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Topology optimization of 2D phononic band gap crystals based on BESO methods

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1. Abstract:
Phononic band gap crystals, which could prohibit the propagations of elastic waves in certain frequency, are consisted of periodically distributed inclusions embedded in a matrix with high contrast in mechanical properties. In recent years, systematic design of phononic band gap crystals has attracted increasing attention due to their wide applications such as sound insulation, waveguides, or acoustic wave filtering. Toward an efficient and reliable optimization for phononic structures, we present a new topology optimization algorithm based on bi-directional evolutionary structural optimization (BESO) method and finite element analysis to maximize phononic band gaps. The optimization of maximizing the relative band gap size between two appointed neighbour bands starts from a unit cell without any band gap and then gradually adjusts the distribution of two materials in the following iteration steps based on the sensitivity analysis and BESO algorithm until the convergence criterions are satisfied. Various patterns of optimal phononic structures for both out-of-plane shear waves and are in-plane mixed waves presented. Numerical results show that the proposed algorithm is very effective and efficient.
2. Keywords: Phononic Band Gap Crystals, Topology Optimization, Bi-directional Evolutionary Structural Optimization (BESO)

3. Introduction
Sparkled by the remarkable work on the photonic crystals (PtCs) with periodic constructions of two dielectrics composite materials, which offer control over the propagation of electromagnetic waves, the study of phononic band gap crystals was first carried out by Kushwaha in 1993 [1, 2]. In analogy to photonic crystals, phononic crystals (PnCs), which prohibit the propagation of mechanical waves in certain range of frequencies, are generally composed of periodically distributed inclusions embedded in a matrix with high contrast in elastic properties. Such novel property makes them desirable for a variety of applications, for instance, sound insulation, waveguides, acoustic wave filtering, negative refraction, shock isolations well as acoustic cloaking [3]. Thus, photonic/phononic crystals have attracted considerable interest during past few decades.
When PnCs are designed for sound insulation or shock isolation, usually it is best to have the band gap as wide as possible. Therefore, how to obtain the optimal band gap structure is of great interest here. A promising mean to achieve this goal is to utilize the topology optimization method for systematic and scientific approach of designing phononic structures. Topology optimization of phononic band gap structures was first performed by Sigmund and Jensen (2003) [4], using finite element method combined with the method of moving asymptotes (MMA) to maximize the band-gap sizes. This pioneering work only presented a few examples and lacked the analysis of coupled problem of in-plane and out-of-plane waves. Later a genetic algorithm (GA) in conjunction with finite element method was proposed for optimizing a two-dimensional phononic crystal for out-of-plane waves (Gazonas et. al) [5]. Hussein et al. [6, 7] used GA to conduct a series of optimization of both one-dimensional and two-dimensional phononic crystals. Rupp et al. [8] developed a gradient-based topology optimization to design two and three-dimensional phononic wave filters, including surface waveguides. Dong et al.[9] reported a more detailed work on topology optimization of two-dimensional phononic crystals using a two-stage GA and FEM for both out-of-plane waves and in-plane waves with and without volume constraint. Liu et al. [10] used a two-stage GA in conjunction with fast plane wave expansion method to optimize the band gap width of phononic crystals for in-plane coupled mode, out-of-plane acoustic mode and mixed mode. It should be noted that aforementioned algorithms often cost significant computations. Taking GA in combination with FEM for example, it usually would take more than several hundreds of steps before the optimal design was achieved [9, 10]. Though parallel computation could reduce the computational cost more easily than before, it is still lack of efficiencies.
Toward an efficient and reliable optimization for phononic structures, in this paper we propose a new topology optimization algorithm based on the bi-directional evolutionary structural optimization (BESO) method and finite element analysis to maximize phononic band gaps. The rest of the paper is organized as follows: governing equations and BESO optimization approach to optimize the band gap width between two adjacent bands are presented in section 4. In section 5, various patterns of optimal phononic band gap structures are presented for both out-of-plane shear waves and in-plane mixed waves. This is followed by conclusions.

4. Formulations

4.1 Analysis of phononic crystals

The propagation of mechanical waves in an elastic inhomogeneous medium is governed by

$$\rho u = \nabla[\lambda(r) + 2\mu(r)](\nabla u) - \nabla \times [\mu(r)\nabla \times u] \tag{1}$$

Where λ and μ are the Lame's coefficients; ρ is the material density; $\mathbf{u=\{u_x,u_y,u_z\}}$ is the displacement vector.

In this paper we only consider the elastic waves that propagate in the x-y plane, i.e. the wave field are independent of z so that $\partial u / \partial z = 0$. Then Eq.(1) can be split into two coupled in-plane equations, which govern the longitudinal and transverse modes, and an out-of-plane equation that governs acoustic mode:

$$\rho \frac{\partial^2 u_x}{\partial t^2} = \frac{\partial}{\partial x}\left[\left(\lambda(\boldsymbol{r}) + 2\mu(\boldsymbol{r})\right)\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y}\right] + \frac{\partial}{\partial y}\left[\mu(\boldsymbol{r})\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)\right] \tag{2}$$

$$\rho \frac{\partial^2 u_y}{\partial t^2} = \frac{\partial}{\partial x}\left[\mu(\boldsymbol{r})\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)\right] + \frac{\partial}{\partial y}\left[\frac{\partial u_x}{\partial x} + \left(\lambda(\boldsymbol{r}) + 2\mu(\boldsymbol{r})\right)\frac{\partial u_y}{\partial y}\right] \tag{3}$$

$$\rho \frac{\partial^2 u_z}{\partial t^2} = \frac{\partial}{\partial x}\left[\mu(\boldsymbol{r})\frac{\partial u_z}{\partial x}\right] + \frac{\partial}{\partial y}\left[\mu(\boldsymbol{r})\frac{\partial u_z}{\partial y}\right] \tag{4}$$

where r=(x,y) denotes the position vector.

According to the Floquet-Bloch wave theory, the displacement vector can represented as the product of a periodic function and an exponential factor as:

$$\boldsymbol{u}(\boldsymbol{r},\boldsymbol{k}) = \boldsymbol{u}_k(\boldsymbol{r})e^{i(\boldsymbol{k}\cdot\boldsymbol{r})} \tag{5}$$

where $\mathbf{u_k(r)}$ is a periodic function of **r** with the same periodicity as the structure; $\mathbf{k=(k_x,k_y)}$ is the Bloch wave vector.

Inserting Eq.(5) into either Eq.(2), Eq.(3) or Eq.(4), with λ(**r**)=λ(x,y), μ(**r**)=μ(x,y) and ρ(**r**)=ρ(x,y); the elastic waves governing equations can be converted to eigenvalue problems within a unit cell. After discretized by finite element method (FEM), these equations can be written as:

$$\left(\boldsymbol{K}(k) - \omega^2\boldsymbol{M}\right)\boldsymbol{u} = 0 \tag{6}$$

where $\boldsymbol{u}=\boldsymbol{u}_k$; **K** and **M** are stiffness matrix and mass matrix respectively. Due to the periodicity of the unit cell, only the wave vectors on the boundary of irreducible Brillouin zone are considered for the calculation of the band diagram.

4.2 Topology optimization problem

Our goal for the optimization of phononic crystals here is to maximize the relative band gap between two adjacent bands (referred as band n and band n+1). The objective function can be stated as follows:

Max:
$$f(x_e) = 2\frac{\min\omega_{n+1}(\boldsymbol{k}) - \max\omega_n(\boldsymbol{k})}{\min\omega_{n+1}(\boldsymbol{k}) + \max\omega_n(\boldsymbol{k})} \tag{7}$$

Subjected to:
$$\sum_{e=1}^{N} x_e \times V_e = V$$

where x_e is the design variable which describes the material distribution in the unit cell. Ve and V are the elemental volume and the prescribed volume of the unit cell, respectively. It should be noted that the frequency is the function of the wave vector.

It is assumed that the phononic crystal is composed of two base materials. We use the linear material interpolation scheme, which has been applied successfully to the design of phononic crystals [4] as

$$\rho(x_e) = (1 - x_e)\rho_1 + x_e\rho_2 \tag{8}$$

$$\lambda(x_e) = (1 - x_e)\lambda_1 + x_e\lambda_2 \tag{9}$$

$$\mu(x_e) = (1 - x_e)\mu + x_e\mu_2 \tag{10}$$

where subscripts '1' and '2' represent the matrix material and the inclusion material respectively. In the traditional BESO method [11-14], the discrete design variable is set x_e=0 or 1 only. However, numerical simulation shows that the optimization process of phononic crystals is very sensitive to the change of design variable. Thus, in this paper the variation of the design variable in each iteration step is limited to be Δx_e=0.1.

4.3 Sensitivity Analysis and BESO algorithm

For a given wave vector **k** and assuming that eigenvectors are normalized to the global mass matrix, the sensitivities of eigenfrequencies $\omega_n(\mathbf{k})$ with respect to a change in an element design variable can be computed as:

$$\frac{\partial \omega_n(\boldsymbol{k})}{\partial x_e} = \frac{1}{2\omega_n} u(\boldsymbol{k})_n^T \left(\frac{\partial K}{\partial x_e} - \omega_n^2 \frac{\partial M}{\partial x_e} \right) u(\boldsymbol{k})_n \tag{11}$$

Thus, the sensitivity of the objective function can be written as:

$$\frac{\partial f(\boldsymbol{X})}{\partial x_e} = 4 \frac{\max\omega_n(\boldsymbol{k}) \dfrac{\partial \min\omega_{n+1}(\boldsymbol{k})}{\partial x_e} - \min\omega_{n+1}(\boldsymbol{k}) \dfrac{\partial \max\omega_n(\boldsymbol{k})}{\partial x_e}}{\left(\min\omega_{n+1}(\boldsymbol{k}) + \max\omega_n(\boldsymbol{k})\right)^2} \tag{12}$$

Originally proposed by Xie and Steven [15] in early 1990s, the essential idea of evolutionary structural optimization (ESO) method is by gradually deleting low efficient materials, remain topology of the structure evolves to an optimal design. Its later version, BESO allows adding materials while removing insufficient ones [16, 17]. Topology optimization of phononic band gap structures starts from a simple unit cell without any band gap. Then based on the sensitivity analysis and BESO algorithm, it will gradually modify the distribution of two materials in the following iteration steps by changing the value of the design variable of every element until the convergence criterions are satisfied. A filter scheme shown below is adopted to avoid checkerboard and mesh-dependency problems [11]:

$$\hat{\alpha}_i = \frac{\sum_{j=1}^{M} w(r_{ij})\alpha_j}{\sum_{j=1}^{M} w(r_{ij})} \tag{13}$$

where r_{ij} denotes the distance between the centre of the element i and node j ; $w(r_{ij})$ is weight factor given as

$$w(r_{ij}) = \begin{cases} r_{\min} - r_{ij}, & for \quad r_{ij} < r_{\min} \\ 0, & for \quad r_{ij} \geq r_{\min} \end{cases} \tag{14}$$

with r_{min} as the radius of the filter.

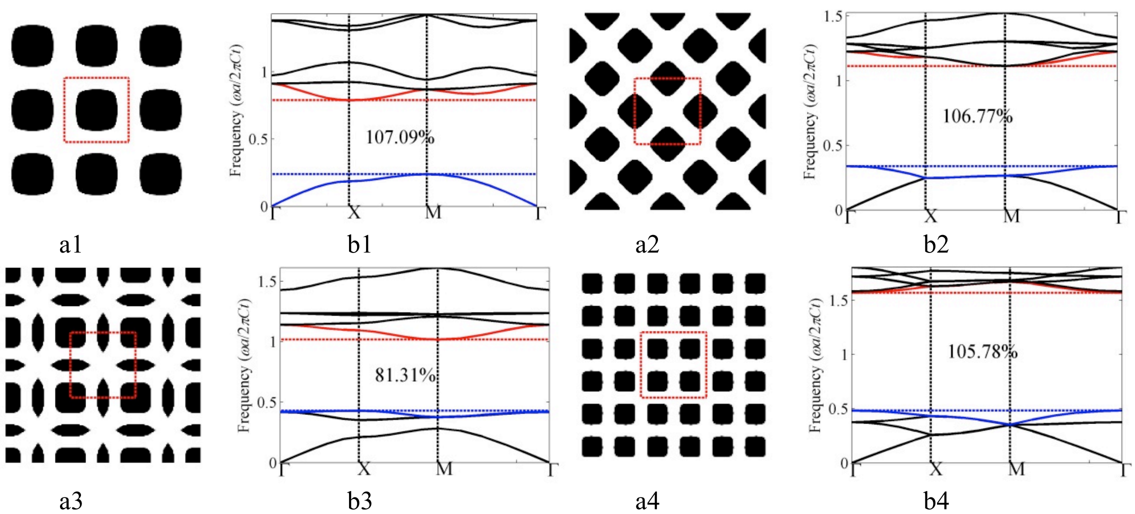
5Numerical Results

In this example, our goal is to maximize the relative band gap between two neighbor bands of a 2D square unit cell for a prescribed material volume fraction. A solid-solid phononic structure design is considered with Epoxy as the matrix and Au as the inclusion material. The material parameters are: ρ_{epoxy}=1200 kg/m^3, λ_{epoxy}=6.38 GPa, μ_{epoxy}=1.61 GPa, ρ_{Au}=19500 kg/m^3, λ_{Au}=65.44 GPa and μ_{Au}=29.94 GPa.

BESO starts from an initial design without band gap and gradually decreases the total volume of the unit cell using an evolutionary rate ER=2%. A mesh-independency filter is used to avoid tiny structures and the radius of the filter is 1/50 of the length of the lattice's diagonal line.

5.1 Out-of-Plane waves (Acoustic modes)

The optimal unit cells and the corresponding band diagrams for the first to eighth band gaps of the out-of-plane waves which propagate in the Au-Epoxy composite are demonstrated in figure 1 with the volume constraint of V_f=0.38. The optimized topologies show the distribution of 3×3 array of unit cells (the representative unit cell is shown within the red dashed box), in which black represents Au and white represents Epoxy. The optimal designs are very similar to those reported by Dong et al. [9] for the first and fifth band gap structures. It demonstrates the effectiveness of the proposed optimization method. It is also noted that the complexity of the optimal topologies increases when the appointed bands grow higher.



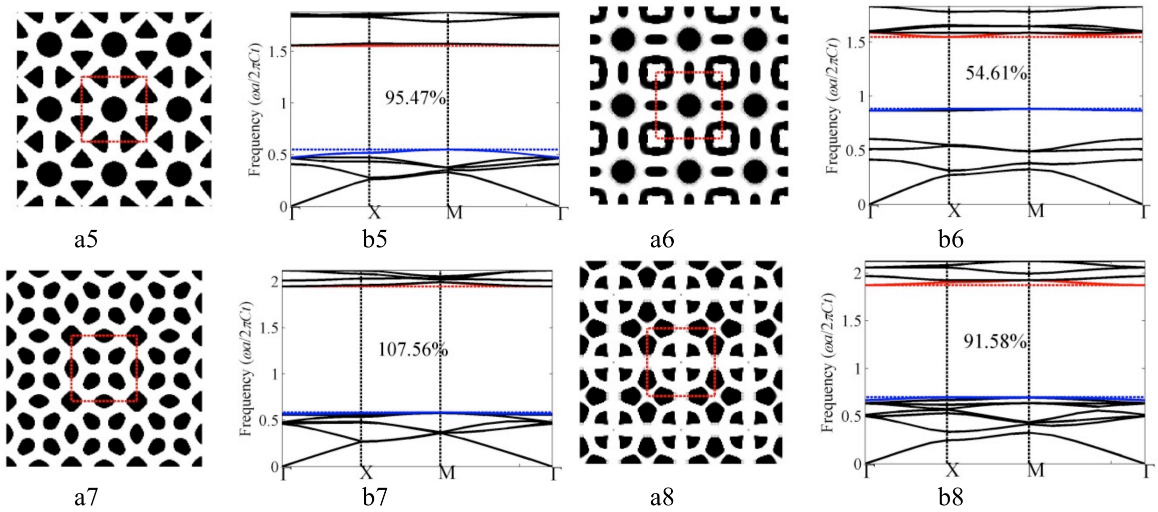


Figure 1: Optimized band gap structures and corresponding band diagrams from the first to eighth band for the out-of-plane mode .The black and white colours represent Au and Epoxy, respectively.

Figure 2 illustrates the evolution history of the first band gap optimization process for the out-of-plane mode. As shown in the figure, there is no initial gap between the first and second bands. The band gap occurs after several iterations and then the total volume of the unit cell gradually increases as the volume fraction decreases to the predefined value. Finally, the optimized gap size stably achieves its maximum value when the volume is kept to be the constraint value. It can also be concluded from figure 2 that the proposed algorithm is of high efficiency since the optimization process would converge in 70 iteration steps, which is much faster than present optimization methods, for instance GA would take nearly 1000 iterations [9].

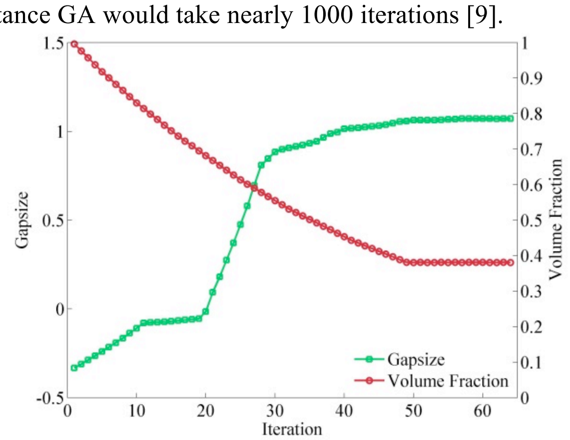


Figure 2: Evolution histories of the first band gap size and volume fraction.

5.2 In Plane waves (Coupled modes)

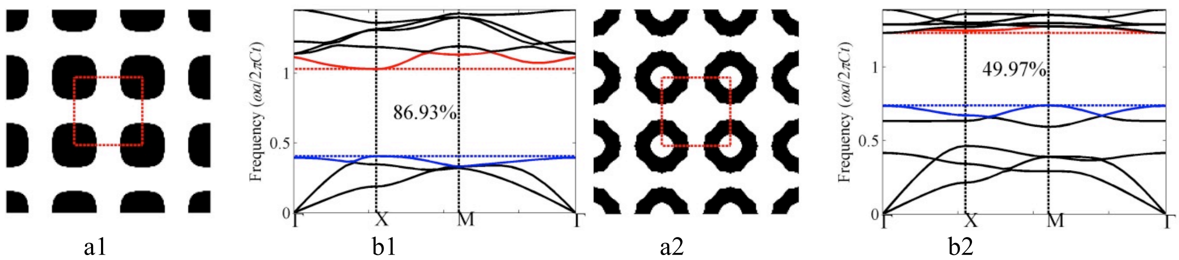


Figure 3: Optimized phononic band gap structures and corresponding band diagrams for third and fifth band gaps of in-plane mode.

The proposed optimization method can also applied to the in-plane waves of phononic crystals. Using the same parameters for the previous examples, the optimization results for the third and fifth band gaps of the in-plane mode are shown in the figure 3. The volume constraint is also set to be V_f=0.38. The optimized topology for the third band gap is analogous to the first band gap structure of the out-of-plane mode. The optimized topology for the fifth band gaps looks like a hollow diamond, which also has a small band gap between the third and fourth bands. It is observed that band gap between the third and fourth band can be easily obtained when optimizing for other band gaps.

6. Conclusions

This paper proposes a new optimization algorithm based on BESO in combination with FEM for the design of phononic band gap structures and systematically investigates the topology optimization of 2D phononic band gap crystals for both the out-of-plane and in-plane wave modes. Numerical results show that optimized topologies for various band gaps has been successfully achieved. The optimized band gap sizes well demonstrate the effectiveness of the proposed optimization algorithm. Moreover, the optimization method proposed in this paper is also efficient as the optimization usually converges within about 100 iterations.

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