Photonic band gap of 2D complex lattice photonic crystal*

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(Received 26 November 2008)

It is of great significance to present a photonic crystal lattice structure with a wide photonic bandgap. A two-dimension complex lattice photonic crystal is proposed. The photonic crystal is composed of complex lattices with triangular structure, and each single cell is surrounded by six scatterers in an hexagon. The photonic band gaps are calculated based on the plane wave expansion (PWE) method. The results indicate that the photonic crystal has tunable large TM polarization band gap, and a gap-midgap ratio of up to 45.6%.

Document code: A **Article ID:** 1673-1905(2009)02-0120-4 **DOI** 10.1007/s11801-009-8162-3

Photonic crystal (PC) structures become a subject of intense research activity because of their remarkable features compared with some common materials since E. Yablonovitch^[1] and S. John's^[2] work in 1987. Owing to the periodic arrangement of dielectric materials in optical wavelength scale, photonic crystals hold photonic band gaps (PBGs), homologizing to the electronic band gaps in semiconductor. One of the most significant features of PCs is that electromagnetic waves with such frequencies within the photonic band gap are prohibited to propagate, regardless of the polarization and propagating directions of the electromagnetic waves. The light propagation is manipulated by introducing defect structures into the periodic lattice [3-5], which leads to many interesting physical phenomena and important applications in many fields, such as optical communications, optical sensors and integrated optics ^[6-9]. Moreover, the photonic crystal gains more flexibility in terms of the wider PBG and band width. In this paper, a two-dimension complex lattice photonic crystal is presented and the PBG structures are studied by using the plane wave expansion (PWE) method.

In order to research the unique properties of photonic crystals, a calculation method is necessary to determine how light propagates through a photonic crystal structure. There are several applied techniques, but one of the most efficient methods is the plane wave expansion method, which was used in some of the earliest studies of photonic crystals. It is simple enough to be easily implemented to obtain the location and the width of PBG, and even to solve the defect problems. The propagation of light in a photonic crystal follows Maxwell equation. The magnetic field H of electromagnetic waves satisfies the following equation

$$\nabla \times [\frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}(\mathbf{r})] = (\frac{\omega}{c})^2 \mathbf{H}(\mathbf{r}) , \qquad (1)$$

where $\varepsilon(\mathbf{r})$ is the dielectric constant of the material, *c* is the speed of light in vacuum, and ω is the frequency of incident light. The transversality constraint on the magnetic field is given by

$$\nabla \cdot \boldsymbol{H}(\boldsymbol{r}) = 0 \quad . \tag{2}$$

The periodic dielectric constant $\varepsilon(\mathbf{r})$ can be expanded utilizing the Bloch theorem to a set of plane waves with respect to reciprocal lattice vectors, as

$$\frac{1}{\varepsilon(\mathbf{r})} = \sum_{G} \varepsilon_{G}^{-1} e^{iG\cdot\mathbf{r}} , \qquad (3)$$

where G is the reciprocal lattice vector and \mathcal{E}_{G}^{-1} depends on the photonic crystal structure. Resorting to the Bloch theorem, the magnetic field H(r) in a periodic dielectric structure is transformed to the form

$$\boldsymbol{H}(\boldsymbol{r}) = \sum_{G,\lambda} \boldsymbol{h}_{G\lambda} \boldsymbol{e}_{\lambda} e^{i(k+G)\cdot \boldsymbol{r}} \quad , \tag{4}$$

where $\lambda = 1,2$, *k* is Bloch wave vector and e_{λ} is unit vector. Combining with Eq.(2), Eq.(3) and Eq.(4), Eq.(1) is expressed as the following equation

^{*} This work has been supported by the Special Foundation for Harbin Young Scientists (Grant Number 2008RFQXG031).and the Basic Research Foundation of Harbin Engineering University.

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$$\sum_{\mathbf{G}'\lambda'} \varepsilon_{\mathbf{G}-\mathbf{G}'}^{-1} \boldsymbol{h}_{\mathbf{G}'\lambda'} [(\boldsymbol{k}+\boldsymbol{G}') \times \boldsymbol{e}_{\lambda'}] \cdot [(\boldsymbol{k}+\boldsymbol{G}) \times \boldsymbol{e}_{\lambda}] = \frac{\omega^2}{c^2} \boldsymbol{h}_{G\lambda}$$
(5)

And Eq.(5) is equivalent to the form below written by

$$\sum_{\mathbf{G}'} \boldsymbol{H}_{\mathbf{G},\mathbf{G}'} \cdot \begin{bmatrix} h_{1\mathbf{k}}(\boldsymbol{G}') \\ h_{2\mathbf{k}}(\boldsymbol{G}') \end{bmatrix} = \left(\frac{\omega}{c}\right)^2 \begin{bmatrix} h_{1\mathbf{k}}(\boldsymbol{G}) \\ h_{2\mathbf{k}}(\boldsymbol{G}) \end{bmatrix}, \quad (6)$$

where

$$\boldsymbol{H}_{\mathbf{G},\mathbf{G}'} = |\boldsymbol{k} + \boldsymbol{G}| \cdot |\boldsymbol{k} + \boldsymbol{G}| \boldsymbol{\varepsilon}_{\mathbf{G}-\mathbf{G}'}^{-1} \begin{bmatrix} \boldsymbol{e}_2 \cdot \boldsymbol{e}_2' & -\boldsymbol{e}_2 \cdot \boldsymbol{e}_1' \\ -\boldsymbol{e}_1 \cdot \boldsymbol{e}_2' & \boldsymbol{e}_1 \cdot \boldsymbol{e}_1' \end{bmatrix} .$$
(7)

Eq.(6) is known as the eigenvalue equation of the plane wave expansion method. Based on Eq.(6) we can solve mode frequencies ω existing in a photonic crystal, but the equation only has roots at specific frequencies. While the frequency range with no roots is considered as PBG. For 1D and 2D photonic crystals, the eigenvalue equation can be simplified by introducing appropriate unit vectors e_1 and e_2 , so that eigenvalue equations of TM and TE modes are written by Eq.(8) and Eq.(9), respectively

$$\sum_{\mathbf{G}'} \left| \boldsymbol{k} + \boldsymbol{G} \right\| \boldsymbol{k} + \boldsymbol{G}' \left| \boldsymbol{\varepsilon}_{\mathbf{G} - \mathbf{G}'}^{-1} h_{\mathbf{lk}}(\boldsymbol{G}') = \left(\frac{\omega}{c}\right)^2 h_{\mathbf{lk}}(\boldsymbol{G}) , \quad (8)$$

$$\sum_{G'} (\boldsymbol{k} + \boldsymbol{G}) \cdot (\boldsymbol{k} + \boldsymbol{G}') \varepsilon_{G-G'}^{-1} h_{2k} (\boldsymbol{G}') = (\frac{\omega}{c})^2 h_{2k} (\boldsymbol{G})$$

The discussed photonic crystal composed of complex lattices is described in Fig.1(a), in which each single cell contains seven circular scatterers with an arrangement of one of triangle lattices surrounded by six scatterers in hexagonal alignment. The material used in the paper is silicon ($\varepsilon = 11$. 4), *a* is the lattice constant of a triangle lattice, *b* is the distance of two adjacent scatterers of neighbor hexagonal alignment, r_a and r_b are the radius of a triangle lattice scatterer and the radius of its surrounding scatterers, respectively. Next, the bandgap structure of complex lattice photonic crystal will be analyzed in details.

In the case of $r_b = 0$, the proposed structure is equal to the photonic crystal with conventional triangle lattices, while the case of $r_a = 0$ is depicted in Fig.1(b). Fig.1(b) shows that each unit cell of triangle lattices is composed of six cylinders arranged in hexagonal alignment.

The band gap map is simulated by use of the plane wave expansion method with the plane wave number of 441, which is enough to guarantee the result's precision, as shown in



(a) The PC structure with complex lattice



Fig.1 Structure of the PC with complex lattices

Fig.2. Assuming that air holes are embedded periodically in silicon, we notice that the PBG does not appear when r_b is quite small no matter how the size of scatterers changes. While the PBG of TE and TM modes begins to appear as r_b increases, but there is not yet any absolute PBG, and the PBG of TM mode is relatively wide, as shown in Fig.2 (a) (b = 0. 33 *a*). On the contrary, dielectric rods are settled in air, the PBG of TM mode tends to emerge, for instance, there are two wide PBGs of TM mode at corresponding high frequencies when r_b is relatively great, shown in Fig.2(b) (b = 0.33 a).

For the complex lattice photonic crystal shown in Fig.1 (a), the parameter r_a will be also taken into account. Assuming that r_a is identical to r_b , the band gap maps are shown in Fig.3. Fig.3(a) shows band gap map of photonic crystal with Si rods in air with b = 0.33 a, and reveals that only the PBG of TM mode exists, and the gap-midgap ratio(defined as the ratio between the band gap width and the frequency at the center of the band-gap) attains 45.6% when r_a is appropriate. Analogous to Fig.2 (b), the width of PBG is broad, however, the frequency of PBG is relatively high. While air holes are embedded in silicon, the PBG width of TE mode is a little broader than that in Fig.2(a), as shown in Fig.3(b) (b = 0.33 a).



Fig.2 Band gap map of PC in Fig.1(b), (a) air holes in Si material. (b) Si rods in air.



Fig.3 Band gap map of PC in Fig. 1(a) ($r_a = r_b, b = 0.33 a$). (a) Si rods in air, (b) air holes in Si material.

In fact, more parameters need to be considered in the complex lattice photonic crystal with different r_a and r_b . The results demonstrate that this kind of photonic crystal has less probability of obtaining an absolute PBG. For the complex lattice photonic crystal with periodic air holes located in the dielectric medium, an absolute PBG will emerge if r_a is larger, as well as simple triangle lattices, but it has no obvious advantages over the conventional photonic crystal. Nevertheless the wide PBG of TE mode appears if r_a is smaller. The band gap map is depicted in Fig.4, where $r_a = 0.2 a$ and b = 0.25 a.



Fig.4 Band gap map of PC with air holes in Si material in Fig.1(a) ($r_a = 0.2 a$, b = 0.25 a)

Further, the complex lattice photonic crystal with Si rods located in the air is analyzed in this section. On the condition that r_a is relatively large, the band gap mainly depends on the central scatterer in each cell rather than surrounding six scatterers in hexagonal alignment, i.e. the band gap is not sensitive to the change of r_b . The simulated result is shown in Fig. 5(a), in which $r_a = 0.35 a$ and b = 0.15 a. On the other hand, when r_a is assumed to be relatively small, six scatterers in hexagonal alignment prominently affect the performance of the photonic crystal, as shown in Fig. 5(b) where $r_a = 0.12 a$ and b = 0.4 a. In Fig.5(b), there is an extremely wide PBG of



TM mode in high frequencies, and its central normalized frequency of PBG is 0.85, and the gap-midgap ratio reaches 35% larger than that of the photonic crystal with simple triangle lattices.



Fig.5 Band gap map of PC with Si rods in air in Fig. 1(a) . (a) $r_a = 0.35 a$, b = 0.15 a, (b) $r_a = 0.12 a$, b = 0.4 a.

Two-dimension complex lattice photonic crystal is presented in the paper. The simulated results demonstrate that this kind of photonic crystal provides an opportunity to obtain tunable polarization photonic band gap. Therefore, it is flexible to achieve broad photonic band gap. In addition, the gap-midgap ratio attains 45.6% in excess of that of simple triangle-lattice photonic crystals. The results are beneficial to design and fabricate micro-structured devices of photonic crystals.

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