Band Gap Optimization Design of Photonic Crystals Material

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Abstract. The photonic crystal has a fundamental characteristic - photonic band gap, which can prevent light to spread in the crystals. This paper studies the width variation of band gaps of two-dimension square lattice photonic crystals by changing the geometrical shape of the unit cells' inner medium column. Using the finite element method, we conduct numerical experiments on MATLAB 2012a and COMSOL 3.5. By shortening the radius in vertical axis and rotating the medium column, we design a new unit cell, with a 0.3*3.85e -7 vertical radius and a 15 degree deviation to the horizontal axis. The new cell has a gap 1.51 percent wider than the circle medium structure in TE gap and creates a 0.0124 wide TM gap. Besides, the experiment shows the first TM gap is partially overlapped by the second TE gap in gap pictures. This is helpful to format the absolute photonic band gaps and provides favorable theoretical basis for designing photonic communication material.

1. Introduction
In 1987, when E.Yablonovitch and S.John studied to control the spontaneous radiation and used periodic structures to control the spread of radiation, they first put forward the concept of photonic crystals. The photonic crystal is a novel optical material made of two or more than two different kinds of materials arranged periodically. When the electromagnetic wave propagates in photonic crystals, the wave obeys the refraction, reflection and transmission laws, and the periodical Bragg scattering of electron, which is similar to electronic bands, modulates the wave to form photonic energy bands. With proper lattice constants and dielectric function ration, the photonic crystals can produce gaps between energy bands. Electromagnetic waves of certain frequencies are completely prevented in band gaps; see Figure 1 [1]. The photonic band gap is an important property of photonic crystals material. The research and use of photonic crystals physical material and components are significant to develop the information and technology industry, and also provide a possible way to acquire the large-scale integrated optical path [2]. For these reasons, there are a lot of scholars dedicating to study the property of photonic crystals today; they design and explore various structures to acquire low frequency band gaps, such as the design of unit cells in direct problem [3-7], the search for structures with optimal gaps in inverse problem [8-11] and considering to optimize gaps within a given frequency range [12].
The two-dimension photonic crystal is a material that the dielectric function changes periodically in two dimensions and be constant in the third dimension; see Figure 2. Different lattice arrangements produce different lattice types. In this paper, we study band gaps of the unit cells with square lattices, while the lattices’ inner shape can be circle, square, hexagonal and any other shapes. If you want to acknowledge more concepts and theories about the two-dimension photonic crystal, you can see lecture [13].

The finite element method is a numerical method based on calculus of variation, approximation theory and partial differential equations; it is widely used in mathematics and physics. The main idea of this method is to make the continuous physical field discrete by finite elements, approximate the physical field by using basic functions in each sub-region and finally composite the total stiffness matrix. The method has good properties in numerical convergence and stability; it has been widely used in finding the gaps of photonic crystals [14].

The main purpose of this paper is to design the shape of unit cells, having low and wide band gaps, in two-dimension square lattice photonic crystals. Numerical experiment results are presented to show qualitative guidance rules for designing unit cells. In the two-dimension polarization modes, we give the related theoretical derivation of the band gap problem and numerical examples using the finite element method. Using the unit cell with a circle inner medium column as an initial structure, we test the effects relating to radius in vertical axis and angle parameters. As is shown by the numerical results conducting on MATLAB 2012a and COMSOL 3.5 software, we can come to the conclusion that it makes for producing low frequency and wide band gaps destroying the symmetry of medium columns and the whole unit cells.

2. The band gap problem and finite element method
When the waves propagate in photonic crystals, they satisfy Maxwell equations. The interactions between waves and medium are given by Material equations. The effects we consider in photonic
crystals are mainly electrostatic effects. That means the electromagnetic waves propagate in the uniform, passive, non-magnetic and periodic dielectric. In this case, the model satisfies the simplified Maxwell equations and Material equations as follows:

\[
\begin{align*}
\nabla \times \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \\
\nabla \times \mathbf{H} &= \frac{1}{c} \frac{\partial \mathbf{D}}{\partial t} \\
\n\nabla \cdot \mathbf{D} &= 0 \\
\n\nabla \cdot \mathbf{B} &= 0
\end{align*}
\]

(1)

where \( E \) is electric field intensity, \( H \) is magnetic field intensity, \( D \) is electric displacement vector and \( B \) is magnetic induction intensity, and the four field quantity are all vectors relaying on coordinates and time. The \( \varepsilon(r) \) is dielectric function of the medium, \( t \) is time, \( c \) is light velocity in vacuum, \( \nabla \) is nabla operator and \( r \) represents the three-dimension location \((x, y, z)\).

Combining with the Material equations (2), the Maxwell equations (1), with the electric field coupled with the magnetic field, can be transferred into wave equations with the separated electric field and magnetic field component. In addition, as the wave equations include the time component, it's difficult to solve by numerical methods. Meanwhile, electromagnetic waves can be decomposed into simple harmonic waves. When \( E \) and \( H \) are simple harmonic waves, the wave equations can be simplified into Helmholtz equations with no time terms:

\[
\begin{align*}
\nabla \times \nabla \times \mathbf{E}(r) &= \left( \frac{\omega}{c} \right)^2 \varepsilon(r) \cdot \mathbf{E}(r) \\
\nabla \times \left( \frac{1}{\varepsilon(r)} \nabla \times \mathbf{H}(r) \right) &= \left( \frac{\omega}{c} \right)^2 \mathbf{H}(r)
\end{align*}
\]

(3)

In particular, considering the two cases - TE mode and TM mode in two-dimension, the problem of photonic crystals band gaps can be reduced. Here, the TM mode refers to that the electric field is polarized along z-axis, \( \mathbf{E}(r) = (0, 0, E_z) \), and the \( E_z \) is a function with variables \( x, y \); the TE mode refers to that the magnetic field is polarized along z-axis, \( \mathbf{H}(r) = (0, 0, H_z) \), and the \( H_z \) is a function with variables \( x, y \). The \( r_z \) here represents the three-dimension location \((x, y)\). So, the Helmholtz equations (3) can be reduced to:

\[
\begin{align*}
\text{TE}: - \nabla \left( \frac{1}{\varepsilon(t_z)} \nabla H(t_z) \right) &= \left( \frac{\omega}{c} \right)^2 H(t_z) \\
\text{TM}: - \nabla \cdot \left( \nabla E(t_z) \right) &= \left( \frac{\omega}{c} \right)^2 \varepsilon(t_z) E(t_z)
\end{align*}
\]

(4)

Now, the band-gap problem satisfies Neumann boundary conditions.

Furthermore, as the two-dimension photonic crystals are periodic, the two-dimension boundary value problem model (4) can be turned into characteristic equations (5) in the unit cell \( \Omega \), basing on the Bloch theory.
\[ \text{TE}_1 - (\nabla + ik_j) \left( \frac{1}{\epsilon(r_i)} (\nabla + ik_j) \right) = \left( \frac{\omega}{c} \right)^2 H_{\epsilon i}(r_i) \]

\[ \text{TM}_1 - (\nabla + ik_j) \left( (\nabla + ik_j) \right) = \left( \frac{\omega}{c} \right)^2 \epsilon(r_i) E_{\epsilon i}(r_i) \]  

(5)

where \( k_{||} = (a, b) \) are wave vectors in two-dimension place space and chosen along the irreducible Brillouin zone boundary. The following Figure 3 gives the corresponding conversion processes for the first and the irreducible Brillouin zone in two-dimension.

\[ \text{Figure 3. The irreducible Brillouin zone in two-dimensional} \]

Now, the electromagnetic field variables satisfy the periodic Floquet boundary conditions on \( \Omega = \partial \Omega \). Choosing base vectors of the unit cell \( \sigma_1 = (a, 0), \sigma_2 = (0, a) \) parallel to the x-axis and y-axis respectively, we can get the following Floquet boundary conditions.

\[ \begin{cases} H_{\epsilon i}(r_i + \sigma_j) = H_{\epsilon i}(r_i) \\ \frac{1}{\epsilon(r_i + \sigma_j)} \partial_{\sigma_j} H_{\epsilon i}(r_i + \sigma_j) = \frac{1}{\epsilon(r_i)} \partial_{\sigma_j} H_{\epsilon i}(r_i) \end{cases} \]  

and

\[ \begin{cases} E_{\epsilon i}(r_i + \sigma_j) = E_{\epsilon i}(r_i) \\ \partial_{\sigma_j} E_{\epsilon i}(r_i + \sigma_j) = \partial_{\sigma_j} E_{\epsilon i}(r_i) \end{cases} \]  

(6)

(7)

where \( n \) is outward normal direction on the boundary of the unit cell.

Then, to derive the process of calculus of variation related to the finite element method, we write the TE mode and TM mode equation as the following uniform form - the eigenvalue form.

\[ \begin{cases} (\nabla + ik_j) \left[ \delta (\nabla + ik_j) u \right] + \lambda \partial u = 0, u \in \Omega \\ u_{\epsilon i}(r_i + \sigma_j) = u_{\epsilon i}(r_i) \\ \partial_{\sigma_j} u_{\epsilon i}(r_i + \sigma_j) = \partial_{\sigma_j} u_{\epsilon i}(r_i) \end{cases} \]  

(8)

where

\[ \delta = \begin{cases} 1 & \text{TE} \\ \frac{1}{\epsilon(r_i)} & \text{TM} \end{cases}, \quad g = \begin{cases} 1 & \text{TE} \\ \frac{1}{\epsilon(r_i)} & \text{TM} \end{cases}, \quad \zeta = \begin{cases} 1 & \text{TE} \\ \frac{1}{\epsilon(r_i + \sigma_j)} & \text{TM} \end{cases} \]

\[ \lambda = \left( \frac{\omega}{c} \right)^2 \]

is the eigenvalue to solve, \( u \) is the field quantity to solve and here it is eigenvector.
Define the periodic Sobolev space

\[ H^1_{k_i}(\Omega) = \left\{ f(\tau_i) \in H^1(\Omega) : f(\tau_i + \sigma_j) = f(\tau_i) \text{ on } \Pi = \partial \Omega, \quad i = 1,2 \right\} \]

(9)

The related norm definitions of Sobolev space can be found in lecture [15]. The eigenvalue equations (8) can be transferred into the following form. To \( \forall k_\parallel \in \mathbb{B} \), find \( (\lambda, u) \in C \times H^1_{k_\parallel}(\Omega) \) satisfy

\[
\int_\Omega \delta(\nabla + ik_\parallel)u \cdot (\nabla + ik_\parallel)v d\Omega = \lambda \int_\Omega \partial u \cdot v d\Omega
\]

(10)

Here, the \( (\nabla + ik_\parallel)v, v \) is the conjugate of \( (\nabla + ik_\parallel)v, v \).

Then, the finite element method is conducted step by step. First, the unit cell is subdivided by triangular and the element stiffness matrix is developed by choosing suitable basis functions in each triangular cell. Second, synthesize the global stiffness matrix and consider the Floquent boundary conditions. Finally, the generalized eigenvalue equation \( AU = \lambda BU \) can be derived in the two-dimension photonic crystals problem. There are several ways to solve the generalized eigenvalue equations; readers who are interested in the problems can consult lecture [16]. Especially, when the matrix \( A \) and \( B \) are positive definite, we can get the reverse of \( B \) or decompose \( B \) by Cholesky algorithm.

3. The numerical experiment

In this chapter, we use the finite element method to solve the band-gap problem of two-dimension square lattice photonic crystals numerically. The numerical experiment was initialized by testing the structure with circle inner medium column, and then studied on changing the radius in vertical axis and rotating the medium column to acquire qualitative guiding theories in the design of unit cells with low frequency and wide gaps. We conducted the experiment on MATLAB 2012a and COMSOL 3.5 software. In detail, we used the TE mode and TM mode 2D eigenfrequency analysis modules in COMSOL 3.5 to build unit cells, and then we imported the models into MATLAB 2012a to plot the band gaps figures.

The related parameters used in COMSOL 3.5 are dielectric functions \( \varepsilon_1 = 1, \varepsilon_2 = 8.898 \) for two-dimension square lattice, the length of the square unit cell \( a = 3.85e-7 \), the initial search frequency \( 2.5e14 \) and the initial circle medium column radius \( r = 0.378a \). First, we change the length of the radius in vertical axis. Then, we rotate the horizontal axis; see Figure 4. In this paper, the seven lowest frequency bands are mainly considered and the gaps between them, namely along the three side of irreducible Brillouin zone boundary.

Figure 4. The change in medium column of COMSOL models

Firstly, when the length of the radius in vertical axis changes among the set \( \{0.4*a, 0.378*a, 0.3*a, 0.2*a, 0.1*a\} \), the corresponding largest TE mode and TM mode band gaps of each unit cell are shown in table 1. The value of band gaps here we referred is the normalized frequency. That is to say, the value will not be affected by the size of the crystals material.
Table 1. The relation between radius in vertical axis and largest band gaps

|        | 0.1*a | 0.2*a | 0.3*a | 0.378*a | 0.4*a |
|--------|-------|-------|-------|---------|-------|
| TE mode| 0.0442| 0.0374| 0.0595| 0.0456  | 0.0390|
| TM mode| 0     | 1.0e-03*0.4189 | 0.0107 | 0   | 1.0e-03*0.3153 |

Table 1 shows that when the vertical axis radius equal 0.3*a, the TE mode gap is 1.39 percent bigger than the corresponding circle structure and a 0.0107 width TM mode gap is created. So, we can draw the conclusion that changing the vertical axis radius is changing the symmetry in some degree which contributes to produce wider gaps.

Then, the changing of angle parameter was considered by rotating the horizontal axis of the structure with a 0.3*a vertical axis radius which have relative largest gaps in table 1. The following table 2 shows the relation between the angles and largest gaps.

Table 2. The relation between angle parameter and largest band gaps

|        | 0°   | 15°  | 30°  | 45°  |
|--------|------|------|------|------|
| TE mode| 0.0595 | 0.0607 | 0.0588 | 0.0557 |
| TM mode| 0.0107 | 0.0124 | 0.0230 | 0.0275 |

Table 2 shows that when the horizontal axis is rotated 15°, a TE mode gap which is 0.12 percent wider than the non-rotating structure and a TM mode gap which is 0.17 percent wider than the non-rotating structure can be obtained. The subsequent changes in angle make no improvement in TE mode gap, but they help to widen the TM mode gaps. In particular, the TM mode gap in the structure rotated 45° is 1.68 percent wider than the non-rotating structure. So, we can come to the conclusion that rotating the elliptical medium column destroys the symmetry of the unit cell further and produces band gaps wider.

The whole changing process, from the circle medium column to the structure with a 0.3*a vertical axis radius and a 15° horizontal rotating angle, makes the TE mode gap increase 1.51 percent and creates a 0.0124 width TM mode gap. In the following Figure 5, we list the TE mode and TM mode energy band diagrams of the structure with a 0.3*a vertical axis radius and a 15° horizontal rotating angle.

From the gaps’ location in Figure 5, we can see that the second gap of TE mode has partly overlapped with the first gap of TM mode. This phenomenon can develop an absolute band gap which provide favourable theoretical basis for designing photonic communication material.

4. Conclusions and future work

We design a novel structure by destroying the symmetry of the circle medium column and the unit cell to acquire low frequency and wide band gaps. The new unit cells with a 0.3*a vertical axis radius and a 15° horizontal rotating angle has both wide TE mode gaps and TM mode gaps.

Many subjects still need to do in this area. They all relate to the optimal of band gaps of two-dimension photonic crystals, including research on more complex butterfly lattices and tessellate lattices structure, exploration to band gaps character of photonic quasi-crystal structure and the reverse problem.
Figure 5. The TE mode and TM mode energy bands of the structure with a 0.3*a vertical axis radius and a 15° horizontal rotating angle

References
[1] Ma X Y 2010 Photonic Crystal Principle and application (Beijing: Science Press)
[2] Ye W M 2010 Photonic Crystal Introduction (Beijing: Science Press)
[3] Wang X H, Gu B Y, Li Z Y and Yang G Z 1999 Phys.Rev.B. 60 11417
[4] Liu D, Gao Y H, Gao D S and Han X Y 2012 Opt.Commun. 285 1988
[5] Li Z Y, Gu B Y and Yang G Z 1998 Phys.Rev.Lett. 81 2574
[6] Zhu N, Wang J, Cheng C and Yan X 2013 Optik 124 309–312
[7] Liu J J, Fan Z G, Kuang M, He G M, Guan C Y and Yuan L B 2013 Opt. Commun. 288 52
[8] Cox S and Dobson D 1999 SIAM J. Appl. Math. 59 2108
[9] Chiu Y K, Stanley O and Eli Y 2005 Appl. Phys. B. 81 235
[10] Han M, Ngoc N, Robert F, Parrilo P and Jaime P. 2010 J.Comput.Phys. 10 3706
[11] Elizabeth H, Andras S, Djidjel Ki, Marc M, Ken T and Cox S 2012 Photonics and Nanostructures - Fundamentals and Applications 10 25.
[12] Cox S and Dobson D 2000 J. Comput. Phys. 158 214
[13] Igor A S and Igor V G 2009 Photonic Crystal (Heidelberg: Springer)
[14] Jin J M 1998 Finite Element Method of Electromagnetic Field (Xi’an: Xi’an electronic science and technology university press)
[15] Li R H and Liu B 2009 Numerical Methods for Differential Equations (Beijing: Advanced Education Press)
[16] Klaus J B 2016 Finite Element Method: Theory, Format and Solution, ed Xuan J P (Beijing: Advanced Education Press)