the system as follows [3]:

$$\mathrm{i}\hbar \frac{\partial|\Psi(t)\rangle}{\partial t} = H|\Psi(t)\rangle. \tag{1}$$

The state $|\Psi(t)\rangle$ is a linear combination of the states $|a,n\rangle$ and $|b,n\rangle$ of the unperturbed atom-field system. Here, $|a,n\rangle$ is the state, in which the atom is under its excited state and the field has n photons. $|b,n\rangle$ is the state, in which the atom is in its ground state and the field has n photons. Taking at time $t = 0$ the atom to be in the state $|a\rangle$ and the field in vacuum mode $|0\rangle$, the state vector can be written as

$$|\Psi(t)\rangle = c_a(t)|a,0\rangle + \sum_{\boldsymbol{k}} c_{b,\boldsymbol{k}}(t)|b,1_{\boldsymbol{k}}\rangle, \tag{2}$$

where $c_a(t)$ and $c_{b,\boldsymbol{k}}(t)$ are time dependent probability amplitudes of state, in which initial conditions $c_a(0) = 1$ and $c_{b,\boldsymbol{k}}(0) = 0$. From the Schrodinger equation, the equation of motions for $c_a(t)$ and $c_{b,\boldsymbol{k}}(t)$ can be obtained, with frequency integration over a Dirac δ function and further approximations, $c_a(\boldsymbol{r},t)$ can be expressed as [4]

$$\begin{aligned} c_a(\boldsymbol{r},t) = & -\frac{d^2}{2(2\pi)^3\varepsilon_0\varepsilon(\boldsymbol{r})\hbar}\int_0^t \mathrm{d}t' c_a(\boldsymbol{r},t') \\ & \times \int_0^\infty \mathrm{d}\omega\omega \mathrm{e}^{\mathrm{i}(\omega-\omega_d)(t'-t)} \\ & \times \int_0^\infty \mathrm{d}\boldsymbol{k}\delta(\omega-\omega_{\boldsymbol{k}})|\boldsymbol{e}_d\cdot\boldsymbol{\Lambda}_{\boldsymbol{k}}(\boldsymbol{k})|^2. \end{aligned} \tag{3}$$

Equation (3) contains the LDOS, which counts the number of modes per unit volume at a given frequency ω, and the atomic dipole oriented along $\boldsymbol{e}_d$ and positioned at $\boldsymbol{r}$ can couple to this frequency. This projected LDOS is defined as [5]

$$N(\boldsymbol{r},\omega,\boldsymbol{e}_d) \equiv \frac{1}{(2\pi)^3\varepsilon(\boldsymbol{r})}\sum_p \int_0^\infty \mathrm{d}\boldsymbol{k}\delta(\omega-\omega_{\boldsymbol{k},P})|\boldsymbol{e}_d\cdot\boldsymbol{\Lambda}_{\boldsymbol{k}}(\boldsymbol{r})|^2, \tag{4}$$

where the summation on the field polarization p has been inserted back. The dielectric function $\varepsilon(\boldsymbol{r})$ must be real here; otherwise the complex mode density $N(\boldsymbol{r}, \omega, \boldsymbol{e}_d)$ is not be defined.

3 Plane-wave expansion method

The plane-wave method is a widespread technique to calculate eigenvalues and the local density of eigenmodes in perfectly-periodic photonic crystal. According to Bloch theorem, which is the base of the plane-wave method, the Bloch modes of a photonic crystal can be expressed as a product of plane waves and functions describing the periodicity of the crystal lattice. These known periodic functions are expanded into Fourier series and inserted into the wave equation. To compute the eigenfrequencies $\omega(k)$ and the expansion coefficients of the eigenmodes $\boldsymbol{u}_{\boldsymbol{G}}^{n,\boldsymbol{k}}$, the infinite equation set is truncated: the reciprocal-lattice vectors $\boldsymbol{G}$ are restricted to a finite set ζ with $N_{\boldsymbol{G}}$ elements [6,7]. This results in a $3N_{\boldsymbol{G}}$ dimensional equation:

$$-\sum_{\boldsymbol{G}'\in\zeta}\eta_{\boldsymbol{G}-\boldsymbol{G}'}(\boldsymbol{k}+\boldsymbol{G})\times\left[(\boldsymbol{k}+\boldsymbol{G}')\times\boldsymbol{u}_{\boldsymbol{G}'}^{n,\boldsymbol{k}}\right] = \frac{\omega_n(\boldsymbol{k})^2}{c^2}\boldsymbol{u}_{\boldsymbol{G}}^{n,\boldsymbol{k}}, \quad \forall\boldsymbol{G}\in\zeta. \tag{5}$$

The transversality of the field gives an additional condition: $(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{u}_{\boldsymbol{G}}^{n,\boldsymbol{k}} = 0$, which eliminates one component of $\boldsymbol{u}_{\boldsymbol{G}}^{n,\boldsymbol{k}}$. For each $\boldsymbol{k}+\boldsymbol{G}$ one needs to find two orthogonal unit vectors $\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}}^{1,2}$ that form an orthogonal triad with $\boldsymbol{k}+\boldsymbol{G}$. By expressing the eigenmode expansion coefficients in the plane normal to $\boldsymbol{k}+\boldsymbol{G}$ as $\boldsymbol{u}_{\boldsymbol{G}}^{n,\boldsymbol{k}} = \boldsymbol{u}_{\boldsymbol{G},1}^{n,\boldsymbol{k}}\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}}^1 + \boldsymbol{u}_{\boldsymbol{G},2}^{n,\boldsymbol{k}}\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}}^2$, one third of the unknown is removed. Equation (5) becomes

$$\begin{aligned} & \sum_{\boldsymbol{G}\in\zeta}\eta_{\boldsymbol{G}-\boldsymbol{G}'}|\boldsymbol{k}+\boldsymbol{G}||\boldsymbol{k}+\boldsymbol{G}'| \\ & \begin{pmatrix} \boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}}^2\cdot\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}'}^2 & -\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}}^2\cdot\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}'}^1 \\ -\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}}^1\cdot\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}'}^2 & \boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}}^1\cdot\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}'}^1 \end{pmatrix}\begin{pmatrix} \boldsymbol{u}_{\boldsymbol{G}',1}^{n,\boldsymbol{k}} \\ \boldsymbol{u}_{\boldsymbol{G}',2}^{n,\boldsymbol{k}} \end{pmatrix} \\ & = \frac{\omega_n(\boldsymbol{k})^2}{c^2}\begin{pmatrix} \boldsymbol{u}_{\boldsymbol{G},1}^{n,\boldsymbol{k}} \\ \boldsymbol{u}_{\boldsymbol{G},2}^{n,\boldsymbol{k}} \end{pmatrix}, \quad \forall\boldsymbol{G}\in\zeta. \end{aligned} \tag{6}$$

The coefficients $\eta_{\boldsymbol{G}-\boldsymbol{G}'}$ are computed by first Fourier-transforming the dielectric function $\varepsilon(\boldsymbol{r})$, truncating and inverting the resulting matrix. Solving Eq. (6) gives the frequencies $\omega_n(\boldsymbol{k})$ and H-field eigenmodes $\boldsymbol{H}_{n,\boldsymbol{k}}(\boldsymbol{r})$ in the photonic crystal. Then, using the Maxwell equations, the E-fields $\boldsymbol{E}_{n,\boldsymbol{k}}(\boldsymbol{r})$ are obtained from

$$\begin{aligned} \boldsymbol{E}_{n,\boldsymbol{k}}(\boldsymbol{r}) = & \frac{1}{\omega_n(\boldsymbol{k})\varepsilon_0}\sum_{\boldsymbol{G}\boldsymbol{G}'\in\zeta}\eta_{\boldsymbol{G}-\boldsymbol{G}'}|\boldsymbol{k}+\boldsymbol{G}| \\ & \times\left(\boldsymbol{u}_{\boldsymbol{G},1}^{n,\boldsymbol{k}}\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}}^2-\boldsymbol{u}_{\boldsymbol{G},2}^{n,\boldsymbol{k}}\boldsymbol{e}_{\boldsymbol{k}+\boldsymbol{G}}^1\right)\mathrm{e}^{\mathrm{i}(\boldsymbol{k}+\boldsymbol{G}')\cdot\boldsymbol{r}}. \end{aligned} \tag{7}$$

To compute the LDOS, the integration over $\boldsymbol{k}$ needs to be discredited. The expression for the LDOS is then written as

$$N(\boldsymbol{r},\omega,\boldsymbol{e}_d) = \sum_{n,\boldsymbol{k}}\delta(\omega-\omega_{n,\boldsymbol{k}})\left|\boldsymbol{e}_d\cdot\boldsymbol{E}_{n,\boldsymbol{k}}(\boldsymbol{r})\right|^2, \tag{8}$$

where the number of k-points should be as large as possible for much better calculation accuracy. In this paper, the LDOS histograms are plotted versus the reduced frequency $a/\lambda = 2\pi c$, where a is the cubic lattice parameter.

4 LDOS in photonic crystal cavity

In the photonic crystal cavity, the eigenmodes $E_{n,\boldsymbol{k}}(\boldsymbol{r}) = \boldsymbol{\Lambda}_{n,\boldsymbol{k}}(\boldsymbol{r})/$ are Bloch functions [8], so that the expression for the LDOS in Eq. (4) becomes

$$N(\boldsymbol{r},\omega,\boldsymbol{e}_d) \equiv \frac{1}{(2\pi)^3}\sum_n\int_{BZ}\mathrm{d}\boldsymbol{k}\delta(\omega-\omega_{n,\boldsymbol{k}})\left|\boldsymbol{e}_d\cdot\boldsymbol{E}_{n,\boldsymbol{k}}(\boldsymbol{r})\right|^2, \tag{9}$$

where n is the band index. In this case, the dipole orientation $\boldsymbol{e}_d$ is averaged over all solid angles, which results in

$$N(\boldsymbol{r},\omega) = \frac{1}{6\pi^2}\sum_n \int_{BZ} \mathrm{d}\boldsymbol{k}\delta(\omega-\omega_{n,\boldsymbol{k}})\left|\boldsymbol{E}_{n,\boldsymbol{k}}(\boldsymbol{r})\right|^2. \quad (10)$$

Further, in order to describe emission dynamics of atoms randomly distributed in photonic crystal cavity, the LDOS can be integrated over the cavity:

$$N_{av}(\omega) = \int_{WSC} \mathrm{d}\boldsymbol{r}\rho(\boldsymbol{r})N(\boldsymbol{r},\omega), \quad (11)$$

where $\rho(\boldsymbol{r})$ is a density of atoms at certain cavity in the crystal [9,10].

To examine the effects of photonic crystal on the LDOS and radiative dynamics of internal sources, an example of an inverse-opal photonic crystal shown in Fig. 2 will be discussed. LDOS calculated with the plane-wave method in inverse-opal photonic crystal is shown in Fig. 3. The LDOSs are at three different positions in the crystal: at point (0, 0, 0), (1/4, 1/4, 1/4) and (1/4, 1/4, 0). At the first two points, the LDOS does not depend on the dipole orientation $\boldsymbol{e}_d$ due to high symmetry, whereas at the third point, the LDOS is strongly orientation-dependent.

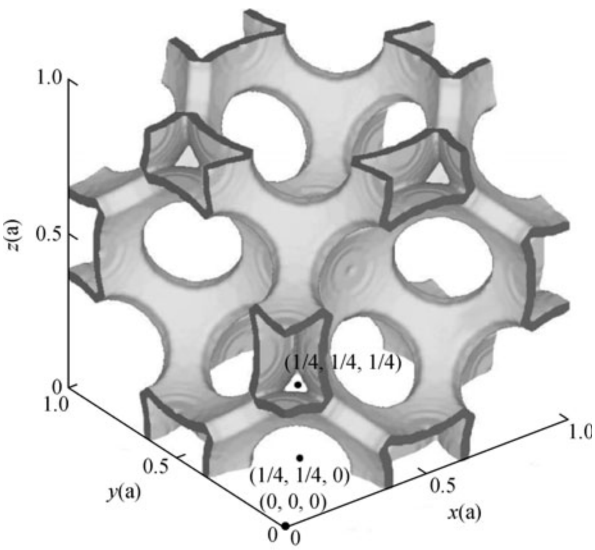

Fig. 2 View of single unit cell of modeled inverse opal

At frequencies near the lowest-order stopgaps, $a/\lambda = 0.6$, the Bloch modes are eliminated for $\boldsymbol{k}$-vectors in a solid angle, which can occupy a considerable part of the whole 4π solid angle. This leads to decreased LDOS and spontaneous-emission rate, especially when the orientation of the transition dipole $\boldsymbol{e}_d$ and its position in the crystal are not favorable for coupling to allowed Bloch modes. At frequencies in the photonic bandgap, $a/\lambda = 0.9$, there are no Bloch modes at all: the LDOS is zero regardless the dipole orientation and position in the crystal. Consequently, spontaneous emission from a dipole emitter vanishes completely. The decay of the excited state in this case can only occur via possible non-radiative channels and via weaker atom-field interaction processes. On the other hand, at frequencies outside the bandgap, the density of Bloch modes is increased leading to enhanced radiative decay rates. Figure 3 reveals sharp peaks in the LDOS just above the band gap, which means that the strong modification of the LDOS in photonic bandgap material can lead to ultimate suppressions as well as enhancements of spontaneous emission.

5 Conclusions

The calculating of LDOS based on plane-wave expansion method was introduced, and its application in an inverse-

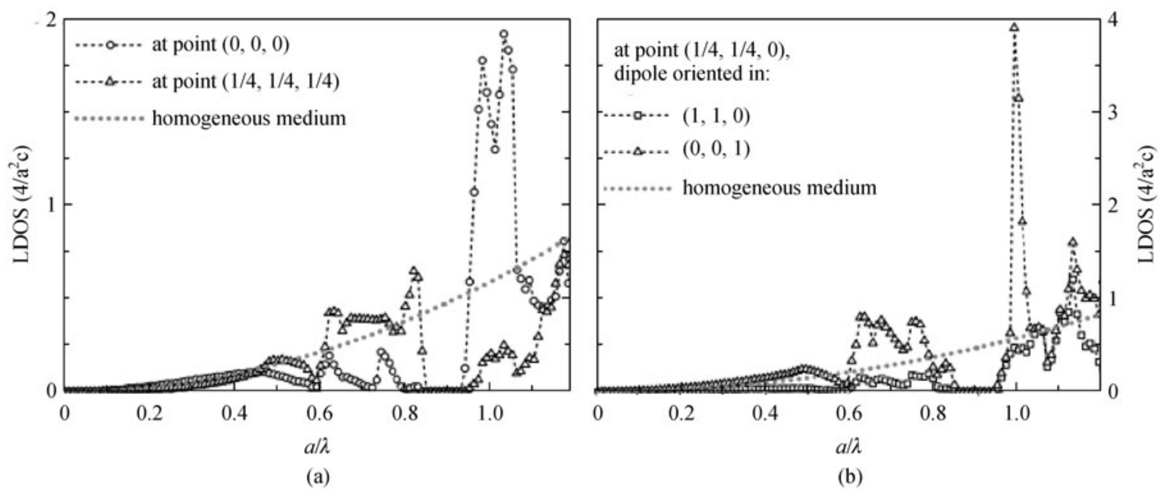

Fig. 3 LDOS calculated with plane-wave method in inverse-opal photonic crystal. LDOS at (a) (0, 0, 0) and (1/4, 1/4, 1/4) are shown by connected circles and triangles, respectively; (b) (1/4, 1/4, 0) projected on (1, 1, 0) and (0, 0, 1) directions are shown by connected squares and triangles, respectively

opal photonic crystal was discussed. Results indicate that the plane-wave expansion method is valid for the calculating of LDOS, and the LDOS can be radically modified in photonic crystal. In addition, it is also proved that in photonic crystal, the LDOS and the rate of spontaneous emission are the functions of position in the crystal unit-cell and orientation of the transition dipole moment. To conclude, LDOS is important for controlling spontaneous decay rates of elementary light sources.

Acknowledgements This work was supported by the Innovation Foundation of Ordnance Engineering College (No. YSCX0905).

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