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A new topology optimization algorithm for photonic band gap structures

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1. Abstract
A new topology optimization algorithm is proposed based on bi-directional evolutionary structural optimization (BESO) method in order to design photonic crystals with maximum band gaps. The optimization process starts from a simple unit cell without band gap, and the photonic crystals are assumed to be periodically composed of two materials with different permittivity. Based on finite element analysis, the BESO algorithm gradually re-distributes dielectric materials within the unit cell until the resulting photonic crystals possess a maximal band gap at appointed position in the band diagram. Numerical results are presented to demonstrate the effectiveness of the proposed optimization algorithm.
2. Keywords: Topology optimization; photonic band gap; bi-directional evolutionary structural optimization (BESO).

3. Introduction
Photonic crystals are optical structures consist of dielectric materials with different refractive indexes. They have lattice constants and periodicity on the wavelength scale in one, two or three dimensions. Photonic crystals are also called photonic band gap (PBG) structures because of their ability of prohibiting the propagation of electromagnetic waves within certain frequency ranges [1]-[2]. In practice, a broader band gap means broader available bandwidth of electromagnetic signals, therefore it is of great significance to design photonic crystals with large band gap. The optical properties of photonic crystals depend not only on the properties of dielectric materials but also on their spatial distributions. For given materials, the design of photonic crystals becomes a typical topology optimization question: how to periodically distribute the materials to maximize the band gap. Due to the polarization of electromagnetic waves, both transverse magnetic polarization (TM modes) and transverse electric polarization (TE modes) should be considered, respectively or simultaneously.
The traditional design approach of photonic band gap structures is a trial-and-error process based on physical intuitions and parametric study. This process can be inefficient and time-consuming [3]. To get photonic crystals with larger band gaps, different topology optimization methods have been introduced, for example, level set method [4], genetic algorithm [5], evolutionary algorithm [6] and semidefinite programming method [7]. These methods have been proved to be useful and many interesting results have been obtained. However, the optimization method starts from an initial design with band gap [6] or a randomly generated initial topology, which makes the method less efficient.
In this paper a new approach based on bi-directional evolutionary structural optimization (BESO) method [9] is proposed to optimize the design of 2D photonic crystal. BESO and its former version evolutionary structural optimization (ESO) are structural optimization method based on finite element analysis. The basic concept of ESO [8] is to achieve the optimal structural topology by gradually removing inefficient materials from initial ground structure. In BESO, materials can not only be removed, but also added to the structure based on the sensitivity analysis. The BESO algorithm proposed by Huang and Xie [9] has been successfully applied to the optimization of mechanical structures, property of electromagnetic materials, and natural frequencies of vibrating structures.
To apply the BESO method, the unit cell of a photonic crystal is meshed into elements and represented by discrete design variables respectively. A simple initial topology without band gap is adopted. The ratio of band gap between two appointed adjacent bands and midgap value is maximized as the objective function. Then sensitivity analysis of the objective function is conducted and a mesh-independency filter is adopted to stabilize the sensitivity number. Based on sensitivity numbers, BESO algorithm gradually evolves the topology of the unit cell until the assigned band gap is successfully obtained and maximized.

4. Topology optimization problem
4.1 Finite element analysis for photonic crystals

Electromagnetic wave propagation in photonic crystals is governed by Maxwell's equations. In 2D cases, there are two possible polarizations of the magnetic and electric fields, namely TM (transverse magnetic) and TE (transverse electric) modes. In TM modes, the magnetic field is confined to the plane of wave propagation and the electric field E = (0, 0, E) is perpendicular to this plane. In contrast, in TE modes, the electric field is confined to the plane of wave propagation and the magnetic field H = (0, 0, H) is perpendicular to this plane. It is assumed that there are no point sources or sinks of electric displacement and magnetic fields in photonic crystal, the time-harmonic Maxwell equations can be decoupled and reduce to two independent equations:

$$-\nabla\cdot(\nabla \mathrm{E}) = \varepsilon\left(\frac{\omega}{\mathrm{c}}\right)^2 \mathrm{E} \quad \text{for TM modes} \tag{1}$$

$$-\nabla\cdot\left(\frac{1}{\varepsilon}\nabla \mathrm{H}\right) = \left(\frac{\omega}{\mathrm{c}}\right)^2 \mathrm{H} \quad \text{for TE modes} \tag{2}$$

where c is the speed of light, ω is the angular frequency of the electromagnetic wave and ε(x) is the dielectric function. Due to the periodicity of the crystal, the dielectric function satisfies ε(x) = ε(x+X), where X is the lattice translation vector.

According to Bloch-Floquet theory, the magnetic and electric fields can be represented as the product of a periodic function and an exponential factor as $H(x) = H_k(x)\exp(ikx)$ and $E(x) = E_k(x)\exp(ikx)$. The Maxwell equations can be converted to eigenvalue problems within a unit cell and only the wave vector k on the boundary of irreducible Brillouin zone needs to be considered for band diagram.

$$-(\nabla + \mathrm{ik})\cdot((\nabla + \mathrm{ik})\mathrm{E}_\mathrm{k}) = \varepsilon\left(\frac{\omega}{\mathrm{c}}\right)^2 \mathrm{E}_\mathrm{k} \quad \text{for TM modes} \tag{3}$$

$$-(\nabla + \mathrm{ik})\cdot\left(\frac{1}{\varepsilon}(\nabla + \mathrm{ik})\mathrm{H}_\mathrm{k}\right) = \left(\frac{\omega}{\mathrm{c}}\right)^2 \mathrm{H}_\mathrm{k} \quad \text{for TE modes} \tag{4}$$

By discretizing the unit cell into square elements as in Fig.1, the above equations can be transformed into matrix format through the usual finite element method (FEM) procedure:

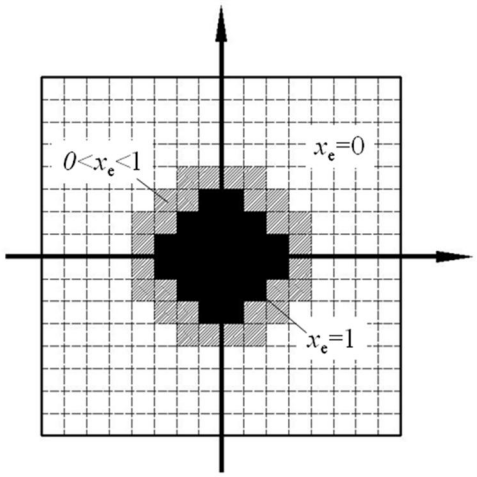


Figure 1: Discretization of a unit cell by square elements

$$\left(\sum_\mathrm{e} \mathrm{K}^\mathrm{e}\right)\mathrm{E} = \left(\frac{\omega}{\mathrm{c}}\right)^2\left(\sum_\mathrm{e} \varepsilon_\mathrm{e}\mathrm{M}^\mathrm{e}\right)\mathrm{E} \quad \text{for TM modes} \tag{5}$$

$$\left(\sum_\mathrm{e} \frac{1}{\varepsilon_\mathrm{e}}\mathrm{K}^\mathrm{e}\right)\mathrm{H} = \left(\frac{\omega}{\mathrm{c}}\right)^2\left(\sum_\mathrm{e} \mathrm{M}^\mathrm{e}\right)\mathrm{H} \quad \text{for TE modes} \tag{6}$$

where e denotes the number of element, and H and E are the eigenvectors for the magnetic and electric fields, respectively. K^e can be expressed by

$$\mathrm{K}^\mathrm{e} = \mathrm{K}_1 + \mathrm{K}_2 + \mathrm{K}_3 + \mathrm{K}_4 \tag{7}$$

where, $\mathrm{K}_1 = \int_\mathrm{A}\left(\frac{\partial \mathrm{N}^\mathrm{T}}{\partial \mathrm{x}}\frac{\partial \mathrm{N}}{\partial \mathrm{x}} + \frac{\partial \mathrm{N}^\mathrm{T}}{\partial \mathrm{y}}\frac{\partial \mathrm{N}}{\partial \mathrm{y}}\right)\mathrm{dA}$

$$K_2 = ik_x \int_A \left(\frac{\partial N^T}{\partial x} N - N^T \frac{\partial N}{\partial x} \right) dA$$

$$K_3 = ik_y \int_A \left(\frac{\partial N^T}{\partial y} N - N^T \frac{\partial N}{\partial y} \right) dA$$

$$K_4 = \left(k_x^2 + k_y^2\right) \int_A N^T N dA$$

M^e is expressed by

$$M^e = \int_A N^T N dA \tag{8}$$

where A denotes the total area of an element. The general form of Eqs. (5) and (6) can be expressed as

$$Ku = \left(\frac{\omega}{c} \right)^2 Mu \tag{9}$$

Where

$$K = \left(\sum_e K^e \right), \quad M = \left(\sum_e \varepsilon_e M^e \right) \quad \text{for TM modes} \tag{10}$$

$$K = \left(\sum_e \frac{1}{\varepsilon_e} K^e \right), \quad M = \left(\sum_e M^e \right) \quad \text{for TE modes} \tag{11}$$

Through sweeping wave vector (k_x, k_y) along the boundary of the first Brillouin zone, we can obtain the band diagram of a specific photonic crystal.

4.2 Objective function

Due to the lack of fundamental length scale in Maxwell's equation, the band gap-midgap ratio, which is independent of the lattice constant of the photonic crystal, is more useful than the absolute value of band gap. Therefore, the objective function in designing photonic structures is to maximize the band gap-midgap ratio between two adjacent bands (referred as band i and band i+1) as

$$f(X) = 2 \frac{\min \omega_{i+1}(k) - \max \omega_i(k)}{\min \omega_{i+1}(k) + \max \omega_i(k)} \tag{12}$$

Where $X = [x_1\ x_2\ \ldots\ x_n]$ is the design variable, n is the total number of elements. For a bi-material photonic crystal optimization, the problem can be stated as

$$\begin{aligned} &\text{Maximize}: f(X) \\ &\text{Subject to}: x_e = 0 \text{ or } 1 \end{aligned} \tag{13}$$

As shown in Fig.1, design variable $x_e = 0$ denotes material 1 with low permittivity and $x_e = 1$ denotes material 2 with high permittivity. In order to get a stable and reliable optimization process, x_e is a discrete value between 0 and 1 with a custom step size. The permittivity ε of element e is interpolated by following functions.

$$\varepsilon(x_e) = \varepsilon_1(1 - x_e) + \varepsilon_2 x_e \quad \text{for TM modes} \tag{14}$$

$$\varepsilon(x_e) = \frac{1}{(1 - x_e)/\varepsilon_1 + x_e/\varepsilon_2} \quad \text{for TE modes} \tag{15}$$

where ε_1 and ε_2 are the permittivity of materials 1 and 2 respectively.

4.3 sensitivity number

For objective function (12), the sensitivity number for element e can be expressed as

$$\alpha = \frac{\partial f(X)}{\partial x_e} = 4 \frac{\omega_{bot} \frac{\partial \omega_{top}}{\partial x_e} - \omega_{top} \frac{\partial \omega_{bot}}{\partial x_e}}{\left(\omega_{top} + \omega_{bot}\right)^2} \tag{16}$$

where $\omega_{top} = \min_k \omega_{i+1}(k)$, $\omega_{bot} = \max_k \omega_i(k)$.

For a given frequency $\omega_i(k)$, and its corresponding eigenvector u_i

$$\frac{\partial \omega_i(k)}{\partial x_e} = \frac{1}{2\omega_i(k)} u_i^T \left(\frac{\partial K}{\partial x_e} - (\omega_i(k))^2 \frac{\partial M}{\partial x_e} \right) u_i \tag{17}$$

The derivatives of matrix K and matrix M for the finite element analysis can be calculated from the interpolation functions (14) and (15) of design variable

$$\frac{\partial K}{\partial x_e} = 0,\ \frac{\partial M}{\partial x_e} = (\varepsilon_2 - \varepsilon_1) M_1^e \quad \text{for TM modes} \tag{18}$$

$$\frac{\partial K}{\partial x_e} = \left(\frac{1}{\varepsilon_2} - \frac{1}{\varepsilon_1}\right)\left(K_1^e + K_2^e + K_3^e + K_4^e\right),\ \frac{\partial M}{\partial x_e} = 0 \quad \text{for TE modes} \tag{19}$$

Based on the eigenfrequency and eigenvector calculated for finite element analysis, combining Eqs. (16)~(19), we can obtain the sensitivity number of each element, and then enhance existing topology by them.

5. Numerical implementation

5.1 Mesh-independency filter

Introducing a filtering scheme can effectively alleviate the numerical instabilities of the checkerboard pattern and mesh-dependency in the BESO method [11]. The modified sensitivity number of element e is

$$\hat{\alpha}_e = \frac{\sum_{i=1}^{n} w_i \alpha_i}{\sum_{i=1}^{n} w_i} \tag{20}$$

where the weight factor w_i is defined by

$$w_i = \begin{cases} r_{min} - r_i^e, & \text{if } r_{min} > r_i^e \\ 0, & \text{if } r_{min} \le r_i^e \end{cases} \tag{21}$$

where r_i^e denotes the distance between the center of element e and i. r_{min} is the radius of the filter, defined to identify the neighboring elements that affect the sensitivity number of element i. r_{min} is taken as 1/50 of lattice constant in this research.

In order to improve the stability and convergence of solution, elemental sensitivity numbers can be further averaged with their corresponding values in the previous iteration as

$$\tilde{\alpha}_e^k = \frac{1}{2}\left(\tilde{\alpha}_e^{k-1} + \hat{\alpha}_e^k\right) \tag{22}$$

where k is the current iteration number.

5.2 Topology evolution

The BESO process starts from an initial design filled up with material 2 which has a relative high permittivity with a pillar of material 1 in the center of the crystal lattice. The total volume of material 2, V, gradually decreases to a prescribed value V_0, and then increases or decreases until the maximum band gap-midgap ratio is achieved. The volume of matrial 2 for the next iteration is calculated by

$$V_{k+1} = V_k(1 - ER) \quad \text{when } V > V_0 \tag{23}$$

$$V_{k+1} = V_k\left(1 + \frac{(f(X_k) - f(X_{k-1}))\cdot(V_k - V_{k-1})}{|f(X_k) - f(X_{k-1})|\cdot|V_k - V_{k-1}|} ER\right) \quad \text{after } V_0 \text{ is reached} \tag{24}$$

where ER is evolution rate, which is taken as 2% in this paper.

The design variables are modified according to the relative values of sensitivity numbers and target volume of material 2. Based on the relative ranking of the elemental sensitivity numbers $\tilde{\alpha}$, a threshold of the sensitivity number, α^*, is determined by using bi-section method so that the target volume of material w in the next iteration is equal to V_{k+1}. 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 of element e is updated as:

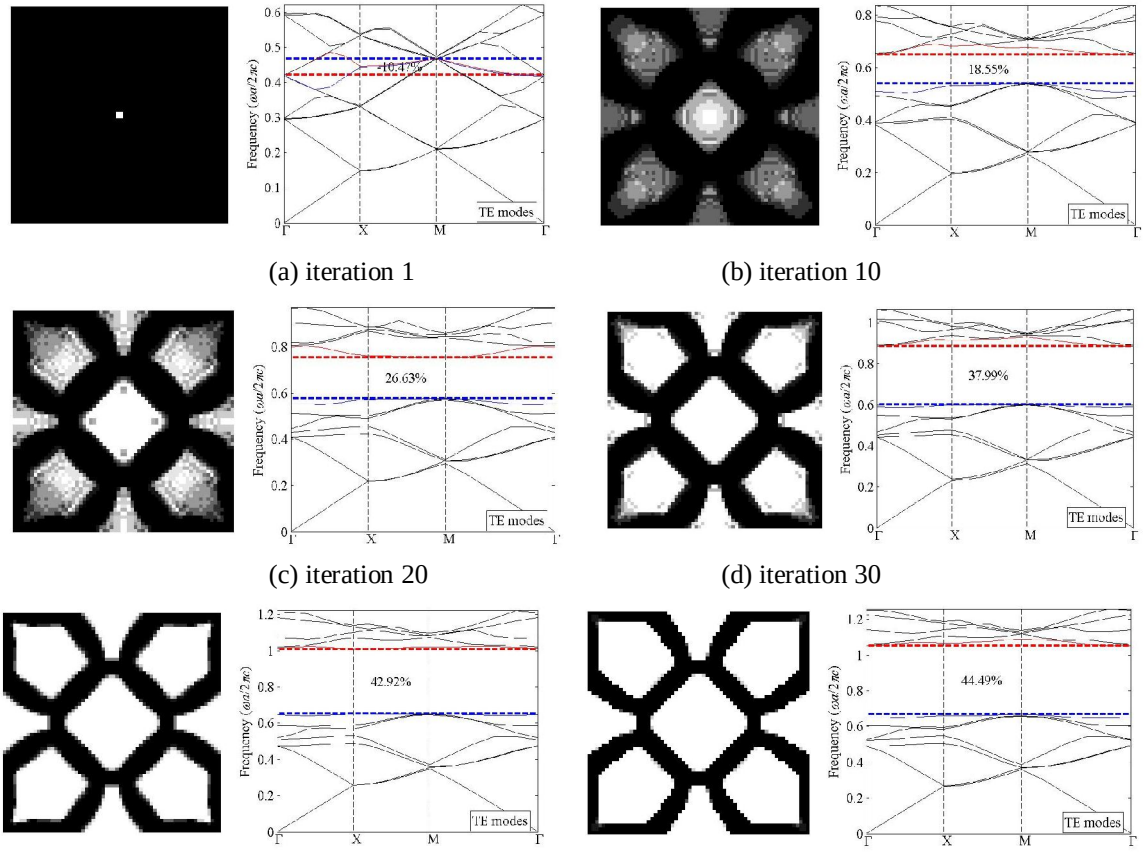
$$x_e = \begin{cases} \min(x_e + \Delta x, 1), & \text{if } \tilde{\alpha}_e > \alpha^* \\ \max(x_e - \Delta x, 0), & \text{if } \tilde{\alpha}_e < \alpha^* \end{cases} \tag{25}$$

6. Numerical results and discussion

The 2D photonic crystal with a square lattice is considered in this paper. The photonic crystal consists of 2 materials: Vacuum background (relative permittivity $\varepsilon_1 = 1$) and GaAs (relative permittivity $\varepsilon_2 = 11.4$). The model is meshed with 64×64 bilinear square elements. The FE analysis is conducted by COMSOL Multiphysics, and the sensitivity analysis is handled in MATLAB.

The optimization process of the 7th band gap of TE modes is illustrated in Fig.2 as an example. The white color denotes air and the black color denotes GaAs. It can be seen that, at the first step, the band gap-midgap ratio is

-10.47%, which means there is no band gap at all. With the optimization continues, the band gap-midgap ratio gradually increases to a positive value and the filling ratio of GaAs gradually decreases from the initial value with almost 100%. At the end of optimization process, the band gap-midgap ratio and volume both tend to be stably convergent. The final band gap-midgap ratio is 44.27%, volume is 39.84%. The whole optimization process needs 60 iterations which demonstrate the high computational efficiency of the proposed optimization algorithm.



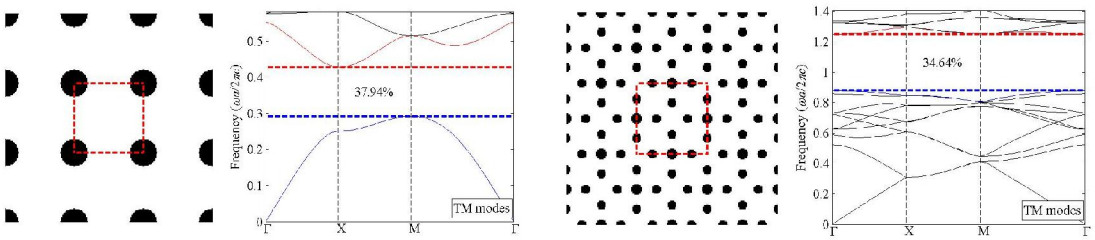
(a) iteration 1 (b) iteration 10

(c) iteration 20 (d) iteration 30

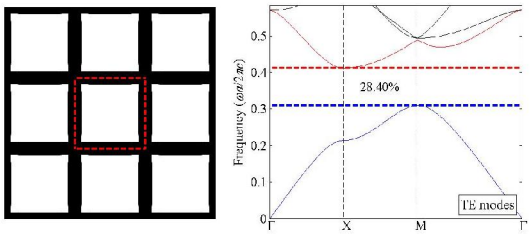
(e) iteration 40 (f) final design

Figure 2: Evolution history of topology and band diagrams for the 7th band gap of TE modes

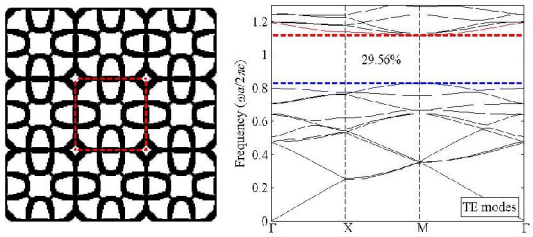
Figure 3 shows the optimized topologies and their corresponding diagrams for the 1st and 10th band gap of TM modes and the 1st and the 10th band gap of TE modes. From the same initial topology without band gap, the topology evolves and the band ratio increase to 37.94%, 34.64%, 28.40% and 29.56% respectively. It can be seen that the proposed BESO algorithm can robustly obtain the optimized results at both low frequency range and high frequency range.



(a) the 1st band gap of TM modes (b) the 10th band gap of TM modes



(c) the 1st band gap of TE modes



(d) the 10th band gap of TE modes

Figure 3: Optimized topologies of phononic crystals and their corresponding band diagrams

7. Conclusions

This paper investigates the topology optimization of 2D photonic crystals for both TM and TE modes. A new optimization method based on BESO is proposed to find the optimal design of photonic crystals with a maximum band gap. Based on the finite element analysis of photonic crystals, BESO gradually re-distrubutes the constituent material with the unit cell until the optimized band gap size is achieved. The numerical results indicate the effectiveness of the algorithm proposed in this paper for the design of photonic band gap structures. This algorithm can be further applied to other optimization problems of photonic crystals.

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9. References

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