Designing photonic crystals with complete band gaps

Fei Meng[1,3], Shuo Li[2], Baohua Jia[2] and Xiaodong Huang[1*]

[1]Centre for Innovative Structures and Materials, School of Engineering, RMIT University, GPO Box 2476, Melbourne, VIC 3001, Australia

[2]Centre for Micro-Photonics, Faculty of Science, Engineering and Technology, Swinburne University of Technology, PO Box 218, Hawthorn, VIC 3122, Australia

[3]School of Civil Engineering, Central South University, Changsha 410075, China

*Presenting author: s3459321@student.rmit.edu.au

†Corresponding author: huang.xiaodong@rmit.edu.au

Abstract

In order to design photonic crystals with complete band gaps, a topology optimization algorithm is proposed based on finite element analysis and bi-directional evolutionary structural optimization method. The photonic crystals are assumed to be periodically composed of two materials with different electromagnetic property. By introducing discrete design variables and calculating the sensitivity of each element, the BESO algorithm gradually re-distributes the dielectric materials within the unit cell until the photonic crystal have a complete band gap between specified photonic bands. The proposed optimization algorithm is efficient and some innovative designs have been obtained.

Keywords: Topology optimization; complete band gap; finite element analysis (FEA); bi-directional evolutionary structural optimization (BESO).

Introduction

Photonic crystals are micro optical periodic structures in 1, 2 or 3 dimensions. Due to the periodic arrangement of dielectric materials with different electromagnetic properties, photonic crystals will be able to modulate the propagation of light and generate some special functions like photonic band gap[1], negative refraction[2] and slow light[3]. Photonic band gap refers to the property that the propagation of electromagnetic waves within a certain frequency ranges are totally prohibited in the photonic crystal. It is an important and fundamental feature which lays the ground for many utilities, for example wave guide[4, 5] and resonant cavity[5, 6]. It has significant meaning to design photonic crystals with large band gaps which can modulate light signals in a broader frequency range.

For two dimensional photonic crystals, electromagnetic wave can be decomposed to transverse magnetic waves, whose electric field is perpendicular to crystal plane, called TM mode, and transverse electric waves, whose magnetic field is perpendicular to crystal plane, called TE mode. Design and optimization of photonic band gap structures for an independent polarization have been reported in many literatures. These methods include the traditional trial-and-error method based on physical intuitions[7, 8] and advanced topology optimization methods such as genetic algorithms[9, 10], level set method[11], SIMP[12] and BESO[13].

Compared with band gaps for a single polarization, complete band gaps, which can prevent electromagnetic waves of both polarizations, are apparently more meaningful. However, the calculation of complete band gap takes the photonic bands of both TM and TE mode into consideration, which makes the optimization process very low-efficient and laborious. Therefore, only limited results have been reported so far [14-19], and most of them are designed based on physical intuitions. Furthermore, some of them share a similar pattern, like the results in Refs. [15], [17] and [18].

While these designs are attractive, it is important to attempt new methods and algorithms in order to find wider complete band gaps or different topologies. In this paper, a new approach based on bi-directional evolutionary structural optimization (BESO) method is proposed. BESO is a structural optimization method based on finite element analysis (FEA). Its key concept is gradually removing inefficient materials from and adding high efficient materials into the design domain, until the optimal design is achieved[20]. BESO has been successfully applied to the optimization of materials with periodic micro structures, including photonic band gap crystals[13].

In this paper, the finite element method used to calculate the photonic bands is firstly introduced. An objective function is put forward and the corresponding sensitivity analysis is conducted. Then based on the FEA and the sensitivity analysis, a BESO algorithm is established by introducing discrete design variables. Starting from a simple initial design without band gap, BESO evolves the topology of the unit cell step by step until a desired complete band gap emerges and enlarges to its maximum. Finally, several numerical examples are presented to demonstrate the effectiveness and efficiency of the proposed optimization algorithm.

Finite element analysis of photonic crystals

The propagation of light in a photonic crystal is governed by the Maxwell's equations. For 2D photonic crystals, when there is no point source or sink of electric and magnetic fields, the Maxwell equations can be reduced to two decoupled master equations as

$$-\nabla\cdot\left(\nabla E(\mathbf{k},\mathbf{r})\right)=\varepsilon(\mathbf{r})\left(\frac{\omega}{c}\right)^2 E(\mathbf{k},\mathbf{r}) \quad \text{for TM mode} \tag{1a}$$

$$-\nabla\cdot\left(\frac{1}{\varepsilon(\mathbf{r})}\nabla H(\mathbf{k},\mathbf{r})\right)=\left(\frac{\omega}{c}\right)^2 H(\mathbf{k},\mathbf{r}) \quad \text{for TE mode} \tag{1b}$$

where $\mathbf{k} = (k_x, k_y)$ is the wave vector and $\mathbf{r} = (x, y)$ denotes the coordinates. $\varepsilon(\mathbf{r})$ is the dielectric function. $E(\mathbf{k}, \mathbf{r})$ is the electric field, $H(\mathbf{k}, \mathbf{r})$ is the magnetic field, c is the speed of light, and ω is the corresponding eigenfrequency.

Due to the periodicity of the crystal, $\varepsilon(\mathbf{r}) = \varepsilon(\mathbf{r}+\mathbf{R})$, $E(\mathbf{k}, \mathbf{r}) = E(\mathbf{k}, \mathbf{r}+\mathbf{R})$ and $H(\mathbf{k}, \mathbf{r}) = E(\mathbf{k}, \mathbf{r}+\mathbf{R})$, where $\mathbf{R}$ is the lattice translation vector. Based on the Bloch-Floquet theory [21], $E(\mathbf{k}, \mathbf{r})$ and $H(\mathbf{k}, \mathbf{r})$ can be represented by the product of a periodic function and an exponential factor

$$E(\mathbf{k},\mathbf{r})=E(\mathbf{r})\cdot\exp(i\mathbf{k}\cdot\mathbf{r}) \quad \text{for TM mode} \tag{2a}$$

$$H(\mathbf{k},\mathbf{r})=H(\mathbf{r})\cdot\exp(i\mathbf{k}\cdot\mathbf{r}) \quad \text{for TE mode} \tag{2b}$$

Substitute Eqs. 2a and 2b into Eqs. 1a and 1b, the governing equations can be converted to eigenvalue problems within the representative unit cell.

$$-(\nabla+i\mathbf{k})\cdot\left((\nabla+i\mathbf{k})E(\mathbf{r})\right)=\varepsilon\left(\frac{\omega}{c}\right)^2 E(\mathbf{r}) \quad \text{for TM mode} \tag{3a}$$

$$-(\nabla+i\mathbf{k})\cdot\left(\frac{1}{\varepsilon}(\nabla+i\mathbf{k})H(\mathbf{r})\right)=\left(\frac{\omega}{c}\right)^2 H(\mathbf{r}) \quad \text{for TE mode} \tag{3b}$$

For a given wave vector $\mathbf{k} = (k_x, k_y)$, Eqs. 3a and 3b can be solved by finite element method. The weak expressions $F_E(v, E(\mathbf{r}))$ and $F_H(v, H(\mathbf{r}))$ corresponding to TM modes and TE modes respectively are

$$F_E(v,E(\mathbf{r})) = v\frac{\partial^2 E(\mathbf{r})}{\partial x^2} + v\frac{\partial^2 E(\mathbf{r})}{\partial y^2} + v\frac{\partial}{\partial x}(ik_x E(\mathbf{r})) + v\frac{\partial}{\partial y}(ik_y E(\mathbf{r})) + ik_x v\frac{\partial E(\mathbf{r})}{\partial x} + ik_y v\frac{\partial E(\mathbf{r})}{\partial y} - k^2 vE(\mathbf{r}) - \left(\frac{\omega}{c}\right)^2 v\varepsilon E(\mathbf{r}) \tag{4a}$$

$$F_H(v,H(\mathbf{r})) = v\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon}\frac{\partial H(\mathbf{r})}{\partial x}\right) + v\frac{\partial}{\partial y}\left(\frac{1}{\varepsilon}\frac{\partial H(\mathbf{r})}{\partial y}\right) + v\frac{\partial}{\partial x}\left(\frac{1}{\varepsilon}ik_x H(\mathbf{r})\right) + v\frac{\partial}{\partial y}\left(\frac{1}{\varepsilon}ik_y H(\mathbf{r})\right) + ik_x\frac{1}{\varepsilon}v\frac{\partial H(\mathbf{r})}{\partial x} + ik_y\frac{1}{\varepsilon}v\frac{\partial H(\mathbf{r})}{\partial y} - k^2\frac{1}{\varepsilon}vH(\mathbf{r}) - \left(\frac{\omega}{c}\right)^2 vH(\mathbf{r}) \tag{4b}$$

where v is the test function. By discretizing the unit cell with 4-node square elements, the above eigenvalue problems can be written in the matrix format as

$$\left[\mathbf{K} - \left(\frac{\omega}{c}\right)^2 \mathbf{M}\right]\mathbf{u} = 0 \tag{5}$$

where $\mathbf{K} = \sum \mathbf{K}_e$, $\mathbf{M} = \sum \varepsilon_e \mathbf{M}_e$ and $\mathbf{u} = \mathbf{E}$ for TM modes, while $\mathbf{K} = \sum \frac{1}{\varepsilon_e}\mathbf{K}_e$, $\mathbf{M} = \sum \mathbf{M}_e$ and $\mathbf{u} = \mathbf{H}$ for TE modes. $\mathbf{K}_e$ and $\mathbf{M}_e$ denote the elemental stiffness and mass matrices, ε_e is the relative permittivity of element e.

BESO process

In this paper, our aim is to design photonic crystals with a large complete band gap. The size of the band gap can be measured by the band gap-midgap ratio, which is independent on the size of the photonic crystal and hence more meaningful than the absolute value of the band gap. The position of the band gap is controlled manually by specify the adjacent TM bands (referred as band ω_i^{TM} and band $\omega_{i+1}^{\mathrm{TM}}$) and TE bands (referred as band ω_j^{TE} and band $\omega_{j+1}^{\mathrm{TE}}$). The upper limit of the band gap is the smaller value of $\omega_{i+1}^{\mathrm{TM}}$ and $\omega_{j+1}^{\mathrm{TE}}$, while the lower limit is the larger value of ω_i^{TM} and ω_j^{TE}. Therefore, the objective function $f(\mathbf{X})$ in can be expressed as

$$f(\mathbf{X}) = \frac{\min(\omega_{i+1}^{\mathrm{TM}}(\mathbf{k}), \omega_{j+1}^{\mathrm{TE}}(\mathbf{k})) - \max(\omega_i^{\mathrm{TM}}(\mathbf{k}), \omega_j^{\mathrm{TE}}(\mathbf{k}))}{(\min(\omega_{i+1}^{\mathrm{TM}}(\mathbf{k}), \omega_{j+1}^{\mathrm{TE}}(\mathbf{k})) + \max(\omega_i^{\mathrm{TM}}(\mathbf{k}), \omega_j^{\mathrm{TE}}(\mathbf{k})))/2} \tag{6}$$

where $\mathbf{X} = \{x_1, x_2 \ldots x_n\}$ is the elemental design variable, n is the total number of elements. Each elemental design variable corresponds to its material property, ε_e,, so $\mathbf{X}$ represents the topology of the unit cell. In the optimization process, the evolution of topology is reflected by the change of design variables.

The design variable is constructed by assuming $x_e = 0$ means element e is consist of material 1 which has a low permittivity ε_1, and $x_e = 1$ denotes material 2 with high permittivity ε_2. According to our numerical experience, in order to have a stable and reliable optimization process, x_e is set to be a discrete value between 0 and 1 with a custom step size. Then, the permittivity of this element is interpolated by following functions.

$$\varepsilon(x_e) = \varepsilon_1(1-x_e) + \varepsilon_2 x_e \quad \text{for TM mode} \tag{7a}$$

$$\varepsilon(x_e) = \frac{1}{(1-x_e)/\varepsilon_1 + x_e/\varepsilon_2} \quad \text{for TE mode} \tag{7b}$$

Finally, the optimization problem can be stated as

$$\begin{aligned} &\text{Maximize}: f(\mathbf{X}) \\ &\text{Subject to}: 0 \le x_{\mathrm{e}} \le 1 \end{aligned} \tag{8}$$

The topology of the unit cell is updated iteratively based on the elemental sensitivity numbers, i.e. the relative ranking of elemental sensitivities, which is the derivative of the objective function with regard to a design variable. Based on the objective function, the sensitivity of element *e* can be expressed as

$$\alpha_e = \frac{\partial f(\mathbf{X})}{\partial x_e} = \frac{\omega_{bot}\dfrac{\partial \omega_{top}}{\partial x_e} - \omega_{top}\dfrac{\partial \omega_{bot}}{\partial x_e}}{(\omega_{top}+\omega_{bot})^2/4} \tag{9}$$

where $\omega_{top} = \min(\omega_{i+1}^{\mathrm{TM}}(\mathbf{k}), \omega_{j+1}^{\mathrm{TE}}(\mathbf{k}))$, $\omega_{bot} = \max(\omega_i^{\mathrm{TM}}(\mathbf{k}), \omega_j^{\mathrm{TE}}(\mathbf{k}))$. Based on the FEA method, for a given frequency $\omega_i(\mathbf{k})$ and its corresponding eigenvector $\mathbf{u}_{\mathrm{i}}$, its derivative to x_{e} can be expressed as

$$\frac{\partial \omega_i(\mathbf{k})}{\partial x_e} = \frac{1}{2\omega_i(\mathbf{k})}\mathbf{u}_i^{\mathrm{T}}\left(\frac{\partial \mathbf{K}}{\partial x_e} - (\omega_i(\mathbf{k}))^2\frac{\partial \mathbf{M}}{\partial x_e}\right)\mathbf{u}_i \tag{10}$$

The derivatives of matrix **K** and **M** can be calculated from the interpolation functions 7a and 7b

$$\frac{\partial \mathbf{K}}{\partial x_e} = 0, \quad \frac{\partial \mathbf{M}}{\partial x_e} = (\varepsilon_2 - \varepsilon_1)\mathbf{M}_e \quad \text{for TM mode} \tag{11a}$$

$$\frac{\partial \mathbf{K}}{\partial x_e} = \left(\frac{1}{\varepsilon_2} - \frac{1}{\varepsilon_1}\right)\mathbf{K}_e, \quad \frac{\partial \mathbf{M}}{\partial x_e} = 0 \quad \text{for TE mode} \tag{11b}$$

In order to improve the stability and convergence of optimization process, a heuristic filter scheme is integrated into the optimization algorithm and the elemental sensitivity numbers are further averaged with their corresponding values in the previous iteration. The specific procedure of the filter and average scheme can refer to Ref. [13].

After obtaining the elemental sensitivity numbers, BESO will modify the design variables based on the specified proportions of two constitutive materials. The BESO process starts from an initial design filled up with material 2 except a tiny void at the center of the unit cell. The total volume of material 2 in each iteration is evolved gradually[13].

BESO will increase design variables for elements with highest sensitivity numbers and decrease design variables for elements with lowest sensitivity numbers simultaneously. Based on the relative ranking of the elemental sensitivity numbers, a threshold of the sensitivity number, α^*, is determined by using bi-section method so that the volume of material 2 in the next iteration is equal to the target volume. The design variable for each element is modified by comparing its sensitivity number with the threshold. Different from other topology optimization methods with continuous

design variable, BESO method uses discrete design variable. In each iteration, the variation of a design variable is a constant Δx ($\Delta x = 0.1$ is used in this paper). The design variable x_e is updated as

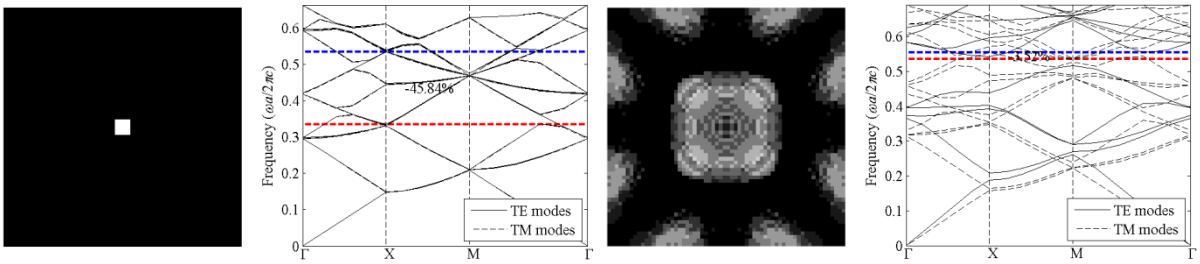
$$x_e = \begin{cases} \min(x_e + \Delta x, 1), & \text{if } \alpha_e > \alpha^* \\ \max(x_e - \Delta x, 0), & \text{if } \alpha_e < \alpha^* \end{cases} \tag{12}$$

Although discrete intermediate design variables are used in the optimization process, the final design tends to be a clear 0/1 design because a larger permittivity contrast leads to a larger band gap[22].

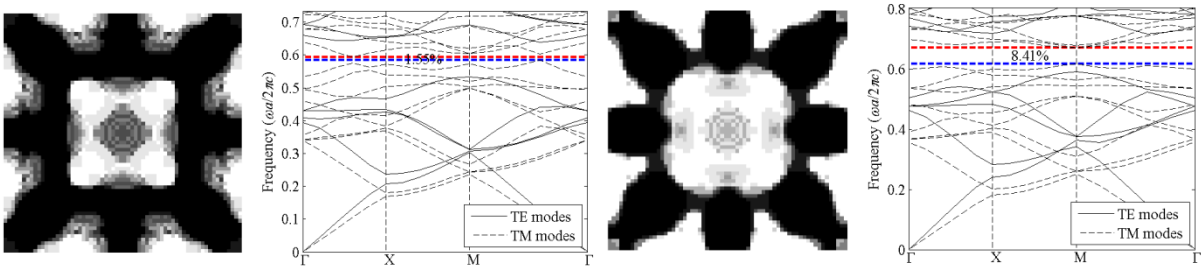
4. Results and discussion

2D photonic crystals with square lattice and C_{4v} symmetry are considered in this paper. The photonic crystals consist of 2 materials: Air, relative permittivity $\varepsilon_1 = 1$ and GaAs, relative permittivity $\varepsilon_2 = 11.4$. In the topology images below, the air is indicated by white color and the GaAs is indicated by black. The model is meshed with 64×64 four-node square elements. The FEA and BESO are programed with MATLAB codes.

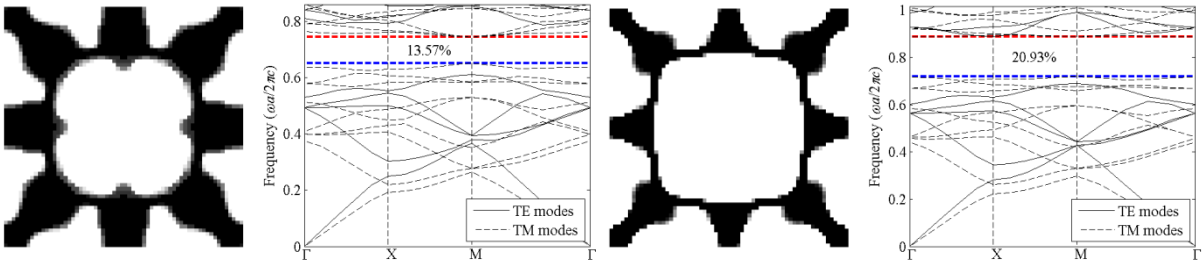
To illustrate the optimization process of BESO method, the evolution history of the topology and band diagrams of an example are shown in Fig. 1. The position of the band gap is between the 5th and 6th TM photonic bands and the 9th and 10th TE bands. For the simple initial design, the band gap-midgap ratio is a negative value, which means there is no band gap at all. With the optimization continues, the topology gradually evolves and the band gap-midgap ratio gradually increases. The volume fraction of GaAs gradually decreases from almost 100% to 30.06% at the end of the optimization process, and a complete band gap with a band gap-midgap ratio of 20.93% emerges. The whole optimization process cost 91 iterations which demonstrate the high computational efficiency of the proposed optimization algorithm.



(a) Initial design **(b) Iteration 10**



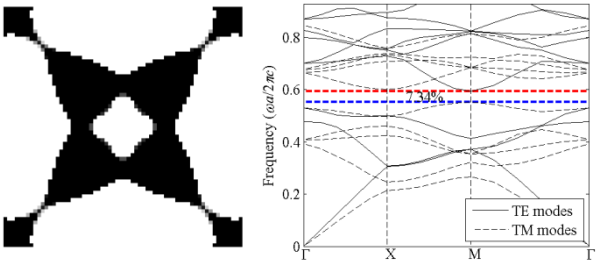
(c) Iteration 20 **(d) Iteration 30**



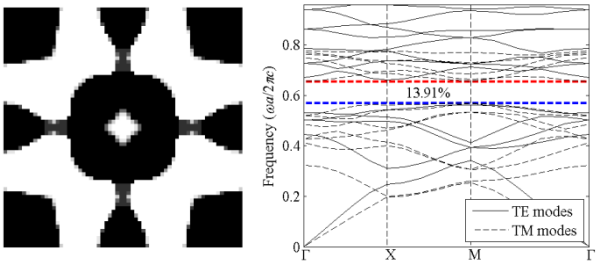
(e) Iteration 40 **(f) Final design**

Figure 1. Evolution history of a complete band gap formed by the overlapping of 9th TM and 5th TE band gap

Although the size of the maximized band gap illustrated in Fig. 1f is slightly larger than the result in Ref. [15], [17] and [18], all of them have a similar structure. However, by appointing different position of the complete band gap, some new designs can be obtained, as illustrated in Fig. 2. These designs are both obtained in less than 100 iterations. The resulting complete band gaps are 7.34% and 13.91%, respectively. It indicates that the solution is highly depended on the specified TE and TM bands for optimization. Therefore, the further study is recommended for finding a maximum complete band gap by appointing appropriate TE and TM bands.



(a) Complete band gap formed by the overlapping of 5th TM and 3rd TE band gap



(b) Complete band gap formed by the overlapping of 8th TM and 5th TE band gap

Figure 2. New designs of photonic crystals with complete band gap

Conclusions

This paper investigates the topology optimization of 2D photonic crystals with complete band gaps. An optimization scheme based on FEA and BESO is proposed to find the optimal design. According to the defined objective function and sensitivity analysis, the initial design gradually evolves to its optimum and a large complete band gap is formed between specified photonic TE and TM bands. The numerical results indicate the high-efficiency of the proposed algorithm and some new topologies with complete band gaps have been obtained. The proposed method can be equally applied for photonic crystals with other lattices.

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