

# NUMERICAL STUDY ON PHOTONIC PROPERTIES IN TWO-DIMENSIONAL COMPLEX PHOTONIC CRYSTALS OF SQUARE LATTICE

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**Abstract:** The photonic properties of a two-dimensional complex photonic crystal (PC) of square lattice were calculated by finite different time domain (FDTD) method. The photonic band structure, photonic density of states, the transmission and reflection coefficients along  $\Gamma X$  direction were obtained. The results indicate a clear correspondence between the photonic band structure and the transmission spectra along  $\Gamma X$  direction. The photonic band structure was also shown by the photonic density of states. Furthermore, the theoretical explanation for the opening of the band gap was given.

**Key words:** photonic crystals; finite different time domain method; density of state; transmission spectra

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## 二维正方形复式晶胞光子晶体的光子特性研究

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**摘要:** 用 FDTD 方法计算了二维正方形复式晶胞光子晶体的光子特性. 通过光子能带结构、光子态密度的分布以及沿  $\Gamma X$  方向透射谱的计算, 发现透射谱光子带隙的位置与能带结构符合得很好. 光子态密度的分布也表明存在全带隙的光子频率范围, 进一步研究给出这种结构光子晶体全带隙存在的物理起源.

**关键词:** 光子晶体; 时域有限差分法; 态密度; 透射谱

### Introduction

Since the pioneering work of Yablonovitch<sup>[1]</sup> and John<sup>[2]</sup>, photonic crystals, which are periodic arrangements of dielectric or metallic materials, have attracted wide attention recently in both theoretically and experimentally<sup>[3]</sup>. PC can exhibit frequency regions where electromagnetic waves cannot propagate in any direction.

These frequency regions are called as photonic band gaps (PBG). Using PC, we can manipulate photons in the same way as we manipulate electrons in semiconductors; this analogy bears promise for PC to influence optical device applications. It is of interest to design photonic crystal with complete bandgap as large as possible.

Although three-dimensional (3D) photonic crystals are considered to be the most interesting ideas for novel

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applications, it is exceedingly difficult to fabricate such 3D crystals with photonic gaps at visible to near-infrared wavelengths. Perhaps for this reason much attention has been drawn towards two-dimensional (2D) lattice structures, where theoretical analysis and fabrication requirements are easier than that of 3D photonic crystals. Furthermore, 2D PBG structures could also have some important uses such as a feedback mirror in laser diodes and channel drop filters<sup>[4,5]</sup>. In this paper, we focus on the 2D PC of a complex square Bravais lattice. This model has been studied in literature<sup>[6]</sup> and the optimizing design gives the largest complete bandgap. However, the physical origin of this band gap and the transmission property are still lack. Thus, we further give theoretical computation and analysis for these problems in this paper.

### 1 Model and Method

As a model system we consider 2D photonic crystal of dielectric columns connected by veins. The schematic diagram of crystals is shown in Fig. 1, where  $r$  is the dielectric columns' radius,  $dx$  and  $dy$  are the half-vein width along  $x$  and  $y$ -directions, respectively. To study the properties of the system, Maxwell's equations are cast into a form similar to Schrodinger's equation,

$$\nabla \times (\nabla \times E(r)) = \left(\frac{\omega}{c}\right)^2 \varepsilon(r) E(r), \quad (1)$$

where  $E(r)$  is the electric field,  $\omega$  is the angular frequency,  $c$  is the velocity of light,  $\varepsilon(r)$  is the dielectric function, and  $r$  is the position vector. The permittivity can be described as

$$\varepsilon(r) = \varepsilon_{av} + \varepsilon_{spatial}(r), \quad (2)$$

where  $\varepsilon_{av}$  is the average value of dielectric function and  $\varepsilon_{spatial}(r)$  is the spatial component of dielectric function, which is analogous to the potential in Schrod-

inger's equation.

The solution to Eq. (1) can be represented in the form of a band structure, which defines some areas with the existence of the band gaps may exist. The theoretical calculation can be solved with either a frequency-domain method such as the plane-wave expansion method<sup>[7]</sup>, or a time-domain method such as the finite-difference time-domain (FDTD) method<sup>[8-10]</sup>. The plane-wave expansion method is initially used for theoretical analysis of photonic crystals structures. It is still limited because the transmission spectra cannot be extracted from the method. This method has another drawback that the time taken for the calculation scales as the cube of the number of plane waves used. FDTD method has been widely adopted to calculate photonic crystal band structure, defect modes, waveguide modes, and transmission spectra. In particular, the method has been proved extremely useful for large system involving irregular unit cell. It is based on the discretization of Maxwell's equations in both time and space. The discretization then leads to a numerical solution of the wave propagation problem. In this work we have used the FDTD method along with the perfectly matched layer absorbing boundary conditions to truncate the computational domain and minimize the reflections from the outer boundary.

### 2 Results and Discussion

Since the first biggest complete band gap exists for this photonic crystal structure when the parameters  $r = 0.317a$ ,  $dx = 0.026a$ ,  $dy = 0.031a$ , where  $a$  is the lattice constant<sup>[6]</sup>, we also choose the same parameters in our calculation. The dielectric rods are GaAs with relative permittivity  $\varepsilon = 11.4$ .

For the band structure and the density of states, the calculation unit cell contains  $21 \times 21$  discretization grids for the FDTD time-stepping formulary. The total number of the time steps is 8 192 with each time step  $\Delta t = 0.004 \times (m_e a_0^2 / \hbar)$ . The calculated band structures are shown in Fig. 2. There is a large complete photonic band gap between the frequencies  $\omega = 0.40086 (\omega a / 2\pi c)$  and  $\omega = 0.47880 (\omega a / 2\pi c)$ . The band gap is  $\Delta\omega = 0.07794 (\omega a / 2\pi c)$ , which is approximately 9.6% larger than the band gap  $0.0711 (\omega a / 2\pi c)$ <sup>[6]</sup> obtained

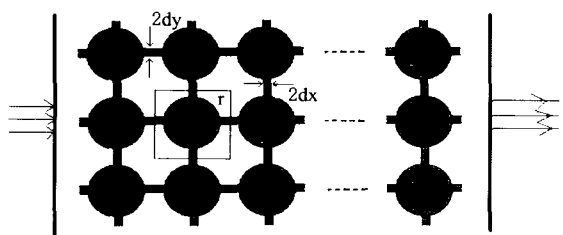


Fig. 1 Schematic diagram of 2D complex photonic crystal of dielectric columns connected by veins  
图1 二维正方形复式晶胞光子晶体的示意图

by the plane-wave expansion method. The density of states is also calculated, which is of benefit to the comprehending of the band structures. Finally, we transform the information from the time domain into the frequency domain by a Fourier transformation.

The photonic band gap is dependent on many parameters (e. g., lattice type, filling fraction, and the shape of filling element). It is well-known that there is no complete two-dimensional band gap for a square lattice of dielectric columns in the background of air under any filling fraction<sup>[11]</sup>. Here we obtain a complete two-dimensional band gap by connecting the high-W regions of the square lattice of dielectric columns by veins. The change of the spatial component of the dielectric function opens the band gap for this structure.

We know that the periodic change of the dielectric function in photonic crystal is analogous to periodic potential in semiconductor, and the spatial component of the dielectric function acts as a perturbation potential. From the band theory, the electrons are forbidden to propagate with a particular frequency in certain directions. If the lattice potential is strong enough, the gap might extend to all possible directions, resulting in a complete band gap. The veins in PC is analogous to perturbation potential in semiconductor. The veins lift degeneracy of bands at high-symmetry points M and open the complete band gap. To get better insight of a veins' role in open the complete band gap, we also give the photonic band structure for the photonic crystal without veins at the same filling fraction as seen in Fig. 3. There is no complete band gap for this structure. The bands are degenerate at M point of high symmetry in the crystal. In addition, the width of the vein along X direction is different from that along Y direction, the band gap of this asymmetric structure is bigger than that of the symmetric one, owing to the lifting band degeneracy by the lattice symmetry reduction.

The electromagnetic waves cannot propagate in any direction in photonic band gaps. This property changes the light-matter interaction. For example, in the photonic band gap, no optical transition is allowed and spontaneous emission of photons is completely forbidden. This can be clearly seen from the density of state diagram, shown in Fig. 2, and the density of states itself in arbitrary

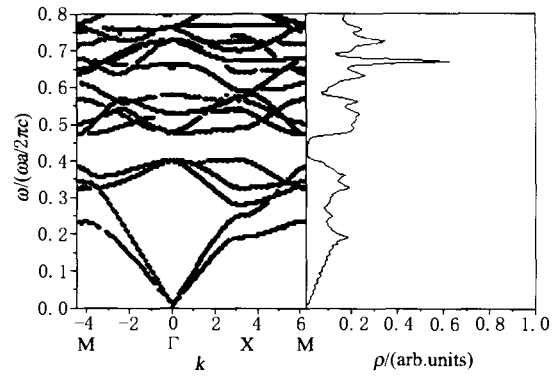


Fig. 2 The photonic-band structure and the density of state of 2D complex photonic crystal of dielectric columns connected by veins

图2 二维正方形复式晶胞光子晶体的光子能带结构和光子态密度

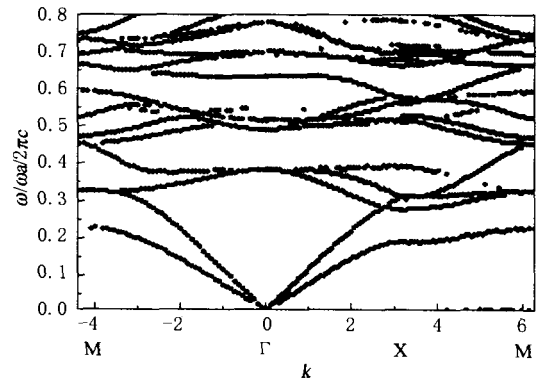


Fig. 3 The photonic-band structure of 2D photonic crystal of dielectric columns

图3 二维正方形光子晶体的光子能带结构

units. The band gap is clearly shown in a frequency window in which the density of states is strongly suppressed. Within the band gap, there are no propagating photonic modes in any direction in space so that the density of photonic modes equals zero.

Finally, we calculate the transmission property along the  $\Gamma X$  direction for the structure. To simulate the described structure, the perfectly matched layers<sup>[12]</sup> (PML) of finite thickness are used at two ends of the system along the  $\Gamma X$  direction. The absorbing layer is essential because even small reflections from the two ends of the system could cause serious errors. Using PML as our absorbing layer, we can simulate the infinite system by finite system. Our calculated system contains four layers. The incident plane wave is assumed to propagate in the  $\Gamma X$  direction. The transmis-

sion and reflection coefficients as a function of frequency are shown in Fig. 4 and Fig. 5 respectively. Results for the TM and TE polarizations are labeled by the dashed and solid lines, respectively. The gaps in TM and TE waves overlap partly. The overlapping region is the complete photonic band gap indicated as the shaded region in Fig. 4. and Fig. 5. The PBG is bound by the lower band edge of TE wave and the upper band edge of TM wave. The frequency ranges where the transmittance is close to 0 and the reflection coefficient is nearly 1 are in perfect agreement with the band gaps. Hence, the band gap can be obtained by the traditional transmission and reflection spectra.

### 3 Conclusion

The photonic properties of two-dimensional complex photonic crystals of square lattice are calculated by FDTD method. We calculate the band structure, the density of

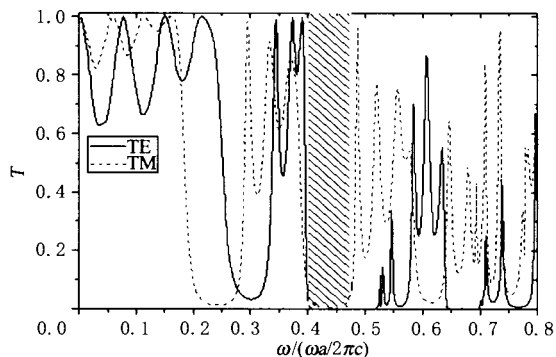


Fig. 4 Transmission spectrum in the  $\Gamma X$  direction calculated for 2D complex photonic crystal of dielectric columns connected by veins.

图4 二维正方形复式晶胞光子晶体的沿  $\Gamma X$  方向的透射谱

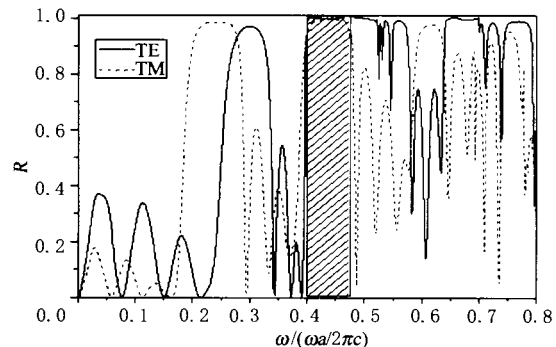


Fig. 5 Reflection spectrum in the  $\Gamma X$  direction calculated for 2D complex photonic crystal of dielectric columns connected by veins.

图5 二维正方形复式晶胞光子晶体的沿  $\Gamma X$  方向的反射谱

state and the transmission and reflection coefficients of the photonic crystals. The comparison between the band structure and the calculated transmittance along  $\Gamma X$  direction shows a clear correspondence for the band gaps. The band gap's width is larger than that obtained by the plane-wave expansion method. This is due to the energy cut-off of the plane wave expansion. We also give the theoretical explanation for the opening of the band gap in the complex two-dimensional photonic crystals.

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