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Absolute photonic band gap from 2D square compound lattices

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We describe the calculation of photonic band structures of 2D square compound lattices made up of three dielectric arrays. In particular, we evaluate the relationships between the existence of absolute photonic band gaps common to E and H polarized waves and the structure parameters, and find that only given large contrast of the dielectric constant and their diameter the absolute photonic band gaps can be created.

Keywords: photonic crystals, 2D square compound lattice, the method of plane wave, photonic band gaps.

1. Introduction

During the last decade, photonic crystals, also known as photonic microstructures or photonic bandgap (PBG) structures, have matured from an intellectual curiosity concerning electromagnetic waves to a field with real applications in both the microwave and optical regime. Recently, considerable interest has been focused on 2D and 3D structures for which one expects to obtain absolute PBG common to E and H polarized waves, by analogy to the electronic band gaps in natural semiconductor crystals [1]. In contrast to the limited experimental successes with 3D structures, work on 2D structures has flourished and produced many interesting results. This progress is mainly due to the fact that 2D structures are easier to make, in particular with the aid of the tools developed for the silicon microchip industry. Lower dimensionality also implies easier manipulation of the photonic lattice to increase functionality, such as the deliberate inclusion of defects, or interfacing with "standard" optical elements, such as waveguides, fibres, light sources and detectors. Experimentally, one needs to fabricate photonic lattices and to integrate them into complex assemblies in appropriate

length scale. In the 2D case, it is commonly believed that the honeycomb structures are the best candidates for the creation of absolute PBGs. In particular, triangle lattices of GaAs voids fabricated by electron beam lithography and reactive ion etching have been studied but giving no conclusive evidence of the existence of absolute PBGs [2]. As we know, the 2D square lattices are the best candidate for fabrication and theoretical computing. But because of its high symmetry, there is no absolute PBG common to E and H polarized waves. In principle, the lower the structure symmetry the lower the band structure degeneracy. A detailed symmetry analysis can be found in [3]. In this paper, we design a 2D square compound lattice and perform theoretical computing using the plane-wave expansion method. We hope that with the symmetry decreasing and the structure parameters being adjusted, the absolute PBG with the structure can be created.

2. Theory

For the general calculation of photonic band gaps in full periodic structures and the modes introduced by structural defects, various methods have been proposed. One of the most widely used is the plane-wave method [4], [5]. This method solves the full-vector wave equation for the magnetic field and, as the name implies, is based on a plane-wave expansion of the field and an expansion of the position-dependent dielectric constant. The method has a very general nature for treating periodic structures and may be applied to one-, two-, and three-dimensional problems. It allows one to calculate the photonic band diagrams of photonic crystals and thereby the possible existence, width, and positioning of any PBG.

In the plane-wave method, Maxwell's equation of electromagnetic waves is

$$\begin{cases} \nabla \cdot \mathbf{D} = 0, & \nabla \times \mathbf{H} = \varepsilon_0 \varepsilon(\mathbf{r}) \dfrac{\partial \mathbf{E}}{\partial t}, \\ \nabla \times \mathbf{E} = -\mu_0 \mu \dfrac{\partial \mathbf{H}}{\partial t}, & \nabla \cdot \mathbf{H} = 0. \end{cases} \tag{1}$$

We consider arrays of parallel cylinders, all oriented in the z-direction. For a single mode and H polarized waves, the full-vector wave equation of the electromagnetic fields $\mathbf{E}(r)$ and $\mathbf{H}(r)$ can be written as:

$$\begin{aligned} \mathbf{H}(\mathbf{r}, t) &= [0, 0, H_z(\mathbf{r})]\exp(-i\omega t), \\ \mathbf{E}(\mathbf{r}, t) &= [E_x(\mathbf{r}), E_y(\mathbf{r}), 0]\exp(-i\omega t). \end{aligned} \tag{2}$$

Taking (2) into (1), we find

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = i\omega\mu\mu_0 H_z,$$

$$\frac{\partial H_z}{\partial x} = i\omega\varepsilon(\mathbf{r})\varepsilon_0 E_y, \tag{3}$$

$$\frac{\partial H_z}{\partial y} = -i\omega\varepsilon(\mathbf{r})\varepsilon_0 E_x.$$

From Eq. (3), we let $\mu = 1$ and take out E_x, E_y and obtain the equation about H_z

$$\frac{\partial}{\partial x}\left[\frac{1}{\varepsilon(\mathbf{r})}\frac{H_z(\mathbf{r})}{\partial x}\right] + \frac{\partial}{\partial y}\left[\frac{1}{\varepsilon(\mathbf{r})}\frac{H_z(\mathbf{r})}{\partial y}\right] = -\frac{\omega^2}{c^2} H_z(\mathbf{r}) \tag{4}$$

where $\varepsilon(\mathbf{r})$ is the position-dependent dielectric constant of the periodic structure. Taking advantage of the periodic nature of the problem, the H-field may be expanded into a sum of plane waves using Bloch's theorem as

$$H_z(\mathbf{r}) = \sum_{\mathbf{G}} H(\mathbf{k}+\mathbf{G})\exp[i(\mathbf{k}+\mathbf{G})\mathbf{r}] \tag{5}$$

where $\mathbf{k}$ is a wave vector in the Brillouin zone, $\mathbf{G}$ represents a lattice vector in reciprocal space, describing the periodic structure and $H(\mathbf{k}+\mathbf{G})$ is the expansion coefficient corresponding to $\mathbf{G}$. The dielectric constant may be expressed as a Fourier series expansion

$$\frac{1}{\varepsilon(\mathbf{r})} = \sum_{\mathbf{G}} \varepsilon^{-1}(\mathbf{G})\exp(i\,\mathbf{G}\cdot\mathbf{r}) \tag{6}$$

where

$$\varepsilon^{-1}(\mathbf{G}) = \frac{1}{A_u}\int \frac{1}{\varepsilon(\mathbf{r})}\exp(-i\,\mathbf{G}\cdot\mathbf{r})\,d\mathbf{r}. \tag{7}$$

In Equation (7), A_u indicates the area of a unit cell, *i.e.*, the smallest region, that may be used to represent the periodic structure. Finally, by substituting Eqs. (5), (6) into Eq. (4), we obtain

$$\sum_{\mathbf{G}'}(\mathbf{k}+\mathbf{G})(\mathbf{k}+\mathbf{G}')\,\varepsilon^{-1}(\mathbf{G}-\mathbf{G}')\,H(\mathbf{k}+\mathbf{G}) = \frac{\omega^2}{c^2} H(\mathbf{k}+\mathbf{G}). \tag{8}$$

By the same method, for a single mode and E polarized waves, we also conclude the equation

$$\sum_{\mathbf{G}'} |\mathbf{k}+\mathbf{G}'|^2 \, \varepsilon^{-1}(\mathbf{G}-\mathbf{G}') \, E(\mathbf{k}+\mathbf{G}') = \frac{\omega^2}{c^2} E(\mathbf{k}+\mathbf{G}). \tag{9}$$

Equations (8), (9) include the sum of infinite reciprocal vectors $\mathbf{G}'$ and we select $N = 15$ reciprocal vectors instead. Then the two equations become a matrix eigenvalue equation, which has the form $ME = \lambda E(\lambda = \omega^2/c^2)$. The matrix M includes $N \times N$ matrix elements, E and λ are a $1 \times N$ matrix. For a fixed wave vector $\mathbf{k}$ we use the Matlab program $\lambda = eig(M)$, then the frequencies ω of the allowed modes in the periodic structure are found. In our calculations, the diagonal PQ of the Brillouin zone is equally divided into one hundred parts and the end point of wave vector $\mathbf{k}$ is selected along the end point of every part of PQ (Fig. 1).

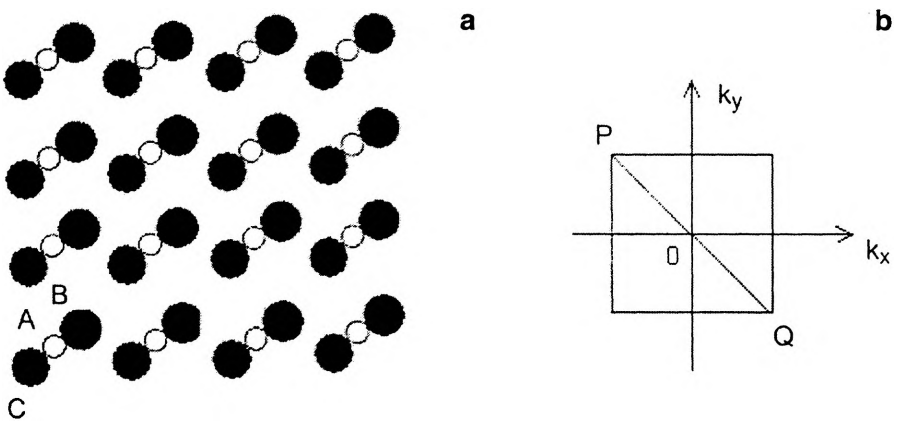

Fig. 1. Two-dimensional square compound structure (**a**) and its first Brillouin zone with $P(-\pi/a, \pi/a)$ and $Q(\pi/a, -\pi/a)$ (**b**).

In the case of our square compound lattice with lattice constant $a = 10^{-6}$ m, the unit cell contains three dielectric cylinders with dielectric constants $\varepsilon_a = 5$ and $\varepsilon_b = \varepsilon_c = 15$ which are embedded in a background of air with dielectric constant $\varepsilon = 1$. The cylinder with dielectric constant $\varepsilon_a = 5$ is placed at $A(0, 0)$ and named A with a diameter of $a/10$, and the cylinders with dielectric constant $\varepsilon_b = \varepsilon_c = 15$ are placed at $B(7\sqrt{2}a/40, 7\sqrt{2}a/40)$ and $C(-7\sqrt{2}a/40, -7\sqrt{2}a/40)$, and named B, C with the same diameters of $a/4$ (Fig. 1). We select the compound lattice as well as the larger values of $\varepsilon_b/\varepsilon_a$ and r_B/r_A in order to decrease the symmetry of the lattice. From the lattice and Eq. (6), we obtain

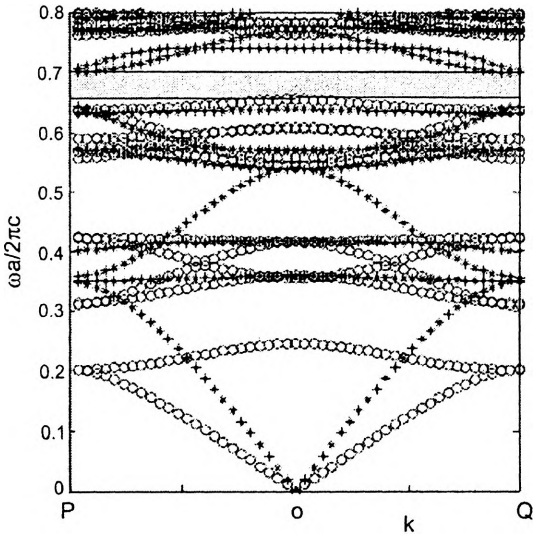

Fig. 2. Photonic band structures for E (denotes as ○) and H (denotes as ∗) polarizations of 2D square compound lattice.

$$\varepsilon^{-1}(\mathbf{G}) =$$

$$\begin{cases} \dfrac{f_a}{\varepsilon_a} + \dfrac{f_b}{\varepsilon_b} + \dfrac{f_c}{\varepsilon_c} + \dfrac{1}{\varepsilon_0(1-f_a-f_b-f_c)}, & \mathbf{G} = 0 \\ \left(\dfrac{1}{\varepsilon_a} - \dfrac{1}{\varepsilon}\right) \times \dfrac{2 f_a J_1(Gr_A)}{Gr_A} + \left(\dfrac{1}{\varepsilon_b} - \dfrac{1}{\varepsilon}\right) \times \dfrac{2 f_b J_1(Gr_B)}{Gr_B} \times 2\cos(\mathbf{G}\cdot\mathbf{d}), & \mathbf{G} \neq 0. \end{cases} \tag{10}$$

In Equation (10), $f_a = \pi r_a^2/a^2$, $f_b = \pi r_b^2/a^2$, $f_c = \pi r_c^2/a^2$ are the fractional filling factors for the three dielectric cylinders and the vector $\mathbf{d}$ points from A to B. With Eq. (10), we solved Eqs. (8) and (9) by the Matlab program. Figure 2 shows the results obtained by using 225 plan waves. The difference between this result and that of the more often used plan waves is less than 1/100. In Fig. 2, the ○ and ∗ lines are for the E and H polarizations, respectively. Clearly, we resolved an absolute PBG in the frequency range from 0.65 to 0.7, respectively (in unit of $2\pi c/a$).

3. Conclusions

To evaluate the structure dependence, we have calculated the PBGs as a function of the dielectric constant with a fixed value of $a/10$ for A and $a/4$ for B, C. With $\varepsilon_a = 5$, only if $\varepsilon_b = \varepsilon_c > 13$, absolute PBGs can be created. The width of absolute PBGs

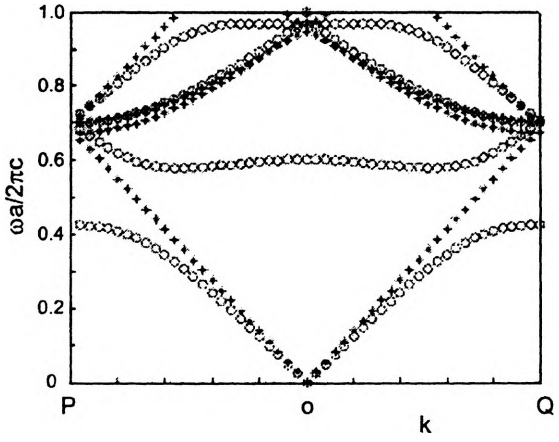

Fig. 3. Photonic band structures for E (denotes as ○) and H (denotes as ∗) polarizations of 2D square single lattice.

increases with increasing ε_b. But if $\varepsilon_b = \varepsilon_c > 20$, the width of absolute PBGs changes a little. On the other hand, fixing $\varepsilon_a = 5$ and $\varepsilon_b = \varepsilon_c = 20$, absolute PBGs can be obtained on condition that $r_B/r_A > 2$. When $\varepsilon_b = \varepsilon_c = 1$ and $\varepsilon_a = 15$, the structure becomes a single lattice and the calculated result is shown in Fig. 3, from which we find a photonic band gap (0.44–0.6) only for the E polarization but no absolute photonic band gap common to the E and H polarizations. We still calculate the PBGs when we turn B and C around A, but the results are almost the same. This may be ascribed to the central symmetry of the cylinders.

In conclusions, we present the photonic crystal of 2D square compound lattice and obtain an absolute PBG common to E and H polarized waves. For the 2D square lattice is the simplest of 2D lattices to be fabricated, our work may be helpful in designing photonic crystals.

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