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Bi-directional evolutionary optimization for photonic band gap structures

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ABSTRACT

Toward an efficient and easy-implement optimization for photonic band gap structures, this paper extends the bi-directional evolutionary structural optimization (BESO) method for maximizing photonic band gaps. Photonic crystals are assumed to be periodically composed of two dielectric materials with the different permittivity. Based on the finite element analysis and sensitivity analysis, BESO starts from a simple initial design without any band gap and gradually re-distributes dielectric materials within the unit cell so that the resulting photonic crystal possesses a maximum band gap between two specified adjacent bands. Numerical examples demonstrated the proposed optimization algorithm can successfully obtain the band gaps from the first to the tenth band for both transverse magnetic and electric polarizations. Some optimized photonic crystals exhibit novel patterns markedly different from traditional designs of photonic crystals.

1. Introduction

Photonic crystals are optical structures consist of dielectric materials with different refractive indexes. They have lattice constants around the wavelength of light and periodicity 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 signals and applications, so it is of great significance to design photonic crystals with large band gaps. The optical properties of photonic crystals depend not only on the properties of dielectric materials but also their spatial distributions [3]. Therefore, for given materials, the design of photonic crystals becomes a typical topology optimization question: how to periodically distribute the materials to maximize the specific band gap. Due to the polarization of electromagnetic waves, transverse magnetic polarization (TM mode) and transverse electric polarization (TE mode) can be considered separately.

The traditional design approach of photonic band gap (PBG) structures is a trial-and-error process based on physical intuitions and parametric studies. This process would be inefficient and time-consuming [4–8], and the resulting design may also be away from the optimum. The systematic way to find the optimal design of photonic crystals is formulating the

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problem with appropriate objective functions and/or constraints, and then solving it by topology optimization methods. The topology optimization methods were originally used in elastic field to seek the best materials layout within a given design space so that the resulting structures had the maximum stiffness or minimum compliance. So far, the commonly used topology optimization methods include Solid Isotropic Material with Penalization (SIMP) method [9–12], level set method [13–17], Evolutionary Structural Optimization (ESO) [18,19] and its later version bidirectional ESO (BESO) [20–22].

In order to obtain photonic or phononic crystals with large band gaps, many researchers have investigated into the design of PBG structures using various topology optimization methods, e.g. genetic algorithms [23–28], level set method [29–31], SIMP [32–35]. These methods have proven to be useful and some interesting designs have been obtained. However, because of the complicate nature of the solution space, a systemic topology optimization for PBG structures with any band gap is still a challenge. Sigmund and Jensen [34,35] proposed two-stage optimization where the first stage using coarse grids generated five best topologically different candidates for each band. Starting from the candidate topologies with the opening of the band gap, the SIMP method was then employed at the second stage to find the optimal PBG structures. Men et al. [36,37] systematically reported the design of PBG structures using semidefinite programming and subspace method. The optimization starts from a series of randomly generated initial designs, the photonic band gap could be obtained but the occurrence of the band gap could not be guaranteed. While these methods are attractive and have successfully obtained the optimized solutions of photonic band gap crystals, the computational cost for the optimization based on finite element analysis (FEA) is still expensive because hundreds, even thousands of iterations are needed. More importantly, the previous research also indicated that the obtained solutions depend highly on the used optimization parameters and algorithm [34–37]. This is because of the fact that a number of different topologies could possess the same band gap property and there is no unique solution for the design of PBG structures. Therefore, it is important to attempt new and different optimization algorithms, such as BESO, in order to find a much wider range of possible solutions to the PBG structures.

Toward an efficient but easy-implement optimization of PBG structures, a new approach based on the BESO method [20–22] is proposed in this paper. Based on FEA, BESO gradually removes elements from or adds elements to the design domain so that the resulting topology evolves towards an optimum. It has been demonstrated that the current BESO method is capable of generating reliable and practical topologies for optimization problems with various constraints such as natural frequency [38], compliant mechanisms [39] and nonlinear structures [40,41]. In recent years, the BESO algorithm has also been extended to the design of materials with mechanical or electromagnetic properties [42,43].

In this paper, we start from finite element discretization of photonic crystals for the propagation of electromagnetic waves. Based on FEA and the sensitivity analysis for the single or multiple eigenfrequencies, a BESO method is established by using discrete design variables. Starting from a simple initial design without any band gap, BESO evolves the topology of the unit cell to the optimized structures with the desired band gap. Finally, numerical examples are given to demonstrate the effectiveness and efficiency of the proposed optimization algorithm for the design of photonic crystals.

2. Finite element discretization

Photonic crystals are usually composed of two or more homogeneous materials distributed periodically as shown in Fig. 1(a). The propagation of electromagnetic waves in photonic crystals is generally governed by Maxwell's equations [1]. However, there are two possible polarizations of the magnetic and electric fields for 2D cases, namely TM (transverse magnetic) and TE (transverse electric) modes. In the TM mode, the magnetic field is confined to the plane of wave propagation and the electric field $\boldsymbol{E} = (0, 0, E(\mathbf{k}, \mathbf{r}))$ is perpendicular to this plane, where the vector $\mathbf{r} = (x, y)$ denotes the coordinates in the plane and $\mathbf{k}$ is the wave vector. In contrast, the electric field of the TE mode is confined to the plane of wave propagation and the magnetic field $\boldsymbol{H} = (0, 0, H(\mathbf{k}, \mathbf{r}))$ is perpendicular to this plane. Since there are no point sources or sinks of electric displacement and magnetic fields in photonic crystal, the time-harmonic Maxwell equations can be reduced to two decoupled equations as

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

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

where c is the speed of light, ω is the angular frequency of the electromagnetic wave and $\varepsilon(\mathbf{r})$ is the dielectric function. Due to the periodicity of the crystal, the dielectric function satisfies $\varepsilon(\mathbf{r}) = \varepsilon(\mathbf{r} + \mathbf{R})$ and $\mathbf{R}$ is the lattice translation vector.

According to the Bloch–Floquet theory [44], the magnetic and electric fields can be represented as the product of a periodic function and an exponential factor as

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

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

Thus, Maxwell equations can be further converted to the eigenvalue problems within a unit cell.

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