Design of porous phononic crystals with combined band gaps

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Abstract

Phononic crystals are periodic structures known for their abilities to alter the propagation of acoustic or elastic waves, and their characteristics are greatly dependent on the topological configurations of constituent materials within the unit cell. Thus it is possible to engineer a phononic crystal for specific functionality by tailoring its topology. Low manufacturing cost as well as light weight gives porous phononic crystals advantages over other kinds of phononic structures. This paper presented a bi-directional structural optimization (BESO) method in conjunction with homogenization theory for the systematic design of porous phononic crystals. On account of sustaining static loads, a bulk or shear modulus constraint is considered in the design of porous phononic structures. A multi-objective optimization was conducted to simultaneously maximize combined band gap width and bulk or shear modulus with a prescribed volume fraction of consisting solid material. The methodology was briefly introduced and several optimized porous phononic structures with exceptionally large band gaps were presented.

Keywords: Porous phononic crystals, Band gap, BESO, Homogenization, Multi-objective optimization

Introduction

Phononic crystals (PnCs) artificially designed to control the propagation of acoustic and elastic waves are periodic structures consisting of different materials usually with high contrast in their mechanical properties [1]-[5]. The most fundamental feature of PnCs is the existence of band gaps, the frequency ranges within which the propagation of mechanical waves is strictly forbidden. This special property gives rise to mangy applications such as noise and vibration control as well as wave filtering and waveguides, *etc.* [6][7]. Over the past two decades, several classes of PnCs differing in the physical nature of the constituent phases have been studied, including solid/solid, solid/fluid, solid/void, fluid/fluid systems, *etc*. [8].Among them, porous phononic crystals with void or air holes embedded in solid matrix have exceptional advantages over other systems, for they can be very light-weighted while easily fabricated with low manufacturing cost. They hold a promising prospect for applications in noise and vibration control of aircraft, automobile and other industries that have restricted control over weight.

Porous PnCs can be easily engineered by adjusting the spatial distributions of air/vacuum holes in a solid substrate. Initially in analog to studies on composite PnCs, positions, shapes, sizes of air/vacuum holes, as well as the layouts of the unit cell have been carefully investigated to disclose their relations with the phononic band gaps [9][10]. It is apparent that such trial-and-error methods are incapable to get the optimal designs when compared with more systematical means such as topology optimization. Systematic design of phononic band gap crystals was first conducted by Sigmund and Jensen based on finite element method (FEM) in combination with a gradient-based optimization algorithm [11]. Later, genetic algorithm (GA) and another gradient-based topology optimization, in conjunction with FEM or the fast plane wave expansion method (FPWE), are developed to maximize the band gap sizes of phononic band gap crystals [12]-[16]. Most of these works focused on the topological design of the composite PnCs while the porous PnCs are less considered [17]. Previous research on composite and porous PnCs has revealed that the stiffer and heavier material

tends to be isolated by the soft and light counterpart in order to get an optimal band gap size. Such characteristic leads to a tricky problem in the optimization of porous PnCs. Since the transverse/ shear waves are not supported in the air, the discontinuous solid materials would only support the propagation of longitudinal waves, which reduces the problem to sonic crystals. However the initial intention is to find the optimal porous phononic structures that exhibit large band gaps for elastic waves. Therefore, it is necessary to make sure that the optimized phononic band gap structures have continuous distribution of solid material to support all components of elastic waves. Dong et al. conducted a multi-objective optimization of 2D porous PnCs for maximizing band gap width and minimizing mass of structure simultaneously by using non-dominated sorting-based genetic algorithm II (NSGA-II) [18]. In this work, an artificial geometrical constraint was adapted to avoid too narrow connections and guarantee the resulting structure is self-support. It is apparent that current research in this area is insufficient and further systematic investigation into the design of cellular phononic band gap crystals is necessary.

Considering the porous PnCs might sustain certain amount of static loads, it is more meaningful to add extra stiffness constraint than simply adding a geometrical constraint to the optimized structures. To the authors' best knowledge, no work has been reported yet to conduct band gap optimization on the porous phononic crystals with a stiffness constraint and volume constraint simultaneously. In the present paper, the focus is the unit cell topology optimization of porous PnCs by using a specific bi-directional structural optimization algorithm. The objective is to maximize the combined out-of-plane and in-plane band gap size for porous phononic crystals subject to bulk or shear modulus constraint with a given volume fraction. In next Section we introduce the essential governing equations and related theories of topology optimization algorithm used in this paper. This is followed by a number of optimization results and conclusions.

Governing Equations and Topology Optimization Algorithm

Governing Equations

In this paper, we consider two dimensional phononic crystals with square lattice and assume the propagation of elastic waves is restricted to the *x*–*y* plane only. The governing equation for out-of-plane transverse waves is given by:

$$\rho(\mathbf{r})\frac{\partial^2 u_z}{\partial t^2} = \frac{\partial}{\partial x}\left[\mu(\mathbf{r})\frac{\partial u_z}{\partial x}\right] + \frac{\partial}{\partial y}\left[\mu(\mathbf{r})\frac{\partial u_z}{\partial y}\right] \tag{1}$$

while the couple in-plane longitudinal and transverse waves are governed by:

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

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

where λ and μ denote the Lame's coefficients; ρ is the material density; and r = (*x*, *y*) denotes the position vector; $\mathbf{u} = \{u_x, u_y, u_z\}^T$ is the displacement vector, and according to Bloch's theorem when waves propagate in periodic structures it should satisfy the form:

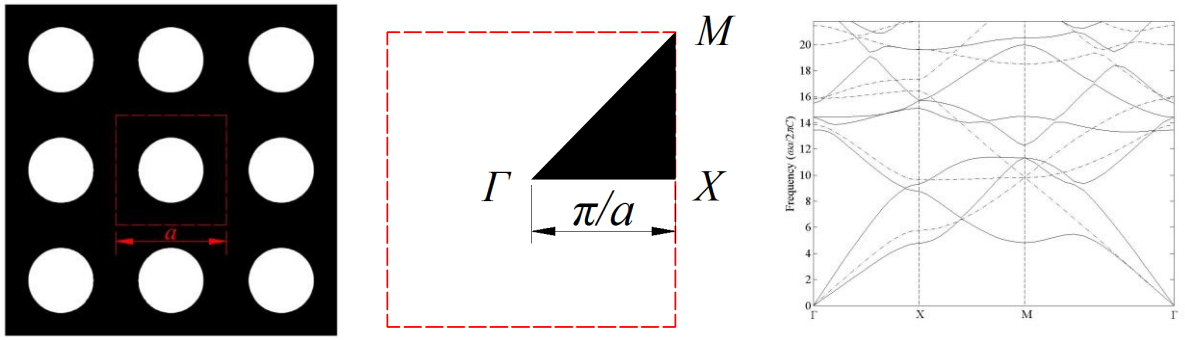
$$\mathbf{u}(\mathbf{r},\mathbf{k}) = \mathbf{u}_k(\mathbf{r})e^{i(\mathbf{k}\cdot\mathbf{r})} \tag{4}$$

where $\mathbf{u}_k(\mathbf{r})$ is a periodic function of $\mathbf{r}$ with the same periodicity as the structure. $\mathbf{k} = (k_x, k_y)$ is the Bloch wave vector. With the Bloch boundary conditions, the governing equations can be converted to two eigenvalue problems for in-plane and out-of-plane waves, respectively, which both can be written as the form:

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

where eigenvectors $\mathbf{u} = \mathbf{u}_k(\mathbf{r})$. $\mathbf{K}$ and $\mathbf{M}$ are the stiffness matrix and mass matrix, respectively.

We could easily solve the problem using the finite-element method and plot the band structures ($\mathbf{k}$-ω) with eigenvalues obtained from above equations. For a 2D phononic crystal with the square lattice shown in Figure 1a, the sweep scope of Bloch wave vector $\mathbf{k}$ can be reduced to the edges of the irreducible first Brillouin zone, which is the triangle *Γ-X-M-Γ* shown in Figure 1b. A schematic band diagram is given in Fig.1c. The dashed lines represent eigenfrequencies for out-of-plane waves while the solid lines denote eigenfrequencies for in-plane waves. Apparently there is no any complete band gap between the out-of-plane waves and in-plane waves in the band diagram.



(a) **(b)** **(c)**

Figure 1. (a) Phononic crystals with 3 × 3 unit cells; and (b) irreducible first Brillouin zone (*Γ-X-M-Γ*); (c) A schematic band diagram without any band gap.

The focus of this paper is to open a complete band gap that exists in both out-of-plane and in-plane mode and gradually enlarge the gap size to obtain an optimal design. For a complete band gap among the n^{th} and $(n+1)^{th}$ dispersion branch of out-of-plane mode and the m^{th} and $(m+1)^{th}$ dispersion branch of in-plane mode, the relative band gap size is computed as the ratio of absolute band gap width and mid-gap value,

$$d_r = 2\frac{\min\left(\omega_{n+1}^{out}(\mathbf{k}),\ \omega_{m+1}^{in}(\mathbf{k})\right) - \max\left(\omega_{n}^{out}(\mathbf{k}),\ \omega_{m}^{in}(\mathbf{k})\right)}{\min\left(\omega_{n+1}^{out}(\mathbf{k}),\ \omega_{m+1}^{in}(\mathbf{k})\right) + \max\left(\omega_{n}^{out}(\mathbf{k}),\ \omega_{m}^{in}(\mathbf{k})\right)} \tag{6}$$

where ω_n^{out}, ω_{n+1}^{out}, ω_m^{in}, ω_{m+1}^{in} are eigenfrequecies at the bottom and top edges of the target band gap for out-of-plane and in-plane modes, respectively. As a result, the band gap size is a relative value with no length scale.

Objective Function

When the porous PnCs might sustain amount of static loads, ideally we want to design these structures as stiffer as possible and the best way is to maximize bulk or shear modulus and the band gaps simultaneously. However, the optimal directions for two goals are opposite to each other. As mentioned in the introduction, the stiffer and heavier material tends to be isolated by the soft and light counterpart to exhibit an optimal band gap size. In the porous case, the solid material will be isolated by air. Such structures clearly could not sustain any

loads as the solid parts are not connected. Instead of maximizing stiffness and band gaps simultaneously, we add an extra bulk or shear modulus constraint to the optimization of the phononic band gap.

The static effective elasticity tensor of a porous material with periodic microstructures can be found by the homogenization theory [19][20] in terms of the material distribution in the unit cell as,

$$E_{ij}^{H}=\frac{1}{|Y|}\int_{\Omega}\left(\left\{\varepsilon_0^i\right\}-\left\{\varepsilon^i\right\}\right)^{T}\left[E\right]\left(\left\{\varepsilon_0^j\right\}-\left\{\varepsilon^j\right\}\right)d\Omega \tag{7}$$

where E_{ij}^{H} is homogenized elasticity tensor, $\left[E\right]$ is the constitutive matrix at a given point, $|Y|$ denotes the area of the unit cell Ω , $i, j=1,2,3$ for two dimensional inhomogeneous structures, $\left\{\varepsilon_0^i\right\}$ are three linear independent test strain fields as $\left\{\varepsilon_0^1\right\}=\{1,0,0\}$, $\left\{\varepsilon_0^2\right\}=\{0,1,0\}$, $\left\{\varepsilon_0^3\right\}=\{0,0,1\}$, $\left\{\varepsilon^i\right\}$ are the introduced strain fields, which are the solutions to the standard finite element equation with periodic boundary condition and subjected to the test strain fields $\left\{\varepsilon_0^i\right\}$. Thus effective bulk or shear modulus of a porous material can be expressed as,

$$\kappa^{H}=\frac{1}{4}\left(E_{11}^{H}+E_{12}^{H}+E_{21}^{H}+E_{22}^{H}\right) \tag{8}$$

$$G^{H}=E_{33}^{H} \tag{9}$$

For simplicity, dimensionless stiffness constraints are used instead of effective bulk or shear modulus in the following numerical examples. Specifically, $\kappa = \kappa^{H}/\kappa_0$ and $G = G^{H}/G_0$ are used as effective bulk and shear modulus constraints, where κ_0 and G_0 are the bulk and shear moduli, respectively, of the solid material.

On account of potential weight limitation, a volume share of the solid in the whole design domain should be restricted. Therefore, the optimization problem under consideration can be mathematically formulated with objective and constraint functions as follows:

$$\text{Maxmize: } f\left(x_e\right)=d_r \tag{10}$$

$$\text{Subject to: } V_f^{*}=\sum_{e=1}^{N}x_e V_e \quad x_e=x_{\min} \text{ or } 1 \tag{11}$$

$$\kappa\geq\kappa^{*} \quad or \quad G\geq G^{*} \tag{12}$$

where the objective function $f(x_e)$ denotes the relative band gap size which is defined by the percentage in the following band diagrams; V_f^{*} is the volume constraint; x_e is the artificial design variable, which denotes the material type (air or solid material) for each element. κ^{*} and G^{*} are effective bulk and shear modulus constraints. It should be noted that the bulk or shear modulus constraint should be not greater than the upper limit of the porous structure with the same volume fraction, otherwise the optimization will tend to purely maximize the bulk or shear modulus. The corresponding dimensionless upper limits of bulk or shear modulus are given by Hashin–Shtrikman bounds for two-phase materials [21]. In the following optimizations, the stiffness constraints are set to $\kappa^{*} = \beta^{*}\kappa_{upper}$ or $G^{*} = \beta^{*}G_{upper}$, where β is the ratio of stiffness constraint over its upper bound value at a same volume fraction and is located in the range between 0 and 1.

Bidirectional Evolutionary Structural Optimization (BESO)

Bi-directional evolutionary structural optimization (BESO) method is a gradient-based topology optimization algorithm in optimum material distribution problems for continuum structures , which is a further developed version of evolutionary structural optimization (ESO) [22][23]. The basic concept of BESO is to gradually remove low efficient materials from the structure and meanwhile add materials to the most efficient regions so that the rest part evolves to an optimum [24]-[26]. BESO method has demonstrated its capability in the design of periodic microstructures [27], and already been successfully applied in the design of photonic and phononic band gap crystals [28][29].

To resolve the multi-objective topology optimization problem defined in Eq. (10)-(12), we apply a similar material interpolation scheme with penalization to avoid artificial localized modes as in the studies on the topology optimization of continuum structures for natural frequencies [30]. The interpolation scheme is given as:

$$\rho(x_e) = x_e \rho_0 \tag{13}$$

$$E(x_e) = \left[\frac{x_{\min} - x_{\min}^p}{1 - x_{\min}^p} \left(1 - x_e^p\right) + x_e^p \right] E_0 \qquad (0 < x_{\min} \le x_e \le 1) \tag{14}$$

where ρ_0 and E_0 represent the density and Young's modulus of solid material, respectively; p is the penalty exponent; x_e stands for a design variable, $x_e = x_{min}$ denotes element e is composed of air, and $x_e = 1$ means element e is composed of solid material. To avoid singularity in finite element analysis, x_{min} in the calculation is usually set to be a very small value that is slightly larger than 0. In the following example, the value is chosen as $x_{min} = 1 \times 10^{-6}$.

BESO starts from an initial design and then calculates the elemental sensitivities, i.e. gradients of objective function with respect to the change of design variable x_e. Based on the relative rankings of the elemental sensitivity, it will gradually modify the distribution of solid material in the following iteration steps by changing the value of the design variable of every element until the convergence criterions are satisfied. Details of sensitivity analysis and evolutionary procedure can be found in the literature [28][31][32].

Results and Discussions

We consider silicon as the solid material as an illustration example. The physical properties of silicon are given as $\rho = 2330$ kg/m3, $\lambda = 85.502$ GPa and $\mu = 72.835$ GPa [18]. The following optimizations are conducted with a volume constraint $V_f^* = 50\%$ and constraint ratio β=0.3. A filter scheme has been applied [30]. The unit cell with dimensionless lattice length a=1 is discretised into 64×64 linear four node. The eigenfrequencies (ω) in the band structures are normalized by $\omega a/2\pi C$, where C =340 m/s denotes wave speed in air. By using the aforementioned optimization algorithm, the following topologies with complete band gap have been obtained with silicon/air system.

As shown in Fig.2 and Fig.3, two optimized structures have been found with bulk modulus constraint and shear modulus constraint, respectively. For both cases, the first complete band gap is between the first and second dispersion branch of out-of-plane mode as well as between the third and fourth dispersion branch of in-plane mode, while the second complete band gap is located in the second and third dispersion branch of out-of-plane mode and the sixth and seventh dispersion branch of in-plane mode. All the optimization results again reveal that the solid material is approaching the limiting case of separate columns in air but still keeping connected by slim constructions to support the propagation of shear waves and the prescribed bulk or shear modulus as well.

When maximizing the complete band gap with bulk modulus constraint, the main parts in the resulting topologies are analogous to square inclusions. In comparison, it is interesting to observe that the main parts of the final designs with shear modulus constraint are more like round columns. The other difference between two cases is the position of thin connections. All the complete band gap sizes we obtained in these porous phononic structures have broken

the record value in the literature [17][18]. All designs are amenable to manufacture with appropriate size scaling to the frequency range of interest.

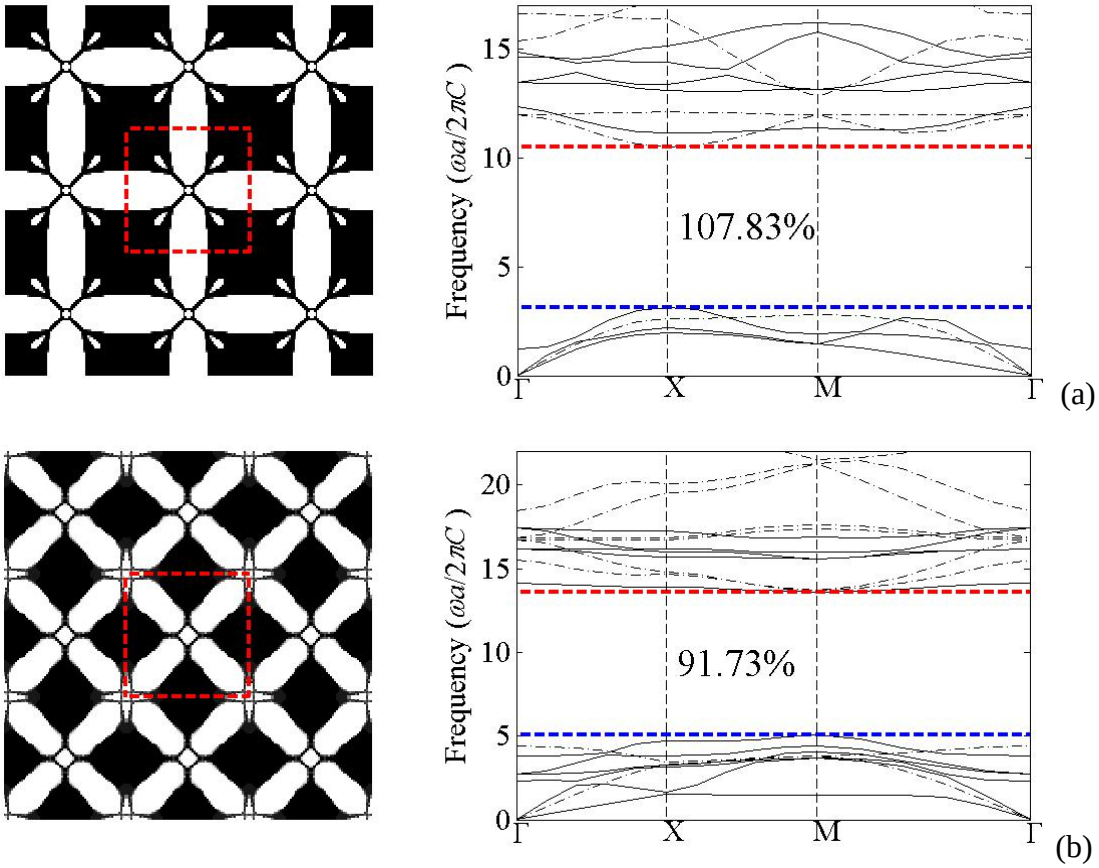
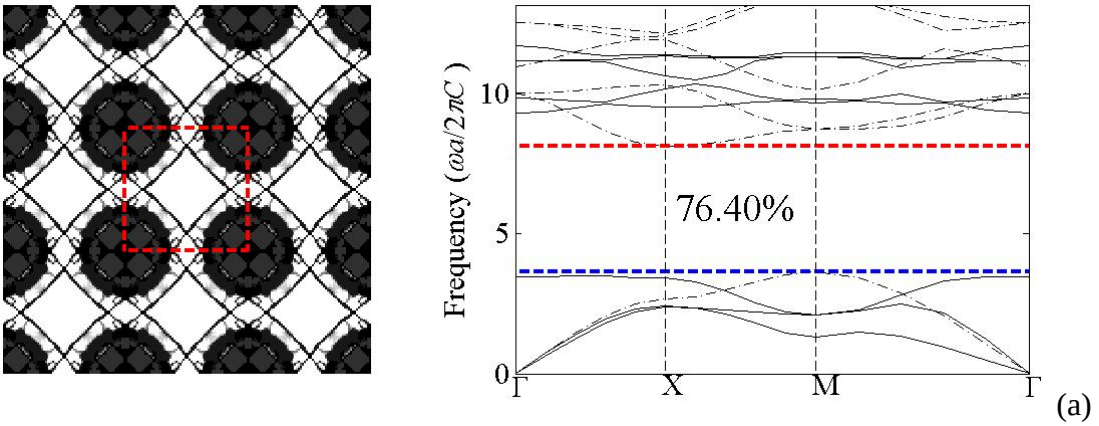


Figure 2. Optimized topologies and corresponding band structures for complete band gap with bulk modulus constraint, (a) between ω_1^{out}, ω_2^{out} and ω_3^{in}, ω_4^{in}; (b)between ω_2^{out}, ω_3^{out} and ω_6^{in}, ω_7^{in}



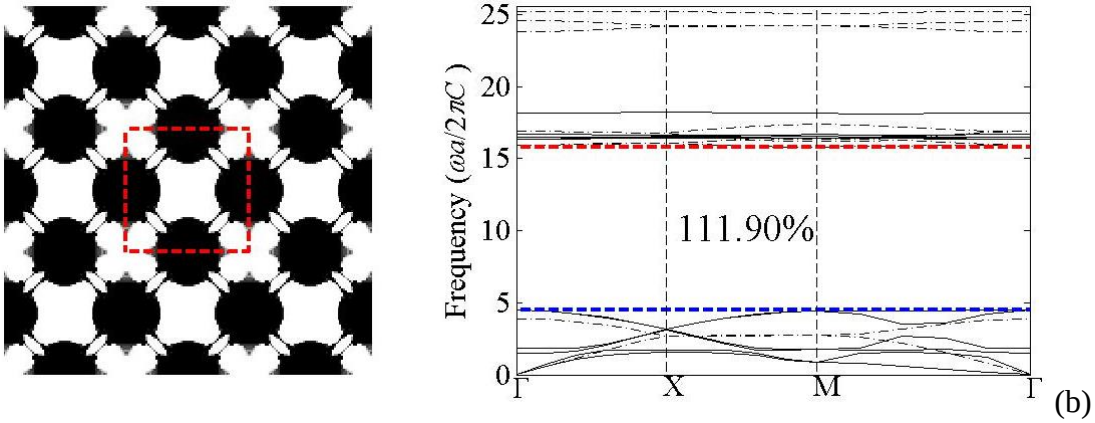


Figure 3. Optimized topologies and corresponding band structures for complete band gap with shear modulus constraint, (a) between ω_1^{out}, ω_2^{out} and ω_3^{in}, ω_4^{in}; (b)between ω_2^{out}, ω_3^{out} and ω_6^{in}, ω_7^{in}

Conclusions

This paper has discussed the topology optimization of porous phononic crystals for maximizing complete band gap between out-of-plane and in-plane mode with a bulk or shear modulus and volume constraint simultaneously. Homogenization theory and BESO algorithm have been adopted to resolve the problem. Several optimization results with bulk and shear modulus constraint were presented. Numerical results showed that there are many slim connections in the optimized topologies of porous phononic crystals. All the presented designs have exceptionally large complete band gaps.

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