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REVIEW PAPER

A comprehensive survey on topology optimization of phononic crystals

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Abstract The objective of this paper is to present a peer-review of the literature and trends surrounding the design of phononic crystals (PnCs) using topology optimization methods. After first providing a brief review of new developments, improvements, and applications of PnCs, this paper investigates the techniques and applications of topology optimization methods for phononic band gaps and functional structures. Both gradient-based and non-gradient-based topology optimization methods have been employed in the design of PnCs. The advantages and drawbacks of the methods used in this area are discussed in detail in this paper. Based on observations of the current state, we highlight suggestions and ideas for future research in the field of phononic crystal design optimization. The paper examines how applying topology optimization techniques into the design of PnCs yields promising performance and functions. This literature survey is designed to provide an overview of the recent advances and novel applications of popular topology optimization methods for the design of PnCs.

Keywords Phononic crystals · Topology optimization · Acoustic and elastic waves · Band gap design · Functional phononic crystal structures

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1 Introduction

Phononic crystals (PnCs) are a class of artificial periodic composite materials which exhibit phononic band gaps (i.e., frequency regimes where the acoustic and elastic waves cannot propagate). The band structure of mechanical waves (i.e., elastic and acoustic waves) was firstly studied in 1992 (Sigalas and Economou 1992), and the idea of "phononic crystals" was firstly introduced in 1993 (Kushwaha et al. 1993) by drawing an analogy to photonic crystals (PtCs). PnCs have for the acoustic and elastic waves all the manipulation capabilities that PtCs have for light. Over the last two decades, PnCs have gained much attention, and the theoretical concept of phononic crystals has been developed extensively. PnCs are of interest because mechanical waves behave differently in them than in homogeneous materials. Significant research has been undertaken to explore the physical properties and potential applications of PnCs; e.g., the constituent materials and the size and spacing of those materials have been studied to determine the maximum band gap width, and to understand the behaviors of the mechanical waves propagating in PnCs to design them for wave guiding. As the topic has become more widely studied, efforts to develop PnCs have focused on practical applications and novel designs.

Research on PnCs requires a combination of multi-physics and engineering; especially, material physics, wave propagation in inhomogeneous and periodic media, acoustics, ultrasonics, mechanical engineering and electrical engineering, and related fields. PnCs can be one, two, or three dimensional periodic structures made of two elastic materials (as shown in Fig. 1). The periodic structures cover a wide range of scales from meter-size (e.g., sound in air) to nanometer size (e.g., radio frequency communication), depending on the propagation characteristics of the waves and application domains of the PnCs. Like PtCs used for the propagation of electromagnetic waves, the properties of PnCs are associated with the scattering of acoustic waves and elastic waves. The former are vector waves, and the latter are tensor waves. As the propagation mechanisms depend on the types of material within which the waves propagate, the mechanical waves propagate as elastic waves in solid material and as acoustic waves in fluid material. Thus, the nonhomogeneous materials used in PnCs are usually made of a combination of solid-solid, fluid-fluid, or solid-fluid materials. Of these three types of nonhomogeneous materials, fluid-fluid PnCs are extremely difficult to form with two liquids of different densities; thus, solid-fluid and solid-solid PnCs are more accessible and more easily to be fabricated. Almost all of the current research is based on solid-fluid or solid-solid PnCs. Thus, from the wave-type point of view, PnCs can be classified into two categories: acoustic PnCs with a fluid matrix, and elastic PnCs with an elastic solid matrix.

The property of periodicity in PnCs leads to constructive or destructive interferences depending on the frequency of the waves. In general, the periodicity of the lattice of a phononic crystal generates Bragg reflections of the acoustic or elastic waves. When the waves are scattered inside PnCs, waves are strongly dispersed from one material to the other, and secondary waves are produced at each interface between them. The secondary waves are reflected backwards and interfere with each other constructively or destructively. This yields ranges of frequencies at which the original waves are either allowed to propagate (pass bands) or in which original waves are blocked in one direction (stop bands) or blocked in any direction (complete band gaps). Thus, the band gaps of PnCs are strongly related to the geometry and the frequency of the waves. As a result, band gap design is of significant interest in the field of PnCs. As a consequence of band gaps, the topological shape of the periodic lattices of a phononic crystal provides a very valuable means to control and manipulate acoustic and elastic waves. Even though the band gap structures of PnCs can also be engineered and tailored by varying the filling ratio and using new materials with different elastic constants, significant attempts have been made to use topology optimization techniques as an alternative process to achieve the best topological shapes of the periodic lattice that yield the largest band gap width in PnCs.

Prior work has found novel effects in PnCs (e.g., band gaps, negative refraction, and defects within band gaps), that

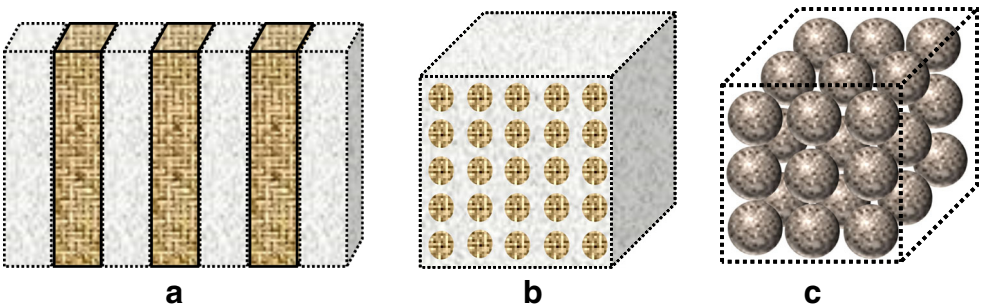


Fig. 1 Phononic crystals with periodicities in (**a**) one, (**b**) two, and (**c**) three dimensions

have been used to create desired functionalities, such as wave guides and filters (Sun and Wu 2006, 2007), imaging (Li et al. 2006), focusing (Chiou et al. 2014), sound collimation (Kaya et al. 2012), energy harvesting (Yang et al. 2015; Yeh 2013), and other features. Most importantly, these novel effects can be tuned to yield excellent performance and functionality of both the infinite and finite phononic crystal structures (i.e., structures extending infinitely and finitely in space). The phenomenon of tunable novel effects of PnCs lays a significant foundation for designing phononic crystal materials and structures for effects of interest and potential applications. Thus, the focus of research on PnCs has extended from the band gap design to the phononic crystal-based structural design. Specifically, the former refers to the design optimization of a unit cell of an infinite phononic crystal structure to seek the largest band gaps in the dispersion relation, which is also stated as the phononic crystal material design sometimes. The latter refers to design optimization of a finite phononic crystal-based device wholly or partly to pursue the best functionalities of interest of the device. In order to obtain the largest band gaps as well as the desired functionalities of the phononic crystal-based structures, topology optimization techniques have been utilized to search for the best phononic crystal-based structures.

Topology optimization is a numerical method for addressing optimized material distributions within a given design domain, such that a desired response of the system is optimized. Because this method is effective to simultaneously deal with geometrical and mechanical/physical performance changes, it is widely used in many structural design problems. Topology optimization was originally presented for structural optimization of mechanical design problems (Bendsøe and Kikuchi 1988; Zhou and Rozvany 1991), and it has been recently extended for use with many design problems that involve multi-physics, such as PtCs (Cox and Dobson 1999; Jensen and Sigmund 2004a; Jensen and Sigmund 2005; Men et al. 2014; Meng et al. 2015), PnCs (Sigmund and Jensen 2003), and other metamaterials (Diaz and Sigmund 2010; Zhou et al. 2011; Otomori et al. 2012). In the field of structural optimization, topology optimization has recently drawn more attention than the other optimization types (e.g., shape optimization) because of its significant benefits (i.e., providing best conceptual design proposals) in achieving required structural performances with minimum cost (i.e., mass or money), or obtaining the stiffest topological shape with a given amount of material. Beginning with the homogenization method (Bendsøe and Kikuchi 1988), various numerical approaches have been developed to perform topology optimization (Sigmund and Maute 2013), including the solid isotropic material with penalization (SIMP) method (Bendsøe 1989; Zhou and Rozvany 1991; Bendsøe and Sigmund 1999), the evolutionary structural optimization method (Xie and Steven 1993), the level set method (Allaire et al. 2004), the Heaviside projection method (Guest et al. 2004; Guest 2008; Ha and Guest 2014), and the phase-field method (Takezawa et al. 2010; Gain and Paulino 2012; Takezawa and Kitamura 2014), among others. Most of these approaches require sensitivity calculation and further cooperation with an optimization algorithm for solutions, such as the sequential quadratic programming (Gill et al. 2002; Yi and Sui 2016a, 2016b), the sequential linear programming (Yang and Chuang 1994; Maute and Frangopol 2003), optimality criteria (OC) (Sigmund 2001a), and the method of moving asymptotes (MMA) (Svanberg 1987). Thus, they are called gradient-based topology optimization (GTO) methods. For those problems where the gradient information is difficult to obtain, especially for those problems involving multi-physics, a heuristic approach, such as genetic algorithm (GA) (Man et al. 1996), is used for topology optimization (Tai and Akhtar 2005; Wang and Tai 2005). Thus, these methods are called non-gradient-based topology optimization (NGTO) methods.

GTO and NGTO methods have both advantages and disadvantages. The GTO methods are efficient for solving problems with a large number of design variables using a limited number of function evaluations; however, they often converge to local optima by iteratively moving a solution in a direction that is derived from gradient information. They are preferred if the gradient information is not too difficult to obtain. The NGTO methods provide alternative means to solve the optimization problems without requiring gradient information, which can be unavailable or unreliable to compute for some engineering problems. Most of the NGTO methods, e.g., GA method, harmony search method, and simulated annealing method, do a good job of spanning the vast majority of the design space because they have a good probability of attaining a global optimum solution. But the computational efficiency of the NGTO method, which strongly depends on the number of design variables, is dragged down significantly due to numerous function evaluations within the design space. On the other hand, several NGTO methods such as GA method and Harmony search method, can handle discrete variables as well as continuous variables. They are easy to implement, but requires tedious work of tuning the algorithm parameters to find generally good global solutions.

Both the above methods have been applied to the topology optimization of periodic structures subject to wave propagation, such as PnCs. Sigmund (2001b) and Sigmund and Jensen (2002, 2003) were the first to attempt to use topology optimization to design phononic band-gaps within finite and infinite structures, and to optimize the response of a finite phononic crystal structure subjected to periodic loading. In their work, a linear interpolation scheme was developed to interpolate the elemental elastic parameters (i.e., mass density and elastic constants) between two different materials, and then the MMA method was used in conjunction with the finite element method to solve the optimization

problems. Later, Gazonas et al. (2006) used the genetic algorithm with finite element method to maximize the band gaps of PnCs with acoustic wave propagation. Following their work, more and more research has examined topology optimization of PnCs. This follow-on work can be classified into two large categories: *phononic band gap design* and *phononic crystal structure design*. Phononic band gap design seeks to find the best topological shape of a phononic lattice or unit cell that exhibits the maximum complete band gap. The optimized lattice or unit cell is based on the assumption that the phononic crystal is infinite and that the wave disperses and scatterers along each edge of the first Brillouin zone (i.e., a uniquely defined primitive cell in reciprocal space). Phononic crystal structure design seeks to optimize the functionalities of PnCs, such as mirrors, cavities, and waveguides, where the PnCs are normally considered as finite structures. Since wave propagation within a phononic crystal structure is quite complicated and basically unknown, phononic crystal structure design is difficult; therefore, more contributions are needed in this field. Thus, the research focused on optimizing the functionalities of finite phononic crystal structures is not as extensive as that focused on optimizing the band gaps. Even though there are many difficulties and challenges that exist in topology optimization of PnCs (e.g., multiple-physics optimization problems, high computational effort, and complex mathematic optimization models), topology optimization remains a powerful means to explore new functionalities and applications of PnCs.

Based on the existing literature, several survey papers have been published for PnCs. Lu et al. (2009) did a review focused on acoustic phononic crystals and acoustic metamaterials; the main properties of acoustic phononic crystals were discussed and summarized. Cadman et al. (2013) provided a critical review of the design of periodic microstructures of multifunctional materials for a range of physical properties, such as elastic stiffness, Poisson's ratio, thermal expansion coefficient, conductivity, fluidic permeability, particle diffusivity, electrical permittivity and magnetic permeability, etc. Topology optimization of phononic band gap materials was simply mentioned in this work; most of the review was devoted to PtCs and metamaterials.

Research on phononic crystal devices and applications was first investigated in a specific micro scale (Olsson and El-Kady 2009). The authors looked into the design techniques, material considerations, microfabrication process, characterization methods, and reported device structures with respect to the micro-PnCs. Pennec et al. (2010) gave a very specific report on examples and applications of two-dimensional PnCs. They studied the properties that contributed to the existence of band gaps, and examined defected PnCs for their special effects and possible applications. Special attention was devoted to the phononic crystal plates, with respect to their potentialities and functionalities. Gazalet et al. (2013) presented a tutorial survey on waves propagating in periodic media, including electronic, photonic, and phononic. They outlined both the real and Fourier domain methods, and provided the basic concepts about eigenfrequencies, reciprocal lattice, Brillouin zones, etc. This work is a very comprehensive study that outlines the physics aspects and the use of Bloch theorem for mathematical deduction of the band structures. Hussein et al. (2014) went through the historical developments of periodic materials and structures, and gave a detailed overview of the developments and trends of PnCs and acoustic/elastic metamaterials while specially considering dynamics, vibrations, and acoustics. They also presented a detailed discussion of the basic concepts and computational analysis techniques for phononic materials and structures, treatment of damping and nonlinearity, and the related experimental research in the field. To the best of the authors' knowledge, there is no comprehensive study on topology optimization of PnCs to date. Hence, it is worthwhile herein to (1) investigate the current trends of topology optimization for phononic band gaps, and (2) study the latest status of topology optimization for phononic crystal structures as it relates to their functionalities and applications.

To start, wave propagation within PnCs and phononic band gaps are introduced in Section 2. Investigation into topology optimization of phononic band gaps is described from an optimization point of view in Section 3, i.e., unconstrained/constrained maximizing band gap problems and GTO/NGTO solution methods. Current topics in topology optimization design for functional phononic crystal structures are studied in Section 4. Section 5 provides a discussion of current and future trends in topology optimization of PnCs. Finally, the conclusions of this review article are given in Section 6.

2 Phononic crystals

2.1 Mechanisms of phononic band gaps

After Kushwaha et al. (1993) initially presented PnCs, research on PnCs initially focused on computing the band gap structures and investigating the mechanisms of the band gap formation. Then, it moved to developing and improving the performance and functionality of PnCs in wave controlling and manipulation. The current trend in research on PnCs is design optimization of PnCs to achieve the best performance for practical applications. In these research studies, it is noted that a fundamental behavior exhibited by PnCs, which has been examined the most by researchers, refers to the phononic band gaps.

Band gaps are the most important characteristic that periodic phononic crystal structures exhibit. They are considered

to be the most fundamental property of PnCs that enables other potential properties, such as the locally resonant mechanism (Liu et al. 2000), simultaneously negative bulk modulus and mass density (Ding et al. 2007), and peculiar transmission peaks (Zhao et al. 2007). Once the PnCs band gaps are known, the propagation of acoustic/elastic waves can be controlled and manipulated for practical uses. The mechanisms surrounding the formation of band gaps in PnCs were investigated by Croënne et al. (2011). According to their research, three different mechanisms for phononic band gaps were identified, namely Bragg, hybridization, and weak elastic coupling effects. Bragg gaps are common features caused by the destructive interference of waves scattered from the inclusions. Hybridization gaps arise from the coupling between scattering resonances of the individual inclusions and the propagating mode of the embedding material. Finally, band gaps that form between the pass bands are created by the weak elastic coupling effects between resonances. Among these three mechanisms, Bragg interference is the most evident reason that can lead to band gaps. It is also the most common and historically it is the first invoked physical mechanism. The phononic band gaps generated by Bragg scattering, based on diffraction and the wavelength of the acoustic/elastic waves that are not allowed to propagate within the PnCs, are on the order of the spatial periodicity of the structure (Kushwaha et al. 1993; Sigalas and Economou 1993). For example, PnCs with periodicities on the order of meters to centimeters will forbid the propagation of mechanical waves in frequencies in range $20 \sim 20 \times 10^3$ Hz, whereas those with periodicities on the order of microns will forbid the propagation of hypersonic mechanical waves with frequencies in the range $10^9 \sim 10^{12}$ Hz (Maldovan and Thomas 2009).

The study of wave propagation in periodic media was first formulated by Floquet (1883) in one dimension. Bloch generalized the work of Floquet to three dimensions in what is now known as *Floquet-Bloch theory*, or the *Bloch theorem* for short. The mechanical waves' propagation in PnCs follows the Floquet-Bloch theory as well. A mechanical Bloch wave that propagates with wave vector $\mathbf{k}$ is represented by the formula

$$\mathbf{u}_\mathbf{k}(\mathbf{r},t) = \mathrm{Re}\left[\mathbf{u}_\mathbf{k}(\mathbf{r})e^{-i\omega(\mathbf{k})t}\right] \quad \text{where} \quad \mathbf{u}_\mathbf{k}(\mathbf{r}) = f_\mathbf{k}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \tag{1}$$

where $\mathbf{r}$ and t, respectively, denote the position vector $\mathbf{r} = (x, y, z)$ and time. $\mathbf{k}$ and ω are, respectively, the wave vector and frequency. The dispersion relation is drawn by $\omega = \omega(\mathbf{k}) = \omega(k_x, k_y, k_z)$. Re is an abbreviation for "the real part of". The function $f_\mathbf{k}(\mathbf{r})$ is a periodic vector function with the same spatial period as the PnCs. $\mathbf{u}_\mathbf{k}(\mathbf{r})$ is the spatial part of the displacement vector of the mechanical Bloch wave propagating with wave vector $\mathbf{k}$ within the crystal. $\mathbf{u}_\mathbf{k}(\mathbf{r},t)$ is the instantaneous displacement vector of the mechanical Bloch wave within the crystal. Then the dispersion relation $\omega = \omega(\mathbf{k})$ for the mechanical Bloch wave propagating in PnCs can be obtained by solving the wave equation for nonhomogeneous solid materials

$$\nabla\cdot\left(\rho c_\mathrm{T}^2\nabla u_i + \rho c_\mathrm{T}^2\frac{\partial \mathbf{u}}{\partial x_i}\right) + \frac{\partial}{\partial x_i}\left(\left(\rho c_\mathrm{L}^2 - 2\rho c_\mathrm{T}^2\right)\nabla\cdot\mathbf{u}\right) = -\rho(\omega(\mathbf{k}))^2 u_i \tag{2}$$

where i represents the i-th Cartesian component in space. $\mathbf{u}$ is the spatial displacement vector $\mathbf{u} = \mathbf{u}_\mathbf{k}(\mathbf{r})$. $\rho = \rho(\mathbf{r})$, $c_\mathrm{T} = c_\mathrm{T}(\mathbf{r})$, and $c_\mathrm{L} = c_\mathrm{L}(\mathbf{r})$ are, respectively, the density and the transverse and longitudinal velocities, which describe the mechanical properties of a phononic crystal.

For acoustic waves, the longitudinal pressure waves propagate as Bloch waves within the PnCs made of fluid/solid inclusions in the fluid background. Both the periodic function and instantaneous displacement are scalar functions. Thus, the governing equation in Eq. (2) can be expressed as the acoustic wave equation

$$\nabla\cdot\left(\frac{1}{\rho}\nabla p\right) = -\frac{1}{\rho c_\mathrm{L}^2}(\omega(\mathbf{k}))^2 p \tag{3}$$

where $p = p_\mathbf{k}(\mathbf{r})$ is the spatial part of the pressure of an acoustic Bloch wave propagating with wave vector $\mathbf{k}$ within the PnCs.

For elastic waves, both the transverse and longitudinal waves can propagate as Bloch waves within the PnCs made of fluid/solid inclusions in solid background. According to the governing equation shown in Eq. (2), for one-dimensional (1D) PnCs (or layered PnCs), as the displacement vector components u_x, u_y, and u_z are independent, elastic waves can propagate independently as longitudinal Bloch waves or as transverse Bloch waves. For two-dimensional (2D) PnCs, as two coupled displacement components determine the displacement vector in the plane of periodicity and the other component oscillates along the direction perpendicular to the plane of periodicity, elastic waves thus propagate as in-plane elastic Bloch waves (coupled elastic waves) and out-of-plane elastic Bloch waves (transverse waves). For three-dimensional (3D) PnCs, elastic waves are neither transverse nor longitudinal because the displacement vector components u_x, u_y, and u_z are generally coupled to each other.

The Bloch waves are obtained by solving the above governing equations. Next the band gap structures in the Brillouin zone can be plotted in diagrams. The periodicity of the PnCs defines the Brillouin zone, and the Brillouin zone determines the set of wave vectors, $\mathbf{k}$, required to plot the dispersion relation $\omega = \omega(\mathbf{k})$. The band gaps appear at symmetry points in reciprocal space and along the irreducible Brillouin zone. Figure 2 shows the irreducible Brillouin zones

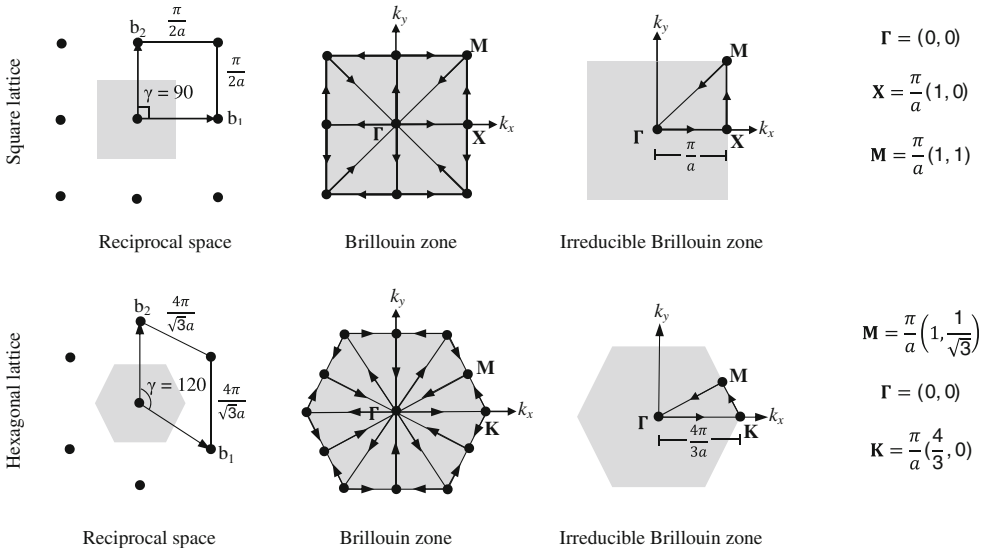


Fig. 2 The irreducible Brillouin zones for (**a**) square and (**b**) hexagonal unit cells in reciprocal space

for square and hexagonal lattices with symmetry imposed at the unit-cell level. The subsequent wave propagation analysis and design representation are needed in only a small portion of the unit cell. The band structure calculation is limited to the corresponding irreducible Brillouin zone. For example, in the case of square and hexagonal lattices, the dispersion relation $\omega = \omega(\mathrm{k})$ will be plotted for wave vectors k along the paths determined by the Γ→X→M→Γ and Γ→K→M→Γ points, respectively.

The above governing equations contain two parameters (k, ω), which can be solved with two techniques: the $\omega(\mathrm{k})$ technique, where the unknown frequencies for a real wave number are calculated from an eigenvalue problem, yields a real band structure; the $\mathrm{k}(\omega)$ technique, where the unknown wave vector for real frequencies is computed from the eigenvalue problem, enables a solution for both complex wave numbers and complex band structures. The former technique is an intuitive and straightforward way to get the dispersion relation; thus, most of the band structures are based on the real bands. The latter one requires the symmetry of the coefficient matrices to be broken, and this requirement has been found to be realized through the extended plane wave method (Laude et al. 2009) and the semi-analytical finite element method (Veres and Berer 2012) by introducing an inverse formalism scheme. For a brief description of the solutions of the real and complex band structures obtained by using the $\omega(\mathrm{k})$ and $\mathrm{k}(\omega)$ techniques, respectively, refer to Ref. Veres and Berer (2012).

Numerous studies on PnCs have shown that the material properties, types of lattice, and scatterer shapes have great influence on the phononic band gaps (Sigalas and Economou 1993; Kushwaha et al. 1994; Min et al. 2006; Su et al. 2012). Generally, a high contrast in material densities, elastic constants, and wave speeds in two constituent materials readily yields a full band gap, such as inclusion of a low mass density in a matrix with a high mass density. In 3D PnCs, the face-centered-cubic structures more easily form a full band gap than the body-centered-cubic structures. These studies confirm that the phononic band gap width depends strongly on the lattice symmetry and on the scatterer shape.

2.2 Large band gaps

Different types of PnCs have been considered in the literature. Every phononic crystal exhibits its own characteristic band structure and has unique band gap properties. It is essential for the phononic band gaps to be as large as possible because extensive practical applications benefit from the feature of phononic band gaps, such as selective frequency waveguides, sound shields and filters, and wave focusing. It is observed that the appearance of band gaps in binary systems (i.e., structures composed of two materials), as well as the size and location of band gaps, depends on the filling fraction, the lattice symmetry, the topology of the constituent material phases, and the contrast between elastic properties of materials (Kushwaha et al. 1993; Lin and Huang 2011). More specifically, the density contrast of the constituent materials plays a crucial role in the appearance of a band gap. For solids, gaps are favored by high-density scatterers in a low-density host (Vasseur et al. 1998). In contrast, for fluids, low-density scatterers in a high-density host provide the most favorable combination for gaps to appear. Also the combination of solid and fluid materials shows promising band gaps (Su et al. 2012). Thus, the ideal (for a wide gap) realistic material combinations are likely to be composites consisting of heavy metal scatterers (e.g., Fe, steel, Pb) in a polymer host (e.g., epoxy) (Kafesaki et al. 1995). On the other hand, the cermet topology (isolated scatterers) is more preferable for a band gap than the network topology (Economou and Sigalas 1993). A volume fraction value between 10 and 50 % is more likely to lead to band gaps. It has been shown that, for a phononic crystal slab

consisting of piezoelectric inclusions placed periodically in an isotropic host material, the ratio of the slab thickness to the lattice period is a key parameter for the existence and the width of the band gaps (Khelif et al. 2006). The width of the band gaps and their frequency domains are strongly affected by the composition of the system and by the lattice parameter (Vasseur et al. 1996). Therefore, by controlling these parameters, a periodic composite for PnCs can be designed to have desired frequency band gaps (i.e., increased band gap width). A structure for PnCs that exhibits excellent performance in practical applications can be realized by design optimization as well. Both theoretical and experimental research related to the design of PnCs has been conducted. The resulting literature will be discussed in Section 3 and Section 4.

2.3 Wave propagation analysis methods

On one hand, the governing equation in Eq. (2) involves solving a complex eigenvalue problem, which makes calculation of the dispersion relation difficult. On the other hand, calculation of the band structures requires performing the eigenvalue calculation numerous times, as the value of the wave vector, **k**, is varied along the edges of the irreducible Brillouin zone. Besides, large dimensions of a unite cell and presence of defects in periodicity can inevitably increase computational effort as well. Hence, the computational calculation of the band structures has a high cost. Several wave propagation analysis methods have been developed for calculating the band structures of acoustic/elastic waves propagating within PnCs. Commonly used methods include the plane wave expansion (PWE) method, the multiple scattering theory (MST) method, the finite-difference time-domain (FDTD) method, and the finite element method (FEM). These methods have the flexibility to construct a variety of 2D and 3D periodic structures, and the phenomena of acoustic/elastic waves propagating inside the PnCs can be investigated as well. Each of them carries particular advantages and disadvantages.

2.3.1 Plane wave expansion method

Based on the periodicity of the inclusions, the PWE method utilizes Bloch's theorem to obtain Fourier coefficients for the elastic displacement field and the material properties in the reciprocal space. An eigenvalue problem is thus formed from the Fourier-transformed propagation equation and its possible solutions. This is basically a list of propagating frequencies calculated over the wave vectors passing through the Brillouin zone edges, which are then obtained as the band structure. The PWE method is highly efficient for calculating band gaps in periodic structures due to the simplicities of theoretical assumption and ease of implementation. However, being a Fourier space method, it suffers from convergence difficulties, especially when dealing with PnCs involving media with a large contrast in their elastic parameters, or with either very high or very low filling fractions (Cao et al. 2004a). Because a large number of plane waves are required to obtain reliable band structures, this is both time consuming and complex in terms of memory requirements. Some modified PWE methods have been developed to alleviate these shortcomings, such as the improved PWE method (Zhang et al. 2011) and the enhanced PWE method (Baboly et al. 2014). It should also be noted that the PWE method cannot be used for the calculation of wave transmittance and reflectance of finite PnCs because of the assumption of a periodic boundary condition in an infinite structure.

The PWE method first applied to PnCs is sourced from the work of Sigalas and Economou (1992, 1993), Kushwaha et al. (1993), and Kushwaha et al. (1994). Kushwaha et al. (1994) gave a detailed description of the PWE method for band structure calculation for periodic inhomogeneity and an analytical expression of the 2D periodicity. Later, the PWE method was utilized to study the first full elastic wave band gap in 2D PnCs and supercell calculation for defected states in the lattice (Sigalas 1997), and to demonstrate the existence of absolute acoustic band gaps in 2D PnCs consisting of Duralumin cylinders embedded in an epoxy resin matrix (Vasseur et al. 1998). Following the revealing of full band gaps in their research, the PWE method has become a popular method used to analyze the band diagram of PnCs for different purposes, for example, the variation in the phononic band gaps upon lattices with different symmetry and scatterers of various shapes, orientations, and sizes (Kuang et al. 2004), and upon the reorientation of the anisotropic cylinders (Lin and Huang 2011).

2.3.2 Finite-difference time-domain method

The FDTD method employs finite differences as approximations for both the space and the time domains. It has been effectively used to solve problems in electromagnetics (Taflove and Hagness 2005; Gedney 2011). Use of the FDTD method for band structure calculation of PnCs is based on the discretization of time-dependent acoustic/elastic wave equations with a small spatial interval and time step. Due to the discretization, the displacement field is expressed as a function of time at any point of the calculation area, which is a unit cell or supercell for the perfect or defect-containing systems, respectively. The difference equations are solved by a large number of time-domain iterations, and fast Fourier transformation is then performed to obtain the eigenfrequencies. Implementation of the FDTD method for PnCs is outlined in the papers by Tanaka et al. (2000) and Zhao et al. (2012). In addition to finding the band structures of wave propagation in PnCs (Tanaka et al. 2000; Cao et al. 2004b; Su et al. 2012), the FDTD method can solve other complicated problems, such as wave trapping and guiding in

PnCs with defects (Khelif et al. 2003; Sun and Wu 2006, 2007), and wave transmission and reflection in finite size PnCs (Lucklum et al. 2012). Unfortunately, it is computationally expensive due to the large amount of memory and computation time required for the discretization of time and spatial domains. In order to overcome this difficulty of the FDTD method, Su et al. (2010) reported a post-processing method based on high-resolution spectral estimation via the Yule-Walker method for improving the efficiency of FDTD calculation of phononic band structures.

2.3.3 Multiple scattering theory method

The essence of the MST method lies in multiple expansions of the elastic field in each region containing an isotropic and homogeneous material. In the MST method, appropriate boundary conditions are applied on interfaces/surfaces between particles (e.g., embedded spheres and its host) to deal with discontinuities. This treatment of discontinuities leads to scattered fields of individual particles and the ensemble of particles yields an aggregate of multiple scatterers. The MST method has excellent convergence speed in the band structure calculation for PnCs composed of cylindrical or spherical scatterers for both periodic and random systems. In addition, it is capable of handling PnCs with components of large mechanical mismatch, such as mixed solid and fluid components. However, the advantage of the MST method sometimes becomes the disadvantage; specifically, the effectiveness of the MST method is limited to solving the band structure of systems containing spherical or cylindrical scatterers. Furthermore, the MST method requires a large number of terms in multiple expansions, which causes a very dense scattering matrix leading to increased computational cost. A description of the fundamental implementation of the MST method in PnCs can be found in Kafesaki and Economou (1999) and Liu et al. (2012). These researchers pointed out that the PWE method was inadequate for accurately calculating band gaps for acoustic waves propagating within periodic composites consisting of solid spheres in a fluid host; instead, they used the MST method based on an extension of the Korringa-Kohn-Rostoker method (Korringa 1947; Kohn and Rostoker 1951) to predict the band structure of the 3D solid-sphere-fluid-host PnCs. Yang et al. (2002) utilized the MST method to calculate the band structure of a face-centered cubic crystal of tungsten carbide beads immersed in water, and they further studied ultrasound tunneling in 3D PnCs. Mei et al. (2005) presented a rigorous multiple-scattering formalism for calculating both the band structure and the transmission coefficients for 2D elastic systems when the wave vector has a nonzero component along the normal of the periodic plane. Liu et al. (2012) extended the MST method by incorporating the interface/surface elasticity theory and they further investigated the interface/surface stress effect on the elastic wave band structure of 2D PnCs. Alonso-Redondo et al. (2015) studied two different types of boundary conditions, perfect boundary conditions and imperfect boundary conditions, on the interface between silica cores and a polystyrene host for the corresponding band structure calculation. Based on the fundamentals of the MST method, a layered MST method has been presented and applied to the calculation of the transmission and reflection coefficients of 2D and 3D PnCs (Yang et al. 2002; Qiu et al. 2005).

2.3.4 Finite element method

The FEM was initially used to solve structural mechanical problems but has been also introduced to calculate the band structures of PnCs. It performs spatial discretization on the displacement field and employs a variational method to express the original problems in a system of linear algebraic equations, which is subsequently solved. The FEM is capable of dealing with the band structure calculation of complex systems. However, the calculation efficiency depends heavily on the size of the discretization domain and the desired accuracy and number of eigenvalues. A detailed description about the finite element discretization of the governing equations and the FEM solutions for PnCs can be found in Veres et al. (2013). Commercially available FEM software packages such as COMSOL Multiphysics (Sigmund and Jensen 2003), ABAQUS (Dong et al. 2014a), and ANSYS (Vatanabe et al. 2014) are broadly used for these purposes. COMSOL Multiphysics allows simulation of the propagation of mechanical / electromagnetic waves in complex structures. The commercial FEM software packages make geometric modeling and wave propagation analysis so much easier, and preprocessing and postprocessing offer more opportunities for engineering design purposes. Thus, the FEM is much more preferable than the other methods for the wave propagation analysis of PnCs, especially in topology optimization process. FEM has been used to study surface acoustic waves in PnCs (Badreddine and Oudich 2011; Li et al. 2014), elastic waves in nano-sized PnCs (Liu et al. 2014b), point and linear defect states of phononic crystal plates (Yao et al. 2013a, 2013b), and topology optimization of phononic band gap width (Dong et al. 2014a, 2014b, 2014c; Hedayatrasa et al. 2015).

2.3.5 Other methods

There are other methods that have been successfully applied for analysis of PnCs. For the sake of completeness, they are briefly mentioned here. The *transmission matrix method* is attractive for analysis of the dispersion relation and the transmission and reflection spectral of PnCs; however, it is limited to 1D PnCs (King and Cox 2007; Chen and Wang 2007; Wu

et al. 2014) or layered PnCs (Fomenko et al. 2014). The *wavelet finite element method* was developed to calculate the dispersion relation of PnCs (Liu et al. 2014a). Compared with the traditional FEM, the wavelet finite element method shows computational efficiency as it requires fewer elements to achieve the same solution quality. However, the application of this method currently is only available for 1D PnCs. The *boundary element method* can calculate the band structures of 2D PnCs with very good performance; however, its convergence and computing speed are dependent on the wave modes, lattice structures, and scatterer shapes (Li et al. 2013a, b). The *variational method* expands the displacement field as a superposition of a finite number of localized functions, and uses a variational principle to solve the eigenvalue problems. Convergence of its numerical results depends on a sufficient number of localized functions. It has been successfully applied into the band structure calculation of 2D PnCs (Sánchez-Pérez et al. 1998; Goffaux and Sánchez-Dehesa 2003). The *inertial amplification method* is another alternative approach for calculating the band structure. It overcomes the shortcomings of previous methods at low frequencies, and it has been successfully applied in the calculation of band structures of infinite and finite periodic structures in two dimensions (Acar and Yilmaz 2013; Yilmaz and Hulbert 2010) and three dimensions (Taniker and Yilmaz 2013).

Regardless of the types of PnCs considered and the methods used to calculate the band structures, the computational effort and the convergence are usually issues of concern. Because the periodicity of PnCs is similar to that of PtCs (Maldovan and Thomas 2009), the methods that are used to analyze the electromagnetic waves propagating in PtCs normally can be extended for analyzing the acoustic and elastic waves propagating in PnCs.

3 Band gap design for PnCs

The larger the PnCs' band gap is, the greater number of applications they can address. In order to obtain wide band gaps of mechanical waves in the modes of interest, the shape and arrangement of scattering phases can be optimized by inverse design of the unit cell. To design a phononic crystal's band gap, the layout of constituent elastic materials is designed to maximize the band gap width. Topology optimization has been efficiently utilized for band gap design of PnCs in 1D, 2D, and 3D, by using either gradient- or non-gradient-based optimization techniques. In addition, under many practical engineering circumstances, one or more kinds of constrained conditions have also been considered while maximizing phononic band gaps. From the perspective of design optimization of the maximal band gap width in PnCs, the following sections thoroughly review the design domain, the optimization model construction, and the optimization techniques.

3.1 Design domain

Due to the periodicity of PnCs, a primitive unit cell is usually taken as the design domain and the shape and size of the unit cell (or lattice) vary with the dimensions and scales of the structures. Generally, the design domain is discretized into a relatively large-size uniform finite element mesh for further topology optimization. Thus, a pixel matrix is defined to describe the material distribution, where the value 1 (or 0) of a matrix element means that the corresponding pixel is filled with one (or the other) of the two component materials. Therefore the element-wise binary design variables are designed to obtain optimal distributions of two constituent materials within the unit cell of PnCs for the maximal band gap width.

Considering the significant computational effort in phononic band structure calculation and optimum search procedure, the design domain is assumed to be highly symmetric. On one hand, lower symmetry of a unit cell means that a large area of the wave vector is needed for band structure calculations, and thus, more computing time is required. Moreover, an asymmetric unit cell means significantly more design variables and a larger optimum search space than a symmetric unit cell. For example, as shown in Fig. 3, for a given meshing of $N \times N$ on a square unit cell, the number of design variables is $2^{N\times N/8}$ for a fully symmetric unit cell, $2^{N\times N/4}$ for a

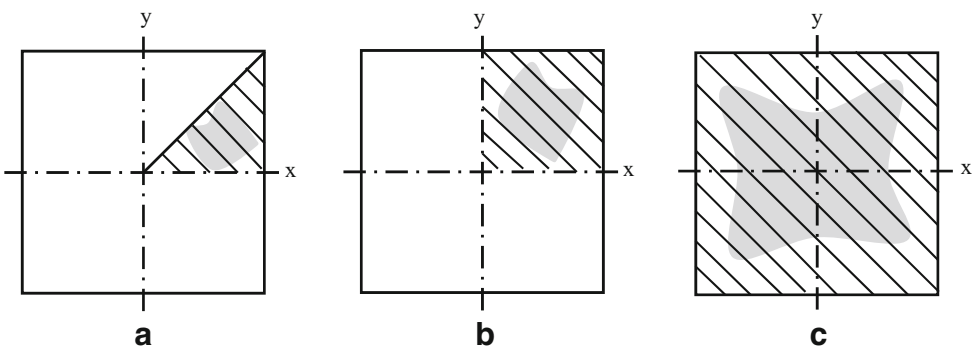


Fig. 3 Examples of symmetry conditions: (**a**) design domain with 1/8 of the unit cell, (**b**) design domain with 1/4 of the unit cell, and (**c**) design domain with a complete unit cell

rotationally symmetric unit cell, and $2^{N\times N}$ for an asymmetric unit cell. The optimization search area for the fully symmetric unit cell can be reduced to the irreducible Brillouin zone. Thus, the assumption of a symmetric unit cell yields incredible calculation efficiency in the design of topology optimization for phononic band gaps. However, it has also been shown that, a symmetry reduction of the unit cell can open wider band gaps or create new band gaps. In the work by Gazonas et al. (2006), the topology optimization design of phononic band gaps for acoustic waves yielded interesting results of asymmetric optimized unit cells with regular polygon inclusion shapes. Dong et al. (2014b) demonstrated that asymmetrical PnCs exhibited a significantly larger relative band gap width than the optimized symmetrical structure. The latest research by Dong et al. (2015) provided a comprehensive study about the effects of the symmetry reduction of the unit cell on the optimized porous PnCs. Different symmetry types (i.e., symmetry, rotational symmetry, and asymmetry) of square/triangular unit cells were numerically studied. The results demonstrated that the changes in symmetry significantly influenced the optimized structures. Topology optimization, combined with symmetry reduction, can discover new structures and offer new degrees of freedom to design phononic-crystal-based devices. Thus symmetry reduction in the design domain has great potential to open another gate for maximizing band gaps of PnCs, if the issue of high computational cost is addressed.

3.2 Definition of the optimization problem

Based on the existing literature, the topology optimization problem for phononic band gap design can be generally defined as

$$\text{Maximize} : f_1(\Sigma) \tag{4}$$

$$\text{Minimize} : f_2(\Sigma) \tag{5}$$

$$\text{s.t.} : g_j(\Sigma) \le g_j^*, j = 1, \cdots, M \tag{6}$$

$$\begin{gathered} \mathbf{u}_{\mathbf{k}}(\mathbf{r},t) = \mathrm{Re}\left[\mathbf{u}_{\mathbf{k}}(\mathbf{r})e^{-i\omega(\mathbf{k})t}\right] \quad \text{where} \quad \mathbf{u}_{\mathbf{k}}(\mathbf{r}) = f_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \\ \nabla\cdot\left(\rho c_{\mathrm{T}}^2\nabla u_i + \rho c_{\mathrm{T}}^2\frac{\partial \mathbf{u}}{\partial x_i}\right) + \frac{\partial}{\partial x_i}\left(\left(\rho c_{\mathrm{L}}^2 - 2\rho c_{\mathrm{T}}^2\right)\nabla\cdot\mathbf{u}\right) = -\rho(\omega(\mathbf{k}))^2 u_i \end{gathered} \tag{7}$$

where Σ denotes the topological distribution within the unit cell of the PnCs. $f_1(\Sigma)$ and $f_2(\Sigma)$ are, respectively, objective functions of the topological distribution that aim to be maximized and minimized. $g_j(\Sigma)$ and g_j^* are, respectively, the constraint value and limit for the j-th constraint condition, whereas M indicates the total number of constraint conditions.

3.2.1 Design variables

Topology optimization of continuum structures refers to find the optimal distribution of the characteristic function (e.g., density function) within a given design domain, which can be solved as a discrete problem where the characteristic function is discretized in an element-wise manner, or relaxing discretized variables to be continuous and introducing penalization to produce a 0–1 design. In the latter case, the discretization is not necessarily done element-wise; there are node-wise discretization (Rahmatalla and Swan 2004), level set method (Allaire et al. 2004), grids of densities independent of the mesh (Nguyen et al. 2010; Wang et al. 2013c), and independent geometric representations of discrete elements (Guo et al. 2014; Norato et al. 2015), etc. The element-wise discretization method, in which a structure's design domain can often be discretized by uniform size finite elements and the characteristic function refers to the material properties on each finite element, is commonly used in topology optimization of continuum structures, including phononic band gaps. Generally, the characteristic function is defined as a function of a parameter (design variable) that determines the mixture of basic materials throughout the domain. During the optimization procedure, the characteristic function requires topological complexity control techniques such as perimeter control techniques (Haber et al. 1996), sensitivity filtering method (Sigmund 1994), density filtering method (Bruns and Tortorelli 2001; Svanberg and Svärd 2013), morphology-based filtering method (Sigmund 2007), and Heaviside projection method (Guest et al. 2004), as the continuum problem would otherwise have an infinite number of holes or suffer from mesh-dependent solutions.

Research on the optimization design of phononic band gaps is mostly element-wise dominated. The design domain is normally discretized with a relatively large number of elements, and each element can have the material properties from material constituent 1 or material constituent 2. The design variables are simply assigned to each element with 0 and 1 values at the beginning of the design. Thus, a string of binary variables control the distributions of the two constituent materials over the design domain. For different dimensions of the design domain, different quantities could be used as design variables. In 1D problems, design variables could be defined as the number of the layers and/or thickness of each layer (Hussein et al. 2006), and the mass at each grid. In 2D and 3D problems, a pseudo-material property (e.g., density or Young's modulus) or an independent mathematical design variable could be used as a design variable. Therefore, in the implementation of topology optimization design for phononic band gaps, either continuous or discrete design variables can be used. In the gradient-based topology optimization techniques, a single continuous design variable is assigned to each element and the material

properties of the element can be obtained by using material interpolation schemes. The optimization problems are solved accordingly based on the sensitivity computation. In the non-gradient-based topology optimization techniques, the discrete 0–1 design variables are kept for the optimization calculation and yield binary optimized solutions. Due to the finite length-scales imposed by the wavelength, the design optimization of phononic band gaps is free from mesh-dependency (Sigmund and Jensen 2003). The aforementioned sensitivity filtering method (Li et al. 2016a, 2016b) and Heaviside projection method (Hedayatrasa et al. 2016b) are often employed to eliminate the checkerboards in the design of phononic band gaps.

3.2.2 Objective functions

Since the goal is to find the optimal topological distribution within the unit cell of the PnCs that exhibits the largest band gap width, Eq. (4) is the objective function of band gap width that will always be considered. For evaluation of the band gap width, some researchers used the difference between two adjacent eigenfrequencies (Jensen and Pedersen 2006; Diaz et al. 2005), called the absolute band gap width, as the objective for the optimization to maximize, specifically

$$f_1(\Sigma) = \omega_{n+1}(\Sigma,\ \mathbf{k}) - \omega_n(\Sigma,\ \mathbf{k}) \tag{8}$$

Most other researchers adopted the size of a particular band gap width normalized with respect to its central frequency, called the relative band gap width, as the objective function (Halkjær et al. 2006; Dong et al. 2014b, 2014c; Liu et al. 2014c; Hedayatrasa et al. 2015), specifically

$$f_1(\Sigma) = \frac{\min_{\mathbf{k}} :\ \omega_{n+1}(\Sigma,\ \mathbf{k}) - \max_{\mathbf{k}} :\ \omega_n(\Sigma,\ \mathbf{k})}{(\min_{\mathbf{k}} :\ \omega_{n+1}(\Sigma,\ \mathbf{k}) + \max_{\mathbf{k}} :\ \omega_n(\Sigma,\ \mathbf{k}))/2} \tag{9}$$

where $\min_{\mathbf{k}} :\ \omega_n(\Sigma, \mathrm{k})$ and $\max_{\mathrm{k}} :\ \omega_n(\Sigma, \mathbf{k})$ denote the minimum and maximum of the n-th eigenfrequency ω_n over the entire discrete wave vector set, $\mathbf{k} = (\mathrm{k}_1, \cdots, \mathrm{k}_{n_k})$, along the boundaries of the irreducible Brillouin zone for a given design, Σ, of the unit cell. n_k is the total number of wave vectors on the irreducible Brillouin zone edges. Alternative expressions for Eqs. (8) and (9) can be formulated by replacing $\omega_n(\Sigma, \mathbf{k})$ and $\omega_{n+1}(\Sigma, \mathbf{k})$ with their square values, $\omega_n^2(\Sigma, \mathbf{k})$ and $\omega_{n+1}^2(\Sigma, \mathbf{k})$, respectively (Sigmund and Jensen 2003; Barbarosie and Neves 2004; Hussein et al. 2007; Bilal and Hussein 2011a, b; Vatanabe and Silva 2011; Dong et al. 2014a, 2015). These replacements have the same meaning because the solutions of the eigenvalue problem in Eq. (2) can be expressed in the form of the eigenfrequencies or as the square of the eigenfrequencies. The expression of the band gap width in Eq. (9) indicates that the band gap exists only when the minimum of the (n+1)-th branch is greater than the maximum of the n-th branch; otherwise, no band gap exists.

The physical benefit of using the relative band gap width lies in that the PnCs can be scaled to change their band of operation. The physical meaning of the above formula is that the optimal band gap structure with the maximum gap width between bands n and n+1 can be realized geometrically by seeking the best distribution of materials in a unit cell that meets symmetry and periodicity requirements. The largest band gap normally exists between two of the first few bands. Thus, it is not necessary to search all of the bands; instead, the optimization focuses on the first few bands, for example, prior work has focused on the first six bands (Sigmund and Jensen 2003), the first five bands (Hussein et al. 2007), and the first nine bands (Dong et al. 2014b).

Other expressions have also been formulated for maximizing the band gap widths. Hussein et al. (2007) reported two objective functions for maximizing the sum of the first five maximum band gap widths, with or without normalization relative to the central frequency of each band gap. In addition to the approach that examines the maximum difference in the frequencies as the optimization objective, Jensen and Pedersen (2006) used two approaches to formulate the objective function, specifically a double-bound formulation for the maximum difference in the frequencies, and a formulation of the maximum ratio of two adjacent eigenfrequencies. The double-bound formulation was also used in the work of Vatanabe et al. (2014).

In multi-objective optimization problems, the number of objective functions is usually limited to two in this field. In addition to maximizing the band gap width, the second objective function, $f_2(\Sigma)$ in Eq. (5), is usually performed to minimize or maximize structural performance and cost. Hussein et al. (2006) constructed a multi-objective optimization problem for maximizing the percentage of stop-bands within a specified large frequency range for minimum wave transmissibility. Dong et al. (2014a) presented research focused on maximizing the relative band gap width for 2D PnCs while minimizing the mass of the design domain. Hedayatrasa et al. (2015) formulated a multi-objective topology optimization model to maximize the sum of the relative band gap widths of several desired modes while minimizing the deviation of the filling fraction of individual solution from the reference filling fraction, which was also aimed to control the structural mass.

3.2.3 Constraints

As Eq. (7) represents the governing equation of acoustic/elastic wave propagation in PnCs, which is the necessary condition for solving the problem, we don't consider it as a constraint from the perspective of optimization, even though it is included in the optimization model. The constraints in topology optimization problems of phononic band gap design

consists of one or more kinds of performance or/and geometrical parameters. Especially in the design of 1D PnCs, some geometrical parameters need to be carefully limited from the viewpoint of convergence. Diaz et al. (2005) considered limiting the non-structural mass added at each design location to control the translation degree of freedom of nodes and rotational inertia of the 1D grid structure. Hussein et al. (2006) constrained the layer thickness and total cell length when designing 1D layered PnCs. Other factors likely to be constrained include the structural volume (Li et al. 2016a), filling fraction (Hedayatrasa et al. 2015), predefined average density (Dong et al. 2014c), double-bound eigenfrequency constraints (Jensen and Pedersen 2006), and predefined band gap width and geometrical width constraint (Dong et al. 2014a, 2015).

3.2.4 Optimization problem types

The topology optimization model described in Eqs. (4) to (7) is a general expression for band gap design of PnCs. The actual optimization problem formulation would depend on the design purpose and requirements. In the existing literature, the specific optimization problems for phononic band gap design can be classified into four types:

Type 1: Single-Objective-Unconstrained Optimization Problem. In this case, the optimization problem is formulated based on Eqs. (4) and (7) to maximize the band gap width without constraint, i.e., maximizing the absolute band gap width (Vatanabe and Silva 2011) or maximizing the relative band gap width (Sigmund and Jensen 2003; Halkjær et al. 2006; Dong et al. 2014b; Liu et al. 2014c).

Type 2: Single-Objective-Constrained Optimization Problem. In this case, Eqs. (4), (6), and (7) are formulated to construct the optimization problem of maximizing the band gap width with one or multiple constraints, such as maximizing the absolute band gap width with non-structural mass constraints on each element (Diaz et al. 2005) or with predefined eigenfrequency constraints (Jensen and Pedersen 2006), maximizing the relative band gap width with a predefined average density constraint (Dong et al. 2014c), maximizing the relative band gap width with a volume constraint (Li et al. 2016a), and maximizing the relative band gap width with a volume constraint and a bulk or shear modulus constraint (Li et al. 2016b).

Type 3: Multi-Objective-Unconstrained Optimization Problem. In this case, the optimization problem is formulated based on Eqs. (4), (5), and (7) to maximize and/or minimize multiple structural performances and characteristics in phononic band gap design. Normally, two conflicting and simultaneous objectives are formulated, for example, maximizing the summation of multiple band gap widths while minimizing the deviation of filling fraction of the optimized solution from the reference filling fraction (Hedayatrasa et al. 2015), and simultaneously maximizing relative band gap width of plate waves in undeformed configuration and maximizing band gap tunability (i.e., relative gradient of the relative band gap width) under a specified externally imposed deformation (Hedayatrasa et al. 2016b).

Type 4: Multi-Objective-Constrained Optimization Problem. In this case, the optimization problem follows the general expression of the phononic band gap design optimization model, which is, for example, multi-objective optimization of maximum relative band gap width and minimum mass with constraints on predefined band gap width and geometric width for 2D porous PnCs with fully symmetrical unit cell (Dong et al. 2014a), or for 2D porous PnCs with reduced symmetrical unit cells (Dong et al. 2015).

3.3 Optimization techniques

Generally, a two-stage topology optimization process is constructed to perform the design optimization of band gaps for PnCs. The first stage is to calculate the band structure of the PnCs for a given design and measure the band gap widths existing in the band structure. The second stage is to mathematically solve the optimization model and address the solution for the current optimization problem. The optimization process is carried out by running the first and second stages repeatedly until the optimization criterion is satisfied. A band structure analysis method (e.g., PWE, FDTD, and FEM), and an optimization solution technique (e.g., gradient- or non-gradient-based optimization method), are used in the first and second stages, respectively. The analysis methods used for calculating the phononic band structures have been discussed in Section 2. The topology optimization problem modeling and optimization solution techniques for phononic band gap design will be reviewed and discussed in the following sections.

3.3.1 Gradient-based optimization techniques

The topology optimization methods that have been developed for mechanical design problems are diversified and efficient; most are gradient-based optimization techniques. In gradient-based topology optimization techniques, the initial discrete problems are relaxed by assuming continuous design variables in the interval [0, 1]. The corresponding material properties at points between 0 and 1 can be interpolated by the material properties at 0 and 1. Thus, the gradient information can be obtained based on the continuity of the design variables. Specifically, the gradient information, or sensitivity

calculation, of the objective and the constraints needs to be provided in the optimization calculation. The gradient information plays a decisive role on the convergence rate and accuracy when updating the iterative solutions to move toward the optimum point. The discrete final designs can usually be obtained using penalization techniques, continuation approaches, post-processing by thresholding (Zhou et al. 2015), projection schemes (Ha and Guest 2014), and robust design formulations (Wang et al. 2011).

The most commonly used gradient-based topology optimization technique for material design is known as the inverse homogenization method (Sigmund 1994), or inverse design of periodic structures by homogenization. This technique was first applied to band gap design of phononic crystal materials by Sigmund (2001b) and Sigmund and Jensen (2002, 2003) through a linear material interpolation scheme. In this approach, the prescribed elastic properties in an element are assumed to be defined as

$$A_e(x_e) = (1-x_e)A_1 + x_e A_2 \tag{10}$$

where subscripts e, 1, and 2, respectively, denote the element number, material phase 1 and material phase 2. A represents material density and elastic properties (i.e., Lame's coefficients or stiffness) and $x_e \in [0, 1]$ is the element design parameter that interpolates the material properties for each element used to discretize the structure. If the design variable is zero, the element has pure phase 1 material. If the design variable is one, the element has pure phase 2 material.

It is obvious that the above interpolation scheme is similar to but different from that in the modified SIMP method for two-phase topology optimization (Sigmund 2001c). In terms of the reason to choose this kind of linear interpolation, Sigmund and Jensen (2003) claimed that it originated in the nature of the band gap phenomenon, where the large contrasts between the involved material phases was favored to yield large band gaps. Thus, there was no need to penalize intermediate artificial relative densities. For the planar wave propagating within the 2D PnCs, each element in the final design has either pure material phase 1 or pure material phase 2. In another words, no intermediate materials appear in the optimal design when considering the in-plane waves and/or the out-of-plane waves. However, the gray elements appear when dealing with the bending wave (Halkjær et al. 2006) and acoustic waves (Jensen and Pedersen 2006). The appearance of gray elements that occur when using the above linear interpolation somehow depends on the waves that propagate within the 2D PnCs. In order to eliminate the gray elements, for the bending wave in a phononic crystal that was composed of a solid material and void, Halkjær et al. (2006) applied an explicit mesh-independent penalization scheme as an extra constraint, as suggested by Borrvall and Petersson (2001); for the acoustic waves, Jensen and Pedersen (2006) used a second-order polynomial based on linear interpolation to penalize the intermediate values for stiffness, whereas for the material density they retained the linear interpolation defined in Eq. (10). In addition, they also proposed interpolations for 1D problems, where the element density was expressed in a complex reciprocal formulation and the element stiffness retained the linear interpolation. No gray elements appeared in this case.

Due to the interpolation schemes, the sensitivities of the objective function and the constraints can be calculated, and the optimization problems can be further solved by using an appropriate optimization algorithm (i.e., MMA). Following the above-mentioned linear interpolation and penalization function schemes, the maximal band gap design problems for PnCs were solved based on a fixed-pattern procedure, where the FEM for the band structure calculation was used in conjunction with a gradient-based optimization algorithm for the optimized solutions. Barbarosie and Neves (2004) considered the unit cell of a double periodic 2D PnCs and performed topology optimization design to maximize the distance between two adjacent frequency curves for the application of frequency filtering. The FEM was used to calculate the band structures within the double periodic solid unit cell, and the topology optimization problem of maximizing the band gap between the two adjacent frequencies was formulated based on the linear material interpolation scheme and solved by using the MMA method. Halkjær et al. (2005) implemented gradient-based topology optimization to design basic bi-material unit cells for maximized phononic band gap for (1) 1D infinite periodic beams modelled by the Timoshenko beam theory, (2) 2D infinite periodic thick and moderately thick plates, and (3) 2D finite thick plates. Diaz et al. (2005) performed the optimization of band gaps in the periodic plane grid structures and explored the effect of the angle between the basic vectors on the band gaps of the structure by using the FEM and the gradient-based MMA method. Vatanabe and Silva (2011) and Vatanabe et al. (2014) also utilized the linear interpolation scheme described above to identify the local effective properties, such as weight, elastic, piezoelectric, or dielectric properties, of the mixture for maximizing the first band gap and maximal absolute band gap of the 2D PnCs composed of non-isotropic materials, i.e., functionally graded piezocomposite materials and regular piezocomposite material, respectively. The optimization problems of phononic band gap design were also solved based on the FEM procedure in combination with MMA. They also found gray elements at the boundary between two materials in the final solution, and a penalized projection method was proposed to successfully remove the gray elements. Based on the above linear-interpolation-based gradient topology optimization approach, Li et al. (2016a) combined an alternative gradient-based optimization algorithm, the bi-directional evolutionary structural optimization (BESO) method, with FEM to optimize the design of phononic band gap for maximum

relative band gap width of two adjacent bands with a volume constraint. Three cases, the in-plane, out-of-plane, and combined in-plane and out-of-plane wave modes, were considered and a small number of gray elements were found in the final results of their research. Meanwhile, Li et al. (2016b) conducted a design optimization of cellular PnCs to maximize relative band gap width with a bulk or shear modulus constraint and a prescribed volume fraction constraint, by using BESO algorithm in conjunction with a homogenization method and FEM. They used the homogenization method to calculate the static effective bulk or shear modulus that satisfied the stiffness requirement of individual topological results. In order to obtain a standard band gap optimization problem, they added the bulk or shear modulus constraint to the relative band gap width through a Lagrangian multiplier to reformulate the objective function. A record-breaking result, the maximum relative band gap width up to 144.41 %, was obtained with the shear modulus constraint in the out-of-plane wave mode in their research.

Even though there are enriched gradient-based approaches developed for topology optimization of mechanical problems, only a couple of them have been applied to the topic of topology optimization of the band gaps of PnCs. We believe that there is a great promise for other alternative methods such as the level set method, the Heaviside projection method, and the phase-field method, to be used in this topic in the future. Regarding the challenges in optimization design of phononic band gaps, a discussion will be given in Section 5.1.

3.3.2 Non-gradient-based optimization techniques

Non-gradient-based optimization techniques are usually based on random processes. The Genetic Algorithm is the most popular approach that has been used for topology optimization of phononic band gaps. As phononic band gap design using the GA method only involves a fitness function and several operation parameters (e.g., population size, mutation, crossover probability, and termination criterion), no material interpolation assumption or complicated sensitivity calculation are required to perform the GA method. This makes the GA method more attractive than gradient-based optimization techniques. However, the operation parameters in the GA method are so important that the selection of their values can be of great influence on the efficiency and convergence of the optimization problems. In addition, their values vary for different problems; thus, there are no standard rules to determine their appropriate values. Since the GA method doesn't require continuity of the design variables or fitness functions, binary variables are usually assigned for the elements (i.e., pixels, grids, or layers) in a unit cell (or a system), where "0" represents material constituent 1 and "1" represents material constituent 2. A 0–1 integer programming formulation is devised for further optimization solutions. Hence, a chromosome consisting of 0–1 binary variables in the GA method is used for population setting, and a string of binary variables will control the distribution of the two constituent materials. The GA method can be easily used for optimization problems with different objective expressions, or different types of optimization problems.

In the topic of topology optimization of phononic band gaps, there has been much research conducted using the GA method as the number of topological design variables searched in a fully symmetric lattice is relatively small and the corresponding computational expense is affordable. Hussein et al. (2007) conducted the phononic band gap design for 2D PnCs based on the FEM and the GA method. The objective function of maximizing the sum of the first five band gap widths, with or without the normalization relative to the central frequency of each band gap, was considered as the fitness function. Based on the GA-driven optimization approach, they studied a range of Young's modulus and density ratios for the optimal unit cell designs in the out-of-plane mode. They found that the lower contrast cases tended to consist of hollow high stiffness/density inclusions while the higher contrast cases tended to produce solid inclusions. Later, Bilal and Hussein (2011a, b) reported a specialized genetic-algorithm-based topology optimization method for maximization of the absolute band gap in 2D solid/void porous PnCs for simultaneous attenuation of out-of-plane and in-plane waves. Their work was a very comprehensive study of the different modes of 2D PnCs. The area between the two dispersion branches of interest was used as an indicator of the fitness of the unit cell design and was added to the maximal relative band gap width as the fitness function. The fitness indicator equaled zero when a band gap existed and equaled the value of the area when no band gap existed. Besides the fitness function, a tournament selection operator and a simple-single-point crossover operator yielded an elegant design with exceptionally large and low frequency band gaps. Dong et al. (2014c) performed design optimization of the maximal relative band gap width of 2D solid PnCs with or without a predefined average density constraint using the FEM and the GA method. For the unconstrained problem, a "coarse to fine" two-stage GA inverse scheme was utilized to reduce the computational load caused by the large-sized search space. The first stage was to perform the GA search on a coarse grid and the second stage was a fine-adjustment stage, where the optimal structure obtained in the previous stage was mapped onto a finer grid and the new GA search space was thus limited to the boundary area between the inclusion and matrix materials. For the constrained problem, an adaptive penalty factor was composed on the constraint and used to transform the constrained optimization into an unconstrained one that could be solved with the same "coarse to fine" two-stage GA procedure that was used for the unconstrained

problem. The penalty factor changed adaptively to prevent premature convergence of the GA. A very large penalty factor was used in the initial stage of the evolution to compensate for the failure of most individuals to meet the filling fraction constraint. The penalty factor became smaller to control the pace of eliminating the unfeasible individuals slowly as the evolution progressed. Eventually, feasible solutions were yielded. This two-stage GA method was also used in the work by Liu et al. (2014c, 2015), where the GA method combined with the PWE method and with the FEM was employed for design optimization of a maximal relative band gap width of 2D solid PnCs. The maximal relative band gap width was considered as the fitness function and the search space was narrowed down to the irreducible Brillouin zone, while considering three modes: in-plane mode, out-of-plane mode, and combined in-plane and out-of-plane mode, respectively.

For the asymmetric lattice, both the areas for band structure analysis and for optimization search are larger than that in the symmetric lattice. Thus, the computational load has been a major challenge in these problems. In these cases, special techniques, such as parallel computation and improved GA method, are employed to alleviate the computational load. Gazonas et al. (2006) used the FEM and the GA method to conduct phononic band gap design for 2D acoustic wave systems with an arbitrarily asymmetric lattice. Based on the binary chromosome scheme, the relative band gap was considered as both the objective and the fitness function. They highlighted that the most expensive part of the entire GA design loop was the evaluation of the objective function itself; this evaluation process could be parallelized for computational cost saving. With computational concerns in mind, Dong et al. (2014b) used the FDTD method and the multiple elitist GA (MEGA) method with adaptive fuzzy fitness granulation (AFFG) for design optimization of the maximal relative band gap width of 2D asymmetrical PnCs in combined out-of-plane and in-plane wave modes. With this approach, this team obtained a larger relative band gap width in the asymmetrical PnCs than that in the symmetrical PnCs. In the AFFG scheme, a Gaussian similarity neighborhood function for each wave vector was defined for the similarity calculation and an evaluation check was performed to estimate the fuzzy fitness of an individual using exact fitness evaluation. Then the granule pool of the generations was updated accordingly. The MEGA method was later used to preserve more excellent genes from each generation. It was claimed by the authors that with the combined approach of AFFG and MEGA, the computational load required for fitness function evaluation was reduced 50 % and the convergence rate was five times faster than that yielded using the conventional evolutionary algorithm with respect to the same final fitness values.

In addition, the GA method is capable of dealing with multi-objective optimization problems. In such problems, there are no single optimal solutions, but rather a set of alternative solutions, which are known as Pareto Front solutions. In multi-objective optimization, the optimal solution is usually selected from the Pareto Front solutions by the human decision-maker. Hussein et al. (2006) used the transfer matrix method and a multi-objective GA (MOGA) to perform design optimization of 1D periodic unit cells for target frequency band structures characterizing longitudinal wave motion. The number of layers in the unit cell and the thickness of each layer were taken as design variables, and binary and mixed formulations were developed for treatment of the optimization problems. Based on the nondominated sorting genetic algorithm (NSGA-II) (Deb et al. 2002), which is a heuristic algorithm capable of efficiently generating quasi-Pareto optimal (noninferior) solutions, three case studies were considered with different multi-objective optimization problems: Case 1, creation of a stop band for maximized wave attenuation at a specified frequency; Case 2, maximization of the percentage of stop bands within a specified large frequency range for minimum wave transmissibility; and Case 3, creation of multiple stop bands/pass bands at specified frequency ranges. The results showed that the pass bands were more difficult to design than the stop bands. Hedayatrasa et al. (2015) reported a comprehensive study on topology optimization of a 1D periodic biomaterial phononic crystal plate for maximization of in-plane Lamb wave (i.e., a complex vibrational wave that propagates parallel to the test surface throughout the thickness of the material) band gap width using the FEM and the NSGA-II method. A specified multilayer FEM model was constructed and the thickness for each layer was considered as a design variable in a symmetrical and a non-symmetrical design domain, respectively. Two different band gap objectives were studied in their research: the widest relative bandwidth of lowest Lamb gap and the widest total relative bandwidth of ten likely gaps within the first eleven in-plane modes of interest. The optimization problem was formulated in two approaches: (1) to maximize the relative bandwidth with a prescribed filling fraction constraint, and (2) to simultaneously maximize the relative bandwidth and minimize the deviation of filling fraction of individual solution from the reference filling fraction. For comparison, two types of design space with symmetric topology as well as constraint-free topology were also examined.

Instead of addressing the best layout of predefined material constituents in the design optimization, Zhang et al. (2013) conducted a multi-band design for 1D PnCs using an optimization algorithm to select appropriate constituents from various material candidates. They derived the analytical expression of elastic wave propagation in a 1D infinite periodic slab based on the Bloch theorem, and considered two objectives in

the optimization algorithm: minimizing boundary frequencies for the band gaps of longitudinal waves and minimizing pass band ranges in the target frequency areas, with constraints on the thickness of each material candidate layer. A total of 22 material candidates were considered and the NSGA-II was utilized to solve the optimization problem. With respect to three different target frequency areas, the design optimization yielded two-material-constituent, four-material-constituent, and six-material-constituent 1D PnCs respectively.

With the help of the efficient MOGA method NSGA-II, multi-objective design optimization of 2D complex phononic crystal structures such as porous PnCs and phononic crystal perforated plates, has also been carried out successfully in the literature. Dong et al. (2014a) and Dong et al. (2015) designed 2D porous PnCs in fully symmetric square lattices and in reduced symmetric square and triangular lattices, respectively, with a simultaneously maximal band gap width and the minimal mass subjected to predefined relative band gap and geometrical constraints by using the FEM and NSGA-II method. According to their research, they found that the symmetry reduction of the unit cell yielded better Pareto-optimal solutions with larger relative band gap widths and smaller mass in three wave modes (i.e., out-of-plane, in-plane and combined out-of-plane and in-plane wave modes) than the full symmetry of the unit cell. Later, Hedayatrasa et al. (2016a) presented topology optimization of single material phononic crystal perforated plates for the widest exclusive band gaps of fundamental symmetric or asymmetric guided wave modes as well as widest complete band gap of mixed wave modes in 3D symmetric and asymmetric unit cells. Even though thinner connections of scattering segments were favored to obtain the largest band gaps, which was also demonstrated in the work by Li et al. (2016b), they easily yielded lower effective stiffness of the structural topologies. Thus, this research team incorporated the in-plane stiffness in the optimization algorithm as an opposing objective to be maximized. They employed a specialized NSGA-II method to get the optimum results. Hedayatrasa et al. (2016b) achieved the optimal design of 2D tunable phononic band gap plates under equibiaxial stretch through two simultaneous objectives, maximum relative band gap width of plate waves in undeformed configuration and maximum band gap tunability, which referred to the relative gradient of relative band gap width with reference to the underformed state when stretched under macromechanical equibiaxial strain of up to 10 %. They utilized the FEM for band structure analysis and nonlinear deformation of the unit cells, the Heaviside projection method for controlling the minimum length scale of designed features, a dimension reduction scheme for adaptively controlling the design space resolution independently of the FEM mesh resolution, and the NSGA-II method for seeking the optimal solutions in the topological design space.

Based on the existing literature, the GA and NSGA-II methods have been very useful to find the optimal solutions of the design problems of phononic band gaps. Even though the computational cost is still a major concern when using these GA-driven NGTO methods, they are able to provide optimized solutions by integrating different computation schemes that scale the computational load effectively.

3.4 Summary

In each of these optimization studies of phononic band gap design, the focus has been primarily on optimizing the unit cells of PnCs in 1D and 2D based on material compositions of one (solid and void), two, or more elastic material phases using GTO or NGTO techniques. A variety of studies have been devoted to the in-plane, out-of-plane, and combined in-plane and out-of-plane waves, as well as the symmetrical and asymmetrical design domains of different lattice shapes. By using appropriate topology optimization techniques, topology optimization of phononic band gaps has been expanded to optimizing the band gaps as well as mechanical performances of complex phononic crystal structures such as porous PnCs, phononic crystal perforated plates, and tunable phononic band gap plates. Seeking for the best mechanical performances of the phononic crystal structures, such as bulk and shear modulus, in-plane stiffness, and band gap tunability, has been incorporated in the design optimization of phononic band gaps.

Regarding the topology optimization techniques used in the literature of design optimization of phononic band gaps, several GTO methods and GA-driven NGTO methods have been studied and presented. The GTO methods are basically developed based on the linear material interpolation scheme and most of them used the MMA for optimization solutions. Besides the BESO method, other topology optimization techniques have not yet been studied in the design optimization of phononic band gaps. The NGTO methods are mostly proposed based on the GA or MOGA methods. In order to alleviate the computational cost of the GA method, computation schemes such as parallel computation, “coarse-to-fine” two-stage strategy, and the AFFG and MEGA approaches, are presented to collaborate with the GA method. However, the diversity of GA-driven NGTO techniques is still quite limited compared to numerous heuristic approaches. Thus there is a high possibility to introduce other heuristic approaches such as multi-objective particle swarm optimization method (Wang et al. 2013a; Fan et al. 2015) into the design optimization of phononic band gaps in future. A detailed discussion and comparison of the advantages and disadvantages of the GTO and NGTO techniques is presented in Sigmund (2011).

With regards to different types of optimization problems, although both the GTO and NGTO methods are capable of

tackling single-objective and multi-objective optimization problems, the proposed GTO methods have been used only in single-objective optimization problems in the literature, whereas the proposed NGTO methods (i.e., GA and NSGA-II) have been used in both single-objective and multi-objective optimization problems. For both single-objective and multi-objective optimization, the GTO methods are relatively more efficient than the NGTO methods as the use of gradient information can be of great benefit. Moreover, the GTO methods such as the topological sensitivity multi-objective method (Suresh 2010, 2013) and the aggregative gradient-based multi-objective method (Izui et al. 2015), have been demonstrated to efficiently find diverse and representative Pareto-optimal sets for multi-objective topology optimization problems. On the other hand, the use of gradient-based methods in multi-objective optimization has been extensively discussed (Bosman 2012; Giacomini et al. 2014; Sato et al. 2016) to search for a high quality Pareto-optimal solution set, which is similar to the solution set obtained from the NSGA-II method but at a much lower computational cost. Therefore, it is expected that the multi-objective GTO methods, as well as the multi-objective gradient-based optimization methods, can be utilized in the multi-objective topology optimization of phononic band gaps.

4 Functional phononic crystal structural design

Building upon the initial research on phononic band gap design, the new field of PnCs design emerged. More recently, numerous novel device designs and functional applications of PnCs have appeared in the literature. Topology optimization design approaches have been identified to create phononic crystal structures and devices with optimized performance and characteristics of interest, normally based on a finite design domain with specified boundary conditions and external wave loading. Here, we review strategies for topology optimization design of phononic crystal structures to enable functional applications.

4.1 Waveguides and filters

Wave guiding and filtering are useful characteristics of finite periodic structures. Phononic crystal wave guides are commonly used in signal transmitting, delaying, bending, and other kinds of processing. For elastic and acoustic waveguides and filters, topology optimization has been effectively used to design novel phononic structures with periodic or periodic-like inclusions. As topology optimization for waveguides and filters has been implemented, two modeling schemes (i.e., frequency- and time-domain topology optimization) and two geometrical construction strategies (i.e., periodic and aperiodic structures) have been considered in the literature.

4.1.1 Frequency- and time-domain topology optimization

Frequency-domain topology optimization is simple and easily implemented. Most topology optimization models are frequency-domain-based, including phononic band gap design (Sigmund and Jensen 2003) and waveguide and filter design (Jensen and Sigmund 2004b). Similar to the FDTD method, where the structure with wave propagation is discretized by time and space, time-domain-based topology optimization is formulated based on time and spatial coordinates. Compared to frequency-domain topology optimization, the main advantage of time domain approaches is the lower computational cost for wave problems consisting of a broad range of frequencies (Lazarov et al. 2011). In addition, time domain methods can model strongly non-linear or time-controllable materials without any limitations. This approach has been used to design complicated filters involving pulse devices (Dahl et al. 2008; Lazarov et al. 2011).

4.1.2 Periodic and aperiodic structures

The first geometrical construction strategy is to create waveguides and filters using a designed periodic unit cell that exhibits the largest band gaps, or to use a promising periodic unit cell. Jensen and Sigmund (2004b) optimized the minimal vibrational response of a 2D phononic crystal structure composed of periodic aluminum square inclusions in an epoxy matrix, subjected to periodic loading at the boundaries. Strong mass-dependent viscous damping was applied in the periodic structure, and a linear material interpolation scheme was used to construct the optimization problems. The gradient-based topology optimization approach, specifically, MMA combined the FEM was used to solve the optimization problem. Two optimization designs with different structural sizes were yielded for the in-plane and out-of-plane modes, respectively. Later, Halkjær et al. (2006) constructed a finite periodic plate using a number of the optimized cells in a post-process version. In order to improve the static stiffness of the structure with the optimized unit cell, a modified objective function, instead of the relative band gap width, was proposed by multiplying the band gap by the square of the mean gap frequency. Halkjær's team manufactured the finite plate with polycarbonate based on the optimized-and-post-processed unit cell, and further investigated the dynamic properties of the finite plate both theoretically and experimentally. The repeated structures with optimized unit cells before and after modifying the objective function, the final finite plate, as well as the comparison of theoretical and experimental results, are

shown in Fig. 4. In the work by Hussein et al. (2007), first, design optimization of unit cells of the 2D PnCs was employed to maximize the band gap width. Next, the designed cells were subsequently used with varying levels of material damping to form a finite vibration isolation structure, subjected to broadband loading conditions. This kind of structure exhibited excellent isolation performance. Another interesting design optimization under this strategy was reported by El-Sabbagh et al. (2008). In this work, topology optimization was used to maximize the fundamental natural frequency of Mindlin plates, while enforcing periodicity. In order to implement this design optimization, the thickness distribution of a local unit cell was designed with a design objective that described the global performance of a periodic assembly of the local unit cell. Thus, a finite structure was generated that was consistent with a finite amount of periodic unit cells.

Instead of considering the unit cell optimization, the second geometric construction strategy is to design a waveguide or filter in a finite design domain with given boundary and loading conditions. As no prior information of the periodicity is provided, the optimized structures normally yield periodic-like or aperiodic inclusions embedded within the background materials. Besides the design optimization of phononic band gap materials, Sigmund and Jensen (2003) conducted the design optimization of a finite phononic crystal structure with strong damping for the purpose of wave guiding. Based on the linear material interpolation scheme, a systematic optimization problem was formulated to minimize the wave magnitude at a point, a line, or an area of a structure subjected to periodic loading. The MMA method in conjunction with the FEM was utilized to solve the optimization. Through the assumptions of different loading locations, absorbing boundary conditions, and output locations, several close-to-periodic finite structures were obtained. In particular, an example of the design of a waveguide that concentrated a wide incoming wave to a narrow and magnified output wave was studied. Rupp et al. (2007) developed a topology optimization approach to design 2D and 3D surface wave filters and waveguides. A topology optimization model for minimizing displacements in certain regions of the design domain was constructed by linearizing the element stiffness and mass matrices with respect to the design variables. Non-reflection boundary conditions (i.e., viscous damping and perfectly matching layers) were imposed wherever the semi-infinite computational domain was cut, and the optimization problems were solved by using the sequential convex approximation-based method of MMA and the commercial large-scale sequential quadratic programming method implementation SNOPT for 3D and 2D problems, respectively. Based on this optimization model, a 3D Bragg grating, a patterned-thin-film surface wave filter device, and a 3D surface waveguide were obtained separately. Figure 5 shows a representative example of topology optimization of the 3D surface waveguide. Later, the same research group (Rupp et al. 2010) reported an interesting and comprehensive study on the response of optimally patterned 2D phononic devices with respect to four switchable applications: a filter, a waveguide, an energy harvester, and a wave actuator. They proposed a polarization-patterned piezoelectric plate uniformly covered by electrodes, by using topology optimization to determine the piezoelectric polarization patterns in this phononic device. A nearly periodic polarization

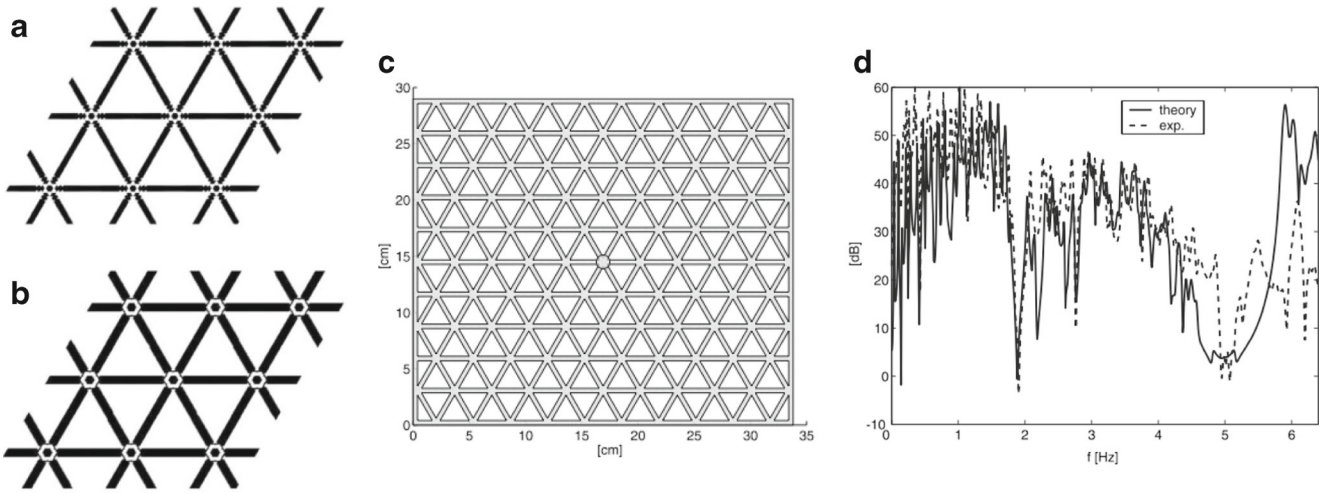


Fig. 4 Example of the finite periodic plate for a wave filter: repeated structures consisting of 3×3 optimized base cells (**a**) with a maximal relative band gap width, and (**b**) with the maximum band gap width multiplied by the square of the mean gap, (**c**) the finite periodic plate consisting of 10×10 post-processed optimized base cells made from Polycarbonate, and (**d**) experimental and theoretical acceleration plots for the finite plate. (By Halkjær et al. 2006)

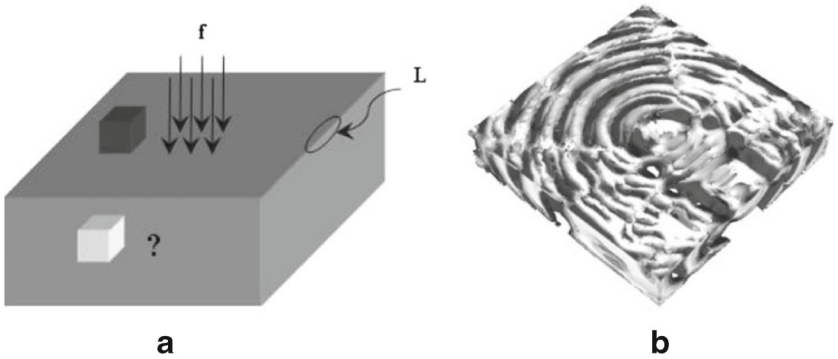


Fig. 5 Example of topology optimization of a 3D surface waveguide: **a** Design domain for a surface wave device which focuses input energy from a normal surface load f into surface waves, which exit the domain at location L. **b** Topology optimization results for the surface wave device problem. Material layout is presented in the same fashion as for the three-dimensional wire Bragg grating. (By Rupp et al. 2007)

distribution was obtained in the wave filter. By switching (on/off) the piezoelectric behavior, they were able to manipulate the propagation of elastic or acoustic waves in the proposed phononic device.

Besides the above 2D and 3D phononic waveguides and wave filters, topology optimization of 1D phononic waveguides and wave filters has also been studied. Evgrafov et al. (2008) presented a synthesis topology optimization design of tunable bi-material elastic wave-guides based on the gradient-based technique (i.e., MMA). Mechanically induced finite elastic pre-straining was proposed to design tunable elastic waveguides with predefined functional properties, such as displacements, periodic/non-reflecting boundary conditions, and external harmonic excitation. A 1D tunable Bragg filter and a 2D tunable elastic switch were presented and designed. By using time-domain-topology-optimization-based methods, Dahl et al. (2008) proposed systematic optimization design of 1D phononic band gap structures and pulse converting structures with possible applications in optical communication. The absorbing boundary conditions at both ends of a finite wave guide and the viscous dampers corresponding to the absorbing terms were considered in a time-integration-based mathematical model for the design domain. The linear material interpolation scheme was used to formulate the optimization problems and the gradient-based optimization algorithm. MMA was utilized to solve the optimization problem. An optimized 1D phononic band gap structure considering vibration-damping and an optimized pulse converting structure are shown in Fig. 6. Subsequently, Lazarov et al. (2011) researched the design of pulse shaping filters using Hilbert transform envelope extraction for pulse shaping and pulse delaying.

4.2 Wave attenuation

In order to improve the acoustic attenuation performance, both gradient- and non-gradient-based topology optimization techniques are used for design optimization of phononic crystal structures. Gradient-based topology optimization to improve acoustic attenuation performance of phononic crystal materials and structures is normally performed based on the inverse homogenization method. Lee and Kim (2009) used the FEM and the gradient-based topology optimization scheme (i.e., MMA) to implement topology optimization of the internal partitions in a muffler for maximizing the acoustical transmission loss at target frequencies. The topology optimization problem was formulated based on a material interpolation of the inverse density and the bulk modulus between two material phases and aimed to maximize the transmission loss with a constraint on the total number of rigid body elements that formed the partitions. Andreassen and Jensen (2014) presented a gradient-based topology optimization strategy combined with the Galerkin FE approach for design of a periodic composite with dissipative materials to maximize the

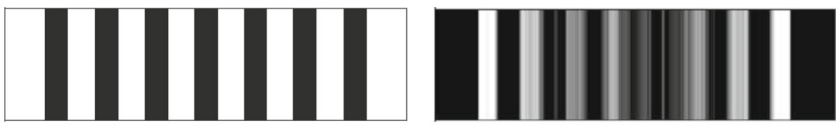


Fig. 6 Example of topology optimization of 1D phononic crystal devices: (**a**) a phononic band gap structure for vibration-damping purpuse, where the device is 20 cm long, the design domain in the device is 16 cm, white material is polymethyl methacrylate, black material is aluminum, and the excitation wave is a Gaussian wave packet with center frequency at 80 kHz and bandwidth 1 kHz; (**b**) a structure optmized for pulse conversion, where the length of device is 45 cm, the white material is fictious material with unit properties (E_1, ρ_1) = (1.0, 1.0), the black material is fictious material with properties (E_2, ρ_2) = (3.5, 2.0), and a pulse-like input excitation is used. (By Dahl et al. 2008)

loss/attenuation of propagating waves. This goal could be realized by optimizing the distributions of a stiff low loss and a soft loss material. The periodic unit cell was designed with high-damping-and-stiffness composites based on quasi-static conditions and the band gap phenomenon for the low and high frequencies, respectively. In communication technology, acoustic wave resonators are designed to realize attenuation. Matsuki et al. (2014) reported an optimal design method for locally resonant sonic material using the inverse-homogenization-based level set method. Based on this optimization method, the locally-resonant optimal sonic material could exhibit roughly a hundred-fold acoustic attenuation at desired frequencies; the optimized design provided excellent attenuation performance. An additional interesting observation from this work was that the combination of different optimal configurations achieved a wider frequency range of attenuation.

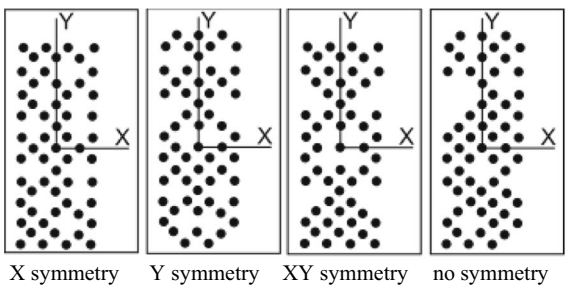
The multi-objective genetic algorithm has also been used for wave attenuation design. Herrero et al. (2009) used the multiple scattering theory and the epsilon variable multi-objective genetic algorithm to optimize sonic crystal attenuation properties by maximizing the attenuation level in a predetermined wide frequency range and minimizing deviation from the average attenuation value within the predetermined frequency range. As shown in Fig. 7, Herrero's team considered four vacancy-creation schemes for the design of sonic crystals. By using a strategy of multiple execution of the optimization algorithm, they obtained results of the four vacancy-creation schemes with high reliability. Using very similar vacancy-creation schemes, Romero-García et al. (2009) worked to improve the attenuation and focusing of phononic crystal arrays. Their team investigated the mechanism for creation of vacancies in a PnCs as a tool for examining interesting acoustic properties by means of the epsilon variable multi-objective evolutionary algorithm in conjunction with the MST method. Later, Romero-García et al. (2012) further reported the optimization of the distribution of vacancies in a 2D phononic crystal, with predetermined acoustic attenuation, by using multi-objective GA combined with the MST method. A quasi-order structure with inverse-designed scattering acoustical elements was thus theoretically created; it experimentally yielded both high and stable values of acoustic attenuation in the given range of frequencies.

4.3 Wave dissipation and transmission

In order to suppress wave propagation in a finite phononic crystal device, wave reflection or dissipation needs to be maximized, or wave transmission needs to be minimized. Jensen (2007) used the FEM and the gradient-based optimization method to address the three-phase-material distributions in a finite design domain to maximize the reflection or dissipation of elastic waves. As three different materials, one host material and two scattering and/or absorbing materials, were considered in the structure, a two-design-variable-based linear material interpolation scheme that had been implemented with two materials and with voids, as described in Bendsøe and Sigmund (2003), was utilized to express the element's properties:

$$\alpha(\mathbf{x}) = (1-x_1)\alpha_h + x_1((1-x_2)\alpha_1 + x_2\alpha_2) \tag{11}$$

in which α represents any of the properties (i.e., Young's modulus, density, Poisson's ratio, and damping coefficient).



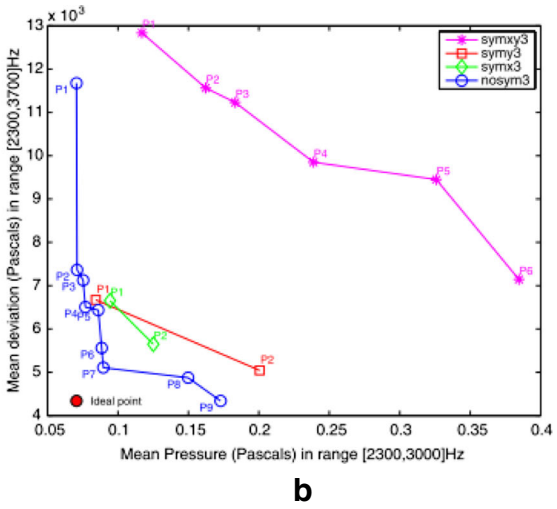


Fig. 7 Example of optimization of sonic crystal attenuation: (**a**) vacancy-creation schemes in a sonic crystal formed by isolated cylinders in a triangular array used as an acoustic barrier; (**b**) comparison of the best results for different symmetry constraints. "symxy3" denotes the XY symmetry-vacancy-based sonic crystal and its solutions obtained by including two times of XY symmetry solutions in the initial population and randomly generating the rest of the population. "symy3", "symx3", and "nosym3" are, respectively, the Y symmetry-, X symmetry-, and no symmetry-vacancy-based sonic crystals, and their solutions are obtained in a similar way as the solution of "symxy3". (By Herrero et al. 2009)

Subscript h, 1, and 2 represent, respectively, the host material, material 1 and material 2. Design field x_1 is an indicator of host material ($x_1 = 0$) or inclusion ($x_1 = 1$), and design field x_2 indicates the inclusion type 1 for $x_2 = 0$ ($x_1 = 1$) and type 2 for $x_2 = 1$ ($x_1 = 1$). Artificial damping was introduced to penalize intermediate design variables in the two design fields. Based on the power balance equations, two optimization problems were formulated to maximize the wave reflection and to maximize the wave dissipation. Both of the 1D and 2D periodic structures, as well as the two-phase and three-phase designs, were examined using the proposed topology optimization approach.

4.4 Self-collimation

Self-collimation of waves is a phenomenon where the wave propagates non-diffractively in the form of a narrow beam. Self-collimation in periodic structures was first studied in PtCs by Kosaka et al. (1999). Park et al. (2015) were the first to use topology optimization techniques for the optimal design of material distribution in a unit cell of a 2D phononic crystal that exhibited the desired self-collimation properties. As wave collimation is dictated by the shape of the equi-frequency contour (EFC), which is a curve connecting two-dimensional wave vectors of propagating modes for a selected frequency, an EFC must have some flat portion to realize self-collimation of waves. Hence, an optimization problem to maximize the curvature of an EFC with a constraint on the slope of the EFC related to the direction of collimation was formulated and it was solved using the modified-SIMP-based MMA method combined with the FEM. The representative results for self-collimation of PnCs are shown in Fig. 8, where the optimized unit cell layouts, and the corresponding EFCs, are shown at different target frequencies.

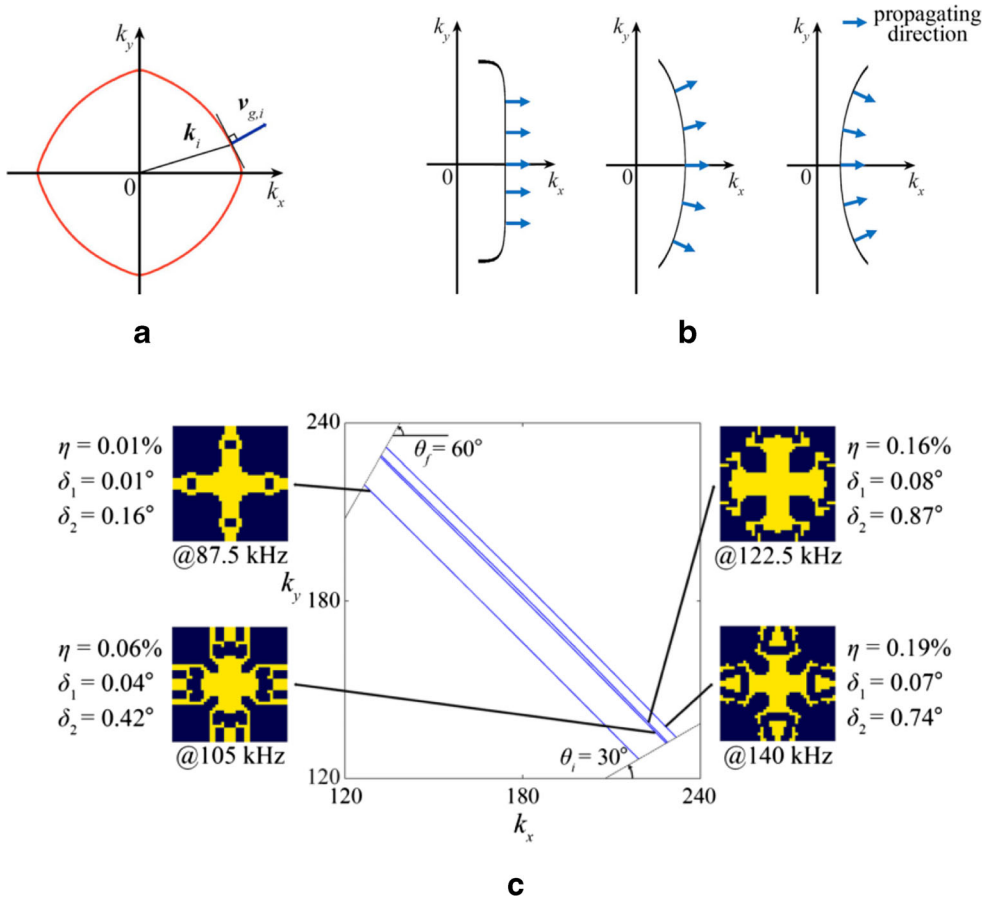


Fig. 8 Example of self-collimation of elastic waves: (**a**) an EFC at a typical frequency where k_x and k_y are, respectively, the wave vector components, $\boldsymbol{k}_i$ is a wave vector, and $\boldsymbol{v}_{g,i}$ is the group velocity perpendicular to the EFC but not necessarily parallel to $\boldsymbol{k}_i$; (**b**) wave diffraction patterns depending on the shape of EFCs, from *left* to *right*: a zero diffraction, normal diffraction, and anti-diffraction, where the arrows denote the directions of wave propagation in the wave vector space plane (k_x, k_y); (**c**) an optimized unit cell at different frequencies and the corresponding EFCs, where the incident wave spreading range of θ is between $\theta_i = 30°$ and $\theta_f = 60°$, η denotes the ratio of the final value of the objective function to the initial configuration, and δ_1 and δ_2 are defined as, respectively, the root mean square value and maximum absolute value of the differences between the direction of collimation and the desired direction of collimation. "@87.5 kHz" means the corresponding optimum unit cell obtained at the target frequency of 87.5 kHz, and so do the other three. (By Park et al. 2015)

4.5 Summary

According to the existing literature, topology optimization design of phononic crystal structures and devices have been successfully conducted to realize functionalities of interest, including waveguides and filters, wave attenuation, wave dissipation and transmission, and self-collimation. Extensive research has been carried out on the topology optimization design of phononic-crystal-based waveguides and filters and relatively less research has been devoted to studying the topology optimization design of phononic crystal structures for other functionalities. Both the unit-cell-based and finite-structure-based design domains are considered in the field of functional phononic crystal designs. Because of the usefulness of band gaps, topology optimization of a unit cell for maximum band gap width is necessarily conducted to find the best topological configuration of the unit cell that can be used repeatedly to form an effective waveguide or wave filter. Designing the functional phononic crystal devices in a finite domain has also been studied and proven to be an efficient means to achieve the desired functionality of the phononic crystal device, except that it may yield periodic-like or aperiodic structures.

Regarding the optimization techniques, both the gradient-based and non-gradient-based topology optimization techniques have been used in the topology optimization of functional phononic crystal structures. According to the number of papers that have been surveyed in this field, the GTO techniques are used more often than the NGTO techniques. Besides, single-objective topology optimization has been studied more than multi-objective topology optimization in this field. Similar to the situation in the design optimization of phononic band gaps, the non-gradient-based topology optimization technique (i.e. GA) has been used to solve the multi-objective topology optimization problems, e.g., distribution of vacancies in phononic waveguide structures. Obviously, in order to get effective desired functionalities, the underlying physics and mechanics of phononic crystal structures related to the specific functionality are required in the design optimization, and essential material properties and mechanisms should be formulated or approximated as accurately as possible when they are not explicitly given. The inverse homogenization scheme is proposed to approximate the material properties and mechanisms. In summary, three formulations have been used for the inverse homogenization scheme in the design of functional phononic crystal structures. These formulations include the linear material interpolation of the element's material properties, the modified SIMP method, and the material interpolation of the inverse density and bulk modulus. The inverse homogenization scheme is perfectly incorporated into the gradient-based topology optimization process.

Currently, 1D, 2D, and 3D phononic crystal structures have been studied, and one-phase, two-phase, and three-phase materials have been considered in these designs. However, the fabrication technologies used for these designs are still in a preliminary stage. More research should be devoted in this area in the future. It is also believed that more and more research will be conducted in the near future to design phononic crystal structures and devices that provide useful and promising functionalities.

5 Challenges and future research directions for design optimization of PnCs

This paper thoroughly examines topology optimization design methods and development trends for phononic band gap design and functional phononic crystal device design. The literature dealing with phononic band gaps is very extensive, while topics related to the design optimization of functional phononic crystal structures are relatively limited. As more of the underlying characteristics and properties are exploited in PnCs, more potential applications and functionalities can be designed for phononic crystal devices. However, because of the inherent complexity of PnCs (e.g., the challenges of multi-phase and multi-physics), analyzing, predicting, and designing the characteristics and performance of phononic crystal devices is difficult. Obviously, challenges remain in topology optimization of PnCs, but there is also great opportunity. Major challenges and future research directions of design optimization of PnCs are discussed in this section.

5.1 Challenges

Currently, much of the research on phononic crystals is based on intuition; then, theoretical and experimental tools are developed to realize the researchers' goals. It is usually time and resource consuming to perform the trial and errors needed to achieve the desired performance of a phononic crystal structure. Design optimization problems aimed at creating functional phononic crystal devices are likely to replace intuitive engineering approaches very soon. In order to perform design optimization of PnCs, several major challenges must first be addressed, including numerical analysis, design, and manufacturing, respectively. These challenges are discussed next.

(1) *Challenges in the analysis of wave propagation in PnCs*: In design optimization of phononic band gaps or functional phononic crystal structures, the dynamics of a periodic material is fully characterized by the application of Floquet-Bloch theory on a single representative unit cell, or on a finite design domain. Currently, simple lattice shapes (i.e., square and triangular lattices) and linear elastic materials have been employed to yield as large a phononic band gap width as possible. To date, only a

couple of complicated cases (e.g., asymmetric design domain and elastic materials with damping), are considered in the literature. It is believed that more research on nonlinear lattices, nonlinear elastic materials, complex wave formats (e.g., time dependent waves, omnidirectional waves, very low or high frequency waves), and multi-physics problems, will be introduced for the design optimization of phononic band gaps and novel phononic crystal engineering devices in the future. Existing wave propagation analysis approaches may not work with these new advances. Thus, relatively complex numerical approaches must be developed to enable analysis of wave propagation in those PnCs. The challenges in addressing the theoretical issues corresponding to the nonlinear lattices, nonlinear elastic materials, complex waves, and multi-physics, among other issues, should be adequately overcome first, and then the scalability and computational efficiency of the new numerical approaches can be addressed. In particular, the 3D structure, which is favored for practical applications, is a large-scale problem, and an efficient analysis solver is in strong demand. In addition, for design optimization of functional phononic crystal structures, even though the FEM is able to deal with many complex structures, the computation time for solving large-scale problems can be a big burden as the size of the discretization domain and the desired accuracy play a critical role in finite element analysis. Therefore, new challenges in the analysis of wave propagation in PnCs will include defining appropriate boundary conditions (i.e., wave absorbing boundary conditions) and constructing simplified sizable and comparable finite element models for the practical engineering problems.

(2) *Challenges in design optimization*: The first challenge in design optimization lies in the sensitivity analysis. On one hand, the complexity of the design engineering problems yields computational complexity in the sensitivity analysis. The multi-physics and multi-phase inherent in phononic crystal structures cause difficulties in formulating the design optimization problems of wave propagation in functional phononic crystal structures. The explicit relationships between the design variables and the desired performances of phononic crystal structures, as well as the corresponding sensitivities, are usually difficult to obtain, especially when the desired performances are implicitly defined in the elastodynamic equilibrium equations. Although this issue is not new in structural optimization problems and some of these problems can be solved by using the direct and adjoint differentiation methods, obtaining analytical performance functions can still be a big bottleneck in design optimization as accurate sensitivities of performance functions are very important in gradient-based optimization to ensure robust and efficient convergence. Inaccurate sensitivities can cause the optimizer to halt or to take a less direct route to the optimum that involves more iterations (Martins and Hwang 2013). On the other hand, the development of efficient computational algorithms used for sensitivity calculation is another issue that needs to be tackled for design optimization of large-scale problems such as phononic crystal-based systems. For instance, efficient sensitivity calculation is especially desired to compute the sensitivities of multiple eigenvectors and eigenvalues in multiple modes with respect to a large number of topological design variables. The computational efficiency of sensitivity analysis can become a great challenge in the design problems involving high dimensions and multiple material phases. The adjoint method, which is efficient as it only requires back-solves and therefore is significantly less expensive than the finite element analysis, has been extensively used in the literature (Jensen 2007; Dahl et al. 2008; Evgrafov et al. 2008). It is unfavorable when a very long time run is required to perform one time of finite element analysis and sensitivity calculation. Thus, more efficient sensitivity computation algorithms will be of fundamental importance for larger-scale and high-dimensional problems.

The second challenge in design optimization lies in optimization approaches as only a small number of optimization approaches have been presented for topology optimization of phononic band gaps and functional phononic crystal structures. As we stated in Sections 3.4 and 4.5, more topology optimization approaches such as the level set method, the Heaviside projection method, and the phase-field method, as well as other optimization algorithms such as multi-objective GTO methods and multi-objective heuristic methods, have great potential to be used to design phononic band gaps and functional phononic crystal structures. How to seamlessly incorporate these topology optimization approaches and optimization algorithms together into the design optimization of phononic band gaps and functional phononic crystal structures will be a big challenge, as the effectiveness and computational efficiency of these approaches should be investigated at first. Combining topology optimization approaches and heuristic algorithms, such as the Heaviside projection method in conjunction with the NSGA-II proposed by Hedayatrasa et al. (2016b), reveals the optimal topological configurations by exploring the strengths of each approach. Regarding designing large-scale phononic crystal-based structures and systems, since the existing optimization approaches often require numerous function evaluations, more efficient optimization techniques that yield less function evaluations and faster

convergence speed should be developed. Nonetheless, the efficiency and accuracy of the optimization techniques should be the most important consideration, as these techniques directly influence the required computational effort and the viability of the optimized design, specifically, its robustness and scalability.

(3) *Challenges in manufacturing*: Even though optimized PnCs with large complete band gaps, as well as optimized functional phononic crystal structures, have been demonstrated by means of theoretical calculations, it is still difficult to directly validate their results through experiments. Some of the optimized structures could be extremely difficult, or impossible, to manufacture. Difficulties associated with manufacturing for physical validation strongly limit the applications of these structures. In addition, the tolerance issue between the optimized structure and the manufactured structure can be a big influence on the experimental results. These factors could result in a structure whose performance is dissimilar to the one that has been designed and optimized. While experimental issues are outside the scope of this paper, the manufacturing process will be easier if the tolerance issues and manufacturing constraints are considered beforehand. New challenges arise when addressing the tolerance issues and modeling the manufacturing constraints.

5.2 Future research directions

In the future, the development of theoretical, computational, and experimental modeling techniques for PnCs will further guide the design optimization of phononic crystal materials and structures. Some future research directions in the area of design optimization of phononic crystal structures include, but are not limited, to the following.

(1) *Topology optimization of PnCs for refractive properties, particularly for negative refraction*. The refraction of waves can be tuned from positive to negative by designing the band structure and dispersion of waves in PnCs. The effects of negative refraction have become one of the most active topics in phononic crystal research. Both experimental and theoretical studies have been performed to examine the novel effects of negative refraction (Zhang and Liu 2004; Li et al. 2006; Farhat et al. 2010; Hladky-Hennion et al. 2011; Al-Lethawe et al. 2012), including wave focusing, imaging, flat lenses, etc. However, most of these novel effects are realized by propagation of acoustic waves in PnCs; only a few research studies have examined the negative refraction of elastic waves. This is mostly because the bi-refraction phenomenon can occur for elastic waves (e.g., combined in-plane and out-of-plane waves) and the case of acoustic waves with only one longitudinal polarization is much easier to deal with than that of elastic waves (Lu et al. 2009). Therefore, additional studies on negative refraction of elastic waves should be considered in the future. On the other hand, no research on design optimization of PnCs for negative refraction has yet been reported. Thus, future research is warranted on topology design optimization for promised negative refraction, as well as for the desired effects of negative refraction on functional phononic crystal structure design.

(2) *Topology optimization of defected PnCs for desired dispersion properties in spite of maximal band gaps, for example, tailoring the dispersion relation by placing defects in a phononic crystal*. PnCs containing point or line defects can produce remarkable features in band structures, such as wave localization in the point defect cavity, or wave propagation in the line defects. Thus, a wide range of functionalities, including wave filtering, guiding, and wave length multiplexing and demultiplexing, etc., can be achieved by taking advantage of these specific features. Kafesaki et al. (2000) created a straight wave guide by simply removing a row of cylinders for elastic waves in 2D PnCs. The phenomenon of wave guidance was due to the existence of extended linear defect modes falling in the band gap of the phononic crystal. Khelif et al. (2002) and Vasseur et al. (2011), respectively, created wave guides for acoustic and elastic waves in 2D PnCs by attaching a stub resonator (point defect) to the side of the structure and placing rods made of different magneto-elastic materials. These theoretical and experimental results indicate that the defects within PnCs can be designed and their corresponding resulting performances can be optimized by using optimization techniques. However, the research on topology optimization related to these defects has not yet been performed. Analogous to the topology optimization of defected PtCs (Jensen and Sigmund 2005), it is believed that this research direction will attract much attention in the future.

(3) *Design optimization of PnCs composed of materials that follow nonlinear elasticity theory*. Research on nonlinear phononic crystal structures (also granular phononic crystals) (Wang et al. 2013b; Ganesh and Gonella 2015) and the effects of damping and viscoelasticity (Oh et al. 2013; Frazier and Hussein 2015; Babaee et al. 2015) has drawn lots of recent attention, because PnCs composed of strongly nonlinear media can exhibit unique characteristics associated with solitary waves, bifurcation, and high tunability. Some fundamental issues related to

nonlinear phononic crystal structures and their dynamic behaviors should be further studied and addressed. New materials and structures with multifunctional properties (i.e., both structural and dynamic functionalities) can be designed by using optimization techniques.

(4) *Topology optimization of PnCs for multifunctional devices involving multi-physics*. Since practical engineering problems normally involve multi-physics, research on phononic crystal material has been extended to thermal conductivity (Yang et al. 2013; Maldovan 2013; Maldovan 2015), electrical and magnetic flow control (Matar et al. 2012; Lan and Wei 2013), phoxonic crystals with dual photonic and phononic bad gaps (Ma et al. 2014), and other physical areas (Anjos and Arantes 2015). However, no research on topology optimization of multifunctional phononic crystal devices involving multi-physics has been conducted yet, with the exception of the study by Dong et al. (2014d) that examined topology optimization of 2D phoxonic crystals for simultaneously maximizing complete photonic and phononic band gaps using the NSGA-II method. Decoupling multi-physics will be one of the fundamental issues for future modeling and analysis of functional structures. Besides pursuing the maximal structural performances and/or minimal cost, special attention should be paid to selecting proper constraints on geometries, mechanical failure, and physical responses related to different physical usages. In order to improve the manufacturability of optimized designs of multifunctional structures for practical engineering applications, manufacturing constraints should be considered simultaneously with the other constraints.

(5) *Topology optimization of phononic band gaps or functional phononic crystal devices under uncertainty.* This research direction has not yet been studied. However, uncertainties in waves, material elastic properties, periodicities, filling fraction, material damping and impedance, and other physical parameters should be considered, as a slight change in these parameters may yield a large change in the phononic band structure, which indicates different band gap widths and passing frequencies, as well as different structural performances. The computational methods for topology optimization in the presence of uncertainty have been well-developed in the field of homogeneous continuum structures (Chen and Chen 2011; Tootkaboni et al. 2012; Lazarov et al. 2012). Likewise, incorporated with the theories and applications of design under uncertainty (Youn et al. 2008; Hu et al. 2013; Jung et al. 2015), reliability-based topology optimization has been extensively studied (Kharmanda et al. 2004; Maute and Frangopol 2003; Jung and Cho 2004; Silva et al. 2010; Nguyen et al. 2011). Once some uncertainties that are sensitive to the phononic band structures are carefully studied, the same computational methods and techniques can be applied to phononic band gap design and design of functional phononic crystal devices in the future.

(6) *Shape and size optimization of PnCs for desired properties, as well as performances of interest*. This research topic is not new, as shape and size optimization has been used in phononic crystal bands to enhance gap properties. For example, Rohan and Miara (2006) performed shape optimization of the inclusions embedded in the matrix to maximize the gap length of the harmonic wave propagation in a 2D phononic crystal structure. Ponge et al. (2015) optimized the cavity length, phononic crystal and transducer positions to increase resonance and anti-resonance frequency shifts as well as the coupling coefficient in a tunable piezoelectric resonator. Open research topics surrounding the tuning of geometric parameters for desired properties or performance using shape or size optimization can be further investigated. New and promising designs of unit cells, or finite functional phononic crystal structures, can be easily achieved as shape and size optimization designs are relatively easier than that of topology optimization.

6 Conclusions

The purpose of this paper has been to provide a comprehensive review of current research examining (1) wave propagation analysis methods for mechanical waves in PnCs, (2) band gap design for PnCs, and (3) the use of topology optimization approaches for design of PnCs for functional applications. Generally, the design of the band gap of PnCs is conducted in the unit cell domain and follows an inverse homogenization formulation or binary optimization model and topology optimization procedure. Thus, both gradient-based and non-gradient-based topology optimization techniques, corresponding to the inverse homogenization formulation and binary optimization model, respectively, have been utilized to solve the optimization problems. The gradient-based topology optimization techniques where the inverse homogenization scheme is used have advantages in that they formulate the underlying material mechanisms of the multi-physical problems and require a relatively small number of function evaluations. In contrast, non-gradient-based topology optimization techniques (i.e., GA, MEGA, MOGA, and NSGA-II) require no gradient information but a large number of function evaluations. They are capable of dealing with multi-objective optimization problems, performing global search, providing binary results directly, and generating quasi-Pareto optimal solutions (i.e., NSGA-

II). They are easily implemented but their usage is limited due to the coarse mesh and the high computational cost.

Design of functional applications for phononic crystal structures and devices is performed in a partial or full structural domain with appropriate boundary conditions. These mostly comply with the inverse homogenization formulations and gradient-based topology optimization techniques. Because the functional application problems of phononic crystal structures and devices are normally complex and involve multi-physics, gradient-based topology optimization is often preferred, as it is capable of revealing the underlying mechanisms and produces reasonable designs with finer resolutions.

It is believed that the methodologies for topology optimization of phononic band gaps and functional devices reviewed in this paper will be of great importance to advanced multi-scale and multi-physical problems in the future.

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