An improved fast plane wave expansion method for topology optimization of phononic crystals

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A B S T R A C T

Phononic crystals (PnCs) are artificially made materials composed of periodically arranged structures capable of manipulating acoustic/elastic wave propagation characteristics. In this paper, an improved fast plane wave expansion method (IFPWEM) is developed to obtain the band structures of PnCs. In the method presented, the continuity of the algorithm has been improved by eliminating the jump discontinuity points as well as decreasing the number of wave vectors used. Implementing these changes results in increased computational efficiency when compared to the traditional fast plane wave expansion method (FPWEM). In order to increase the band gap width produced by the PnCs, an adaptive genetic algorithm is adopted to optimize the PnCs structural topology for in-plane wave mode (xy mode). The numerical results yielded from optimization of two-dimension (2D) PnCs with a symmetric square lattice microstructure verifies that the efficiency of the IFPWEM is significantly greater than the conventional FPWEM and finite element methods.

1. Introduction

Phononic crystals (PnCs) are composed of periodically arranged structures that allow for the creation of band gap regions, in which the propagation of acoustic or elastic waves is completely prohibited [1–11]. Sigalas and Economou [12] firstly presented the band structures of elastic waves propagating in a two-dimension (2D) periodic fluid-solid system in 1993. Since then, there has been a great deal of work devoted to the characterization of PnC band structures. Betsabe et al. [13] presented an experimental demonstration of an omnidirectional band gap formation in a finite multilayer composite composed of two elastic layers. Then in 2006, Lin et al. [15] experimentally obtained the reflection transfer function of a phononic band gap by using a single-quantum-well in a phononic cavity. Tan [14] presented a generalized eigenproblem with a hybrid matrix method for stable analysis of Floquet wave propagation in one-dimensional (1D) PnCs in 2010. Meanwhile, Liu and Fang [16] proposed the lumped-mass method for the band structure analysis of elastic wave propagation in a 1D PnC rod. Afterwards, Yudistira et al. [17] introduced the finite element method (FEM) to demonstrate the existence of non-radiative surface acoustic wave band gaps in 2D piezoelectric phononic crystals with holes. Meanwhile, Gao et al. [18] also investigated the band gap properties of a 2D local-resonant phononic crystal by the FEM with a homogenous matrix. Cao et al. [35] investigated the singularity of the Bloch theorem in a fluid/solid phononic crystal, in which a plane wave expansion method (PWEM) was used to calculate the band structure and transmission spectrum of the air/rigid system. Later, Cao et al. [36] also proposed a revised formulation of eigenproblem for phononic crystals, which significantly improves the convergence in band structure calculations. Based on Cao's researches, Quan et al. [20] developed a plane wave expansion method using a parallel shift scheme to evaluate the band gap formation in a 2D PnC with L-shape scatterers. Afterwards, the fast plane wave expansion method (FPWEM), which was proposed by Liu et al. in 2014, had been employed to investigate the band gap structures of PnCs with arbitrary or pixel scattering elements [21]. Besides the traditional pure PnCs above, the band structures of PnCs with multi-fields coupling materials, such as piezoelectric and piezomagnetic PnCs, had been investigated in [19,37–41].

In PnCs, the band structure characteristics are highly dependent on the topology of the constituent unit cells that make up the materials microstructure. The design and optimization of the PnC unit cell geometry has attracted a great deal of interest recently with the objective of creating structures capable of producing extremely wide band gap regions. Sigmund and Jensen [22] used a topology optimization method to design PnCs capable of exhibiting pure band gaps over specific frequency regions. Bilal and Hussein [23,24] presented a vacuum-soli-porous PnC, in which the band gap with a normalized width exceeded 60%. A 2D PnC with an arbitrarily asymmetric lattice
was also obtained by combining the genetic algorithm (GA) with the FEM [25]. Zhong et al. [26] maximized the band gap width in a PnC by using a GA combined with the fast plane wave expansion method (GA-FPWEM). Meanwhile, Liu et al. [21] applied a GA-FPWEM to the topology optimization of PnCs with square lattices. A bi-directional evolutionary inspired optimization method with a penalization parameter was also developed to achieve convergent optimal solutions for structures comprised of one or multiple materials [27]. Dong et al. [28,29] used the non-dominated sorting-based GA for optimal PnC design which yielded both large band gap width and as well as a reduction in overall mass. Li et al. [30] recently developed a bi-directional evolution based structure optimization algorithm combined with the homogenization method to yield a maximum band gap width between the two adjacent bands in a square unit cell.

Although past researches have been conducted with the objective of optimizing PnC topology utilizing various iterative methods, there remains a lot of works need for further investigation and improvement. For instance, although the topology optimization of PnCs based on the FEM has high accuracy, its efficiency is extremely low which causes the optimization procedure is very time-consuming. The FPWEM is proposed to improve the calculation efficiency while guaranteeing the necessary computational accuracy. But the FPWEM also has drawbacks, which need to be eradicated. If the individual components of the unit cell are highly contrasting, the continuity of the interfacial material boundaries is poor. It means that the concurrent jump discontinuities (or the jump discontinuity points) exist at the boundaries of different materials. In order to ensure the calculation accuracy, the number of wave vectors considered for each band gap needs to be substantial in size. The need for an increase in the number of wave vectors used during computation means that the efficiency of the FPWEM is significantly reduced. In this paper, the IFFPWE model is introduced for calculating band structures of PnCs. Based on the Lauren inverse theorem, By eliminating the jump discontinuity points on the boundaries of different materials, the continuity of algorithm has been improved, and the number of wave vectors used for the band structure analysis is decreased. Thus, compared with the FPWEM, the IFFPWE model can achieve a much higher computational efficiency without loss of precision. Moreover, the GA optimization process alone is not capable of generating an optimal unit cell topology using conventional settings. Thus, the iteration times of conventional GAs can be considerable. Similarly, the adaptive genetic algorithm (AGA), which can generate the optimal unit cell topology in the early stages of the optimization process, is also introduced to reduce the overall iteration times required and improves the convergence of GA. In short, an adaptive genetic algorithm is implemented alongside the improved fast plane wave expansion method (AGA-IFPWEM) in pursuit of the optimal PnC design for the in-plane elastic wave attenuation.

The rest of the paper is organized as follows. In Section 2, the IFFPWE model for topology optimization of PnCs is detailed in Section 3. In Section 4, three numerical examples are employed to investigate the efficiency and effectiveness of the proposed 2D AGA-IFPWEM model. Conclusions are then presented in Section 5.

2. Improved fast plane wave expansion method

2.1. Elastic wave equation

Based on the elastic dynamics theory, the wave propagation in a three-dimensional inhomogeneous elastic medium is governed by

\[
\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x} (\lambda \nabla u) + \nabla \cdot (\mu (\nabla u + \frac{\partial u}{\partial x})),
\]

(1)

\[
\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial y} (\lambda \nabla u) + \nabla \cdot (\mu (\nabla u + \frac{\partial u}{\partial y})),
\]

(2)

\[
\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial z} (\lambda \nabla u) + \nabla \cdot (\mu (\nabla u + \frac{\partial u}{\partial z})).
\]

(3)

where \( \rho \) is the material density, and the Lamé coefficients are denoted by \( \lambda \) and \( \mu \). The displacement vector is written as \( u = (u_x, u_y, u_z)^T \), and its divergence is defined as \( \nabla \cdot u = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \).

Assuming the propagating elastic waves are constrained within \( x \)-plane, such that, \( \partial u/\partial z = 0 \). The resulting elastic wave equations can then be expressed as

\[
\rho \frac{\partial^2 u_x}{\partial t^2} = \frac{\partial}{\partial x} (\lambda \nabla u_x) + \nabla \cdot (\mu (\nabla u_x + \frac{\partial u_x}{\partial x})),
\]

(4)

\[
\rho \frac{\partial^2 u_y}{\partial t^2} = \frac{\partial}{\partial y} (\lambda \nabla u_y) + \nabla \cdot (\mu (\nabla u_y + \frac{\partial u_y}{\partial y})),
\]

(5)

\[
\rho \frac{\partial^2 u_z}{\partial t^2} = \frac{\partial}{\partial z} (\lambda \nabla u_z) + \nabla \cdot (\mu (\nabla u_z + \frac{\partial u_z}{\partial z})).
\]

(6)

Combining Eq. (4) and (5) results in the coupled in-plane equation (governing \( xy \) mode), and Eq. (6) can be used to describe the out-of-plane equation (governing \( z \) mode).

2.2. Fast plane wave expansion method

Periodic variations of material properties, such as elastic constants and mass densities, are intrinsic properties associated with PnCs. In a PnC, the material parameters (\( \rho \), \( \lambda \), and \( \mu \)) are periodic functions of the spatial coordinate \( r \). Based on the spatial coordinate \( r \), the characteristic of any pixel (point location) in the unit cell can be calculated by its location in reference to the center pixel (illustrated in Fig. 1). The Fourier series expansion of material constants at arbitrary spatial locations is then obtained to quantify these spatially varying material properties. In Eq. (7) below, \( g \) denotes the material parameter as a function of spatial location. The Fourier series expansion of material constant \( g \) can be written as

\[
g(r) = \sum_G g(G) e^{G \cdot r},
\]

(7)

where \( g(G) \) is a Fourier coefficient and can be expressed as

\[
g(G) = \frac{1}{S} \int_S g(r) e^{-G \cdot r} d^d r.
\]

(8)

where \( S \) and \( G \) are the unit cell area and the reciprocal vector, respectively.

Fig. 1. The structure of phononic crystal in which the material parameter of the pixel \( P \) can be calculated by the center pixel \( P_0 \) and the spatial coordinate, \( r \). Note that in Fig. 1, the black and white represent lead and epoxy resin, respectively.
Assuming that $P_0$ is a set of pixel elements filled with lead (Pb) in the unit cell, the Fourier transformation of the material constant $g_0$ at the unit cell $(P_i \in P_0)$ is defined as

$$g_0(G) = \begin{cases} g_0 + (\bar{G}_i - \bar{G}_0), & G = 0 \\ (\bar{G}_i - \bar{G}_0)P(G), & G \neq 0 \end{cases}$$  

(9)

In Eq. (9), $g_A$ and $g_B$ are the material constants of lead and epoxy resin, respectively and $f = (1/N^3)$ is the ratio of a pixel in the unit cell. $P(G)$ is the structure function which is defined as

$$P(G) = f \sin c \left( \frac{G_i}{2N} \right) \sin c \left( \frac{G_i}{2N} \right)$$  

(10)

where $a$ is the lattice constant of unit cell and $(G_x,G_y)$ are components of reciprocal vector $G$. Finally, $N$ is used to denote the specific pixel number/location in the spatial domain.

According to the spatial reference, the Fourier transformation of any pixel $(P_i \in P_0)$ filled with lead can be calculated as

$$g_i(G) = g_0(G)e^{iG}r.$$  

(11)

The Fourier transformation of the spatially variant material constants is expressed as

$$g(G) = \sum_{r \in P_0} g_i(G) = \sum_{r} g_i(G)\delta(r) = g_0(G)\sum_{r} e^{iG} r \delta(r),$$  

(12)

where $\delta(r)$ is the material distribution of the unit cell which can be defined as

$$\delta(r) = [\delta(r_1), \delta(r_2), \ldots, \delta(r_N)] = \begin{cases} 1 & P_i \in P_0 \\ 0 & \text{other} \end{cases}$$  

(13)

where $r_k$ denotes the center location of the $k$th pixel and $L$ is the total number of pixels in the unit cell.

Assuming that $e(G) = [e^{iG_1}, e^{iG_2}, \ldots, e^{iG_N}, \ldots, e^{iG_N}]$, Eq. (12) can be rewritten in its equivalent form as

$$g(G) = g_0(G) e(G) \cdot \delta(r).$$  

(14)

Based on the Bloch theorem, the displacement field, $u$, can be defined as

$$u(r, t) = e^{i(k \cdot r - \omega t)} u_k(r),$$  

(15)

where $k$ is the Bloch wave vector which is restricted to the first irreducible Brillouin zone. The Fourier series expansion of $u_k(r)$ can be expressed as

$$u_k(r) = \sum_{G} e^{iG \cdot r} u_k(G')$$  

(16)

and inserting Eq. (16) into Eq. (15), the displacement $u$ is readily obtained as

$$u(r, t) = e^{-i\omega t} \sum_{G} e^{iG' \cdot r} u_k(G').$$  

(17)

Substituting Eqs. (14) and (17) into Eqs. (4), (5) and (6), the eigenproblem system of equations for the PnCs are expressed as

$$\omega^2 \sum_{G} \rho(G'' - G') u_k^{G'} + \sum_{G} [\mu(G'' - G') (k + G'), (k + G'')] + \mu(G'' - G') (k + G'), (k + G'')] + 2(k + G') (k + G'')] u_k^{G'} + \sum_{G} [\mu(G'' - G') (k + G'), (k + G'')] + \mu(G'' - G') (k + G'), (k + G'')] u_k^{G'}$$  

(18)

Based on the spatial coordinate $r$, the material constant of any pixel in the unit cell is obtainable based on its location in reference to the center pixel. Thus, the structural properties of the unit cells at arbitrary distributions can be readily obtained. The PWEM is a conventional method for band structure calculations of PnCs with regular shaped scatterers, such as circular, rectangle and etc. Compared to the PWEM, the FPWEM can analyze band structures of PnCs with arbitrarily shaped scattering elements. However, if the components of the unit cell contrast greatly, the continuity of the interfacial material boundaries is hindered and the efficiency of the FPWEM is reduced. To overcome this problem, an improved fast plane wave expansion method (IFPWE) will be proposed to improve the computational efficiency.

2.3. Improved fast plane wave expansion method

From Eq.'s (4), (5) and (6), $g$ (which expresses the material parameters $\rho, \lambda, \mu$ and $\partial u/\partial r$) are piecewise continuous, interstitially smooth and bounded periodic functions, in which the concurrent jump discontinuities (or the jump discontinuity points) exist at the boundaries of different materials. However, the function, $h_0 = g - \partial u/\partial r$, is continuous along the material boundaries. According to the Lauren inverse theorem, by eliminating the contact discontinuity points when solving for $h_0$, a continuous function can be obtained across these boundaries. The Fourier coefficient of $h_0$ can be defined as

$$h_0 = \sum_{n=-\infty}^{n=M} \sum_{m=-\infty}^{m=M} g_{-n-M} e^{inx},$$  

(21)

where $g_{nm}$ is the Fourier coefficient of $g$.

The Fourier series expansion of the function $h(x)$ can be expressed as

$$h(x) = \sum_{n=-\infty}^{n=M} \sum_{m=-\infty}^{m=M} \sum_{n=-\infty}^{n=M} \sum_{m=-\infty}^{m=M} [f^n_{-m-M} g_{-n-M}] e^{inx},$$  

(22)

or, when combined with the limit theory, the function $h(x)$ can also be written as

$$h(x) = \lim_{N \to \infty} \sum_{n=-N}^{n=M} \sum_{m=-N}^{m=M} [f^n_{-m-M} g_{-n-M}] e^{inx}.$$  

(23)

For practical applications and without loss of generality, Eq.’s (22) and (23) are rewritten as

$$h^{(M)}_n = \sum_{m=-M}^{m=M} [f^n_{-m-M} g_{-n-M}] e^{inx},$$  

(24)

$$h^{(M)}(x) = \sum_{n=-M}^{n=M} h^{(M)}_n e^{inx}.$$  

(25)

The material parameters and displacements are periodic functions of space such that, $r = (x,y,t)$. Substituting Eq.’s (7) and (15) into Eq.'s (4), (5) and (6), the eigenproblem system of equations are expressed as
\[
\sum_{G} \rho(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r})) = \frac{d}{dt}(2\sum_{G} \rho(G)e^{G}\epsilon), \\
+ \sum_{G} j(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r})) + \sum_{G} j(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r})), \\
+ \frac{d}{dy}(\sum_{G} \rho(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r}))),
\]

(26)

\[
\sum_{G} \rho(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r})) = \frac{d}{dt}(2\sum_{G} \rho(G)e^{G}\epsilon), \\
+ \sum_{G} j(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r})) + \sum_{G} j(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r})), \\
+ \frac{d}{dx}(\sum_{G} \rho(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r}))),
\]

(27)

\[
\sum_{G} \rho(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r})) = \frac{d}{dt}(2\sum_{G} \rho(G)e^{G}\epsilon), \\
+ \sum_{G} j(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r})) + \sum_{G} j(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r})), \\
+ \frac{d}{dy}(\sum_{G} \rho(G)e^{G}\epsilon^{2}(\epsilon_{k}^{G\tau(-\text{rot})u}^{G}(\mathbf{r}))),
\]

(28)

From Eqs. (26), (27) and (28), it is apparent that \( u_{k}(\mathbf{r}) \) is also a periodic function in the spatial coordinate, \( r \). Substituting Eq. (16) into Eq.'s (26), (27) and (28), the eigenproblem equations are rewritten as

\[
-\omega^{2} \sum_{G} \rho(G)e^{G}\epsilon^{2} \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}) = \left([2\sum_{G} \rho(G)e^{G}\epsilon] \right) + \sum_{G} j(G)e^{G}\epsilon \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \sum_{G} j(G)e^{G}\epsilon \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \left(\sum_{G} \rho(G)e^{G}\epsilon \right) \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \left(e^{2\omega^{2}} \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0})\right),
\]

(29)

\[
-\omega^{2} \sum_{G} \rho(G)e^{G}\epsilon^{2} \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}) = \left([2\sum_{G} \rho(G)e^{G}\epsilon] \right) + \sum_{G} j(G)e^{G}\epsilon \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \sum_{G} j(G)e^{G}\epsilon \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \left(\sum_{G} \rho(G)e^{G}\epsilon \right) \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \left(e^{2\omega^{2}} \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0})\right),
\]

(30)

\[
-\omega^{2} \sum_{G} \rho(G)e^{G}\epsilon^{2} \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}) = \left([2\sum_{G} \rho(G)e^{G}\epsilon] \right) + \sum_{G} j(G)e^{G}\epsilon \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \sum_{G} j(G)e^{G}\epsilon \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \left(\sum_{G} \rho(G)e^{G}\epsilon \right) \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \left(e^{2\omega^{2}} \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0})\right),
\]

(31)

eigenproblem system can be expressed as

\[
-\omega^{2} \sum_{G_{0}} \left((2\rho(G_{0})e^{G_{0}} + j(G_{0})e^{G_{0}}) \right) u_{k}^{G_{0}} (G_{0}) = \left([2\sum_{G} \rho(G)e^{G}\epsilon] \right) + \sum_{G} j(G)e^{G}\epsilon \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \sum_{G} j(G)e^{G}\epsilon \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \left(\sum_{G} \rho(G)e^{G}\epsilon \right) \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \left(e^{2\omega^{2}} \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0})\right),
\]

(32)

Finally, the formulation of the eigenproblem of PnCs is revisited by the IPPWEM which can be defined as

\[
\sum_{G_{0}} \frac{1}{\rho(G_{0})e^{G_{0}} (G_{0})} \left([2\sum_{G} \rho(G)e^{G}\epsilon] \right) + \sum_{G} j(G)e^{G}\epsilon \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \sum_{G} j(G)e^{G}\epsilon \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \left(\sum_{G} \rho(G)e^{G}\epsilon \right) \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0}), \\
+ \left(e^{2\omega^{2}} \sum_{G_{0}} e^{G_{0}G} u_{k}^{G_{0}} (G_{0})\right).
\]

(33)

The jump discontinuity points are still present in the eigenproblem equations above. However, based on the Laurent inverse theorem, substituting Eq.'s (14) and (24) into Eq.'s (29), (30) and (31), the
Based on the Laurent inverse theorem, by eliminating the jump discontinuity points at the boundaries of different materials, the continuity of the boundaries is significantly improved and the formulation of the eigenproblem has been revised. Compared to the FPWEM, the IFPWEM with a lower number wave vectors can achieve the same calculation accuracy, and thus, the calculation efficiency of the IFPWEM is much higher than that of the FPWEM.

2.4. Accuracy of the improved fast plane wave expansion method

The IFPWEM and the FPWEM are used to analyze the band structure of the 2D PnC with the FEM result considered as the reference value. The calculations are carried out in MATLAB R2009a on a 3.30 GHz Xeon(R) CPU E3 1230 v3. The 2D unit cell and its corresponding Brillouin zone are shown in Fig. 2.

The material parameters of the 2D PnC above are listed in Table 1 below. From Table 1, the elastic constants in the steel-epoxy resin 2D PnC are quite different which means that it possesses large elastic mismatch [35,36].

The band structures of the PnC calculated with the IFPWEM, the FPWEM and the FEM, and the band gaps obtained by the proposed methods are illustrated in Fig. 3. The resulting band gap frequency ranges and overall computation times are listed in Table 2.

From Fig. 3(a), only 81 wave vectors are employed for the band structure analysis by the IFPWEM, its band structure (the green dots) is approximate to the result (the red dashed line) yielded with the FPWEM by 625 wave vectors. Moreover, both of the results calculated with the IFPWEM and the FPWEM are a fine alternative to that of the FEM (the black solid line), it means that the accuracy of the IFPWEM is enough for calculating band structures of 2D PnCs, even in the large elastic mismatch [35,36].

From Table 2, the band gap range of the 2D PnC calculated by the IFPWEM, is [15.367 kHz, 24.983 kHz]. Compared with the result yielded with the FPWEM ([15.283 kHz, 24.802 kHz]), the relative error is less than 1%. Moreover, both of these results obtained by the IFPWEM and the FPWEM are very close to the result obtained through the FEM model. This means that the IFPWEM model can be regarded as a valid alternative to the FEM model for band gap analysis in 2D PnCs. The computing time of the IFPWEM model is 3.58 s which is much shorter compared to that of the FPWEM (57.49 s) and the FEM (85.12 s) models. Thus, the calculation efficiency of the IFPWEM is much higher than either the FPWEM or the FEM.

3. Phononic crystals topology optimization

A pure band gap region is a significant intrinsic characteristic of PnCs. Within the band gap region, the propagation of the elastic waves with frequencies that lie within the band gap frequency range are completely prohibited. This means that PnCs have promising applications in noise filtering and elastic/acoustic wave attenuation. The filling ratio, lattice parameter and scattering element shape all significantly affect the band gap structure characteristics. Topology optimization methods, combined with an adaptive genetic algorithm (AGA), solves the problem of poor convergence in the conventional GA, and obtains PnCs with broad band gaps ranges.

\[
\omega^2 \sum_{G_0} \left[ \frac{1}{\mu_i(G' - G_0)} \frac{1}{\varepsilon(G' - G_0)} \frac{1}{\delta(r)} \right] u_i^*_k(G_0) \\
= \sum_{G_0} \left[ \frac{1}{\mu_i(G' - G_0)} \frac{1}{\varepsilon(G' - G_0)} \frac{1}{\delta(r)} \right] (k + G_0) \cdot (k + G') u_i^*_k(G_0) \\
+ \sum_{G_0} \left[ \frac{1}{\mu_i(G' - G_0)} \frac{1}{\varepsilon(G' - G_0)} \frac{1}{\delta(r)} \right] (k + G_0) \cdot (k + G') u_i^*_k(G_0)
\]

(37)

Table 1
Material parameters of the steel-epoxy resin 2D PnC.

<table>
<thead>
<tr>
<th>Material</th>
<th>Steel</th>
<th>Epoxy resin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density: (\rho_{\text{steel}})</td>
<td>7780 (kg/m(^3))</td>
<td>1180 (kg/m(^3))</td>
</tr>
<tr>
<td>Elastic Modulus: (E_{\text{steel}})</td>
<td>21.06 × 10(^9) (Pa)</td>
<td>4.35 × 10(^9) (Pa)</td>
</tr>
<tr>
<td>Shear Modulus: (G_{\text{steel}})</td>
<td>8.10 × 10(^9) (N/m(^2))</td>
<td>1.59 × 10(^9) (N/m(^2))</td>
</tr>
</tbody>
</table>

3.1. The optimization problem of band gap

The optimization objective employed is to maximize the band gap width, where the objective function can be expressed as

\[
\text{Maximize: } \text{BG}(\Sigma) =: \min_{k} a_{\Sigma,k} - \max_{k} a_{\Sigma,k}, \quad (38)
\]

where \(\text{BG} \) denotes the effective band gap width for the in-plane wave mode, \(a_{\Sigma,k} \) denotes the \(n\)-th eigenfrequency of the PnCs constitutive equations, \(\Sigma\) denotes the topological distribution of the unit cell, and \(n\) is the serial number of bands.

In this paper, only 2D bi-component PnCs with a square lattice configuration are considered. The design of PnCs transforms into the distribution of material in a unit cell. The unit cell is divided into 10 × 10 pixels (see Fig. 4). A quarter of which is taken into consideration when the unit cell is symmetric about \(x\) and \(y\) axis. The values 0 and 1 which respectively represent elements filled with epoxy resin and lead, are distributed randomly for each pixel.

The design variable \(x\), is defined as

\[
x = \begin{cases} 
1 & x \in P_1 \\
0 & x \notin P_1 
\end{cases}
\]

(39)

where \(P_1\) and \(P_0\) are the pixels filled with lead and epoxy resin, respectively.

3.2. Adaptive genetic algorithm

In the GA, the crossover probability directly affects the convergence of an optimization problem. The excessive crossover probability may prematurely discard the individuals with high fitness values. In contrast, the optimization process becomes very slow when the crossover probability is too small [31,32]. In a AGA, the crossover probability is updated according to the fitness to overcome this inherent drawback. When an individual’s fitness is higher than the average fitness, a small crossover probability is assigned to retain the individual in the population carried over to the next generation. On the contrary, if
an individual's fitness is lower than the average fitness, a high crossover probability is assigned to eliminate the individual. The adaptive crossover probability $P_c$ can be defined as

$$P_c = \begin{cases} 0.9 \frac{f_{\text{max}} - f}{f_{\text{max}} - T}, & f \geq T \\ 0, & f < T \end{cases}$$

(40)

where $f$, $T$ and $f_{\text{max}}$ are the individual fitness, the average fitness and the maximum fitness of the population, respectively.

In the GA, the mutation probability can prevent the optimization process from locking into the local optimum. When the mutation probability is big enough, genetically diverse offspring can be created which avoids the chance of choosing the locally optimal solution. If the mutation probability is exceedingly large however, the optimization process can be unstable [33,34]. In the AGA, the mutation probability is determined by the previous fitness values. If the adaptability of the generation is big enough, the mutation probability is small, otherwise, the mutation probability is high. The adaptive mutation probability, $P_m$, is expressed as

$$P_m(n) = P_{mn} + \lambda \left( P_{mn+1} - P_{mn} \right)$$

(41)

where $P_{mn}(n)$ and $P_{mn+1}(n+1)$ are the mutation probabilities of the $n$-th and $(n+1)$-th generations, respectively. $\Delta_n$ is the difference operator, which can be expressed as

$$\Delta_n(\alpha) = \sum_{i=0}^{n-1} \sum_{j=1}^{N_p} \left( f_{i,j}(x) - f_{i-1,j}(x) \right)$$

(42)

where $0 \leq \lambda < 1$ and $f_k$ is the individual fitness of the $k$-th generation.

### 3.3. Optimization procedure

The optimization procedure is shown in Fig. 5. The detailed procedures are as follows.

1. **Initialization:** Initialize the parameters, such as the population size, the iterative times, etc. Calculate the reciprocal vector $G$, the material constant $g_0$ and the structural parameter $e(G)$ which are used for the IFPWEM.

2. **Create initial population:** Considering the symmetry of unit cell, only 1/4 unit cell (see Fig. 4) needs to be initialized. The genes of the initial chromosomes are generally assigned randomly as 1 or 0. The initial population with $N_p$ chromosomes can be defined as

$$f_{\text{arm}} = \{X_1, X_2, \ldots, X_{N_p}\}$$

(43)

3. **Crossover operation:** Mate individuals in the selection pool randomly to create two offspring, which are used to replace their parents. $a$ is defined as a random number between 0 and 1. When $a$ is less than the adaptive crossover probability, $P_c$, the crossover operation is carried out. $b$, which is either 1 or 2, is created to determine the crossover mode. If $b=1$, the horizontal crossover mode is selected. Otherwise, the vertical crossover

![Fig. 3. (a) Band structures calculated with different methods, and the band gaps obtained from (b) the IFPWEM, (c) the FPWEM and (d) the FEM models. Note: The shaded areas represent the frequency regions occupied by band gaps.](image)

![Fig. 4. Discrete structure of unit cell.](image)
mode is selected. Values of 0 and 1 are created randomly to label the gene positions, and the chromosomes exchange their genes at the positions with the value 1. Thus, the new population is expressed as

\[ \text{newfarm} = \{X_1^1, X_2^1, \ldots, X_j^1, \ldots, X_m^1\}. \] (44)

(iv) Increase the population size: Combine the population of the parent with the population of the offspring to enlarge the overall population size. The merged population can be expressed as

\[ \text{Farm} = \{\text{farm, newfarm}\}. \] (45)

(v) Evaluation (fitness) check: First, the band structures of PnCs are calculated with the IFPWEM. The band gap width is then used to define the fitness of individual. If no band gap exists, a small value (0.01) is assigned as the fitness value to avoid the randomly generated individual from being prematurely eliminated in the initial stage of optimization.

(vi) Selection operation: Based on the elitist selection strategy, \( c \) and \( c' \), which are between 1 and \( 2 \times N_p \), are created randomly for the double-random-paired competition. By comparing the fitness of each of the two individuals, \( N_p \) chromosomes are selected to construct a new mating pool.

(vii) Mutation operation: Mutate each chromosome with the adaptive mutation probability \( P_m \). \( d \), which is between 0 and 1, is a

![Fig. 5. Flowchart of optimization procedure.](image1)

![Fig. 6. (a) The initial unit cell and (b) its corresponding band structure.](image2)

<table>
<thead>
<tr>
<th>Material parameters of PnCs.</th>
<th>Lead (Pb)</th>
<th>Epoxy</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Density:</strong> ( \rho_{\text{Pb}} = 11600 \text{ (kg/m}^3) )</td>
<td>( \rho_{\text{Epoxy}} = 1180 \text{ (kg/m}^3) )</td>
<td></td>
</tr>
<tr>
<td><strong>Elastic Modulus:</strong> ( E_{\text{Pb}} = 4.20 \times 10^{10} \text{ (Pa)} )</td>
<td>( E_{\text{Epoxy}} = 4.43 \times 10^{10} \text{ (Pa)} )</td>
<td></td>
</tr>
<tr>
<td><strong>Shear Modulus:</strong> ( G_{\text{Pb}} = 1.49 \times 10^{10} \text{ (N/m}^2) )</td>
<td>( G_{\text{Epoxy}} = 1.59 \times 10^{10} \text{ (N/m}^2) )</td>
<td></td>
</tr>
</tbody>
</table>
random number. If \( d \) falls within the interval \([0, P_m]\), the gene switches to its opposite (1 changes into 0 or 0 changes into 1).

(viii) Convergence check: Repeat steps (iii) to (vii) until the truncation criterion is satisfied.

4. Results and discussions

Three numerical examples are employed to 2D bi-component PnCs with square lattice geometries for in-plane wave mode. The material parameters are listed in Table 3 below.

4.1. The effectiveness and efficiency of the proposed method

The unit cell, which is filled with a random distribution of lead or epoxy resin, is regarded as the initial unit cell for the optimization. The initial unit cell and its corresponding band structure are shown in Fig. 6. The population size is 50, and the number of interactions is set to 100.

The results obtained with the GA-FPWEM and the AGA-IFPWEM methodologies are illustrated in Figs. 7 and 8, respectively and the

<table>
<thead>
<tr>
<th>Method</th>
<th>Iterations</th>
<th>Population</th>
<th>Optimum (kHz)</th>
<th>Band gap (kHz)</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GA-FPWEM</td>
<td>100</td>
<td>50</td>
<td>20.164</td>
<td>[38.282, 58.446]</td>
<td>1.0137×10^6</td>
</tr>
<tr>
<td>AGA-IFPWEM</td>
<td>100</td>
<td>50</td>
<td>20.641</td>
<td>[38.627, 59.268]</td>
<td>5.6952×10^4</td>
</tr>
</tbody>
</table>

Fig. 7. The results yielded by the GA-FPWEM: (a) the optimized unit cell topology, (b) the phononic crystal microstructure and (c) the band structure.

Fig. 8. The results obtained by the AGA-IFPWEM: (a) the optimized unit cell topology, (b) the phononic crystal microstructure and (c) the band structure.

Fig. 9. Initial unit cells with different shapes of scatterers including: (a) square scatterer (b) cross scatterer, and (c) ring scatterer.

Fig. 10. The evolutionary curves of the optimization problem.
results are listed in Table 4.

From Figs. 7 and 8, the optimal structures obtained by the GA-FPWEM and the AGA-IFPWEM models are almost identical. The band gap yielded with the AGA-IFPWEM is [38.627 kHz, 59.268 kHz]. Compared to the result obtained by the GA-FPWEM ([38.282 kHz, 58.446 kHz]), the discrepancy is about 1%.

According to Table 4, the AGA-IFPWEM only spends $5.6952 \times 10^4$ s for 100 iterations while the GA-FPWEM costs $1.0137 \times 10^6$ s. The GA-FPWEM model has to expand 625 wave vectors for each calculation. For the AGA-IFPWEM model, the number of wave vectors used for the band structure analysis decreases from 625 to 81. This significantly reduces the overall computation time, and thus, the efficiency of the AGA-IFPWEM model is much higher than for the GA-FPWEM approach.

4.2. Convergence of the proposed method

In this section, three different initial unit cell shapes are used to verify the convergence of the AGA-IFPWEM model. The structures of initial unit cells are shown in Fig. 9.

The initial unit cells are divided into $10 \times 10$ grids and the length of the chromosome for each unit cell is 100. The population size is 50, and the number of iterative steps is 100. The evolutionary curves of three different initial unit cells are illustrated in Fig. 10.

From the results illustrated in Fig. 10, it's apparent that the optimal values of three different initial unit cells eventually converge to the
same value. However, the convergence speeds are different for each of the three initial cases. For the square scatterer, the optimized result was obtained quickly at the 5th iteration. Meanwhile, the optimal solutions of the cross scatterer and ring scatterer were achieved at the 38th and the 9th iterations, respectively. As the unit cell containing the square scatterer is similar to the optimized result (see Fig. 8), the optimization process with the square scatterer is much faster than the other two unit cells.

4.3. The topology optimization of PnCs

The unit cell is divided into 20×20 grids, and the length of chromosome for each unit cell is 400. Lead and epoxy resin are randomly distributed amongst each pixel. The population size is 100, and the number of iterative steps is set to 250. The results of the fitness values are shown in Fig. 11.

From Fig. 11, with the increase in the generation number, the fitness value of the individual also increases. When the generation number is over 143, the fitness value tapers off asymptotically. This means that the optimization process has achieved convergence where the maximum fitness value attained is 25.542 kHz.

The optimization results at the different generation numbers are shown in Fig. 12. In each case, the left and right subfigures respectively represent the phononic crystal and the corresponding band gap structures.

From Fig. 12(a), it is obvious that there is no band gap formation after the 1st generation step. The first band gap is obtained at the 5th generation for in-plane wave mode. The band gap region is relatively narrow, and its width ranges from [56.987 kHz, 58.612 kHz]. With the increasing generation number, the band gaps sizes also increase. When the 10th generation is reached, the band gap width ranges from [47.633 kHz, 50.995 kHz], which then expands further to [42.557 kHz, 55.922 kHz] at the 35th generation. By the 55th generation, the band gap frequency range reaches [38.627 kHz, 59.268 kHz]. When the generation is over 143, the band gap width remains unchanged, which means that the optimized topology of PnC has been achieved, with a band gap width ranging from [34.433 kHz, 59.975 kHz]. Compared to the result (the band gap range of [38.627 kHz, 59.268 kHz]) mentioned previously in Section 4.1, the final width of the band gap is widened about 23.8%. Furthermore, if the number of grids is further refined, the optimized band gap width can be increased further.

Meanwhile, the first band gap appears between the fourth and fifth eigenfrequencies, then the positions of the band gaps gradually decline. The maximum band gap ultimately stabilizes between the third and fourth eigenfrequencies.

5. Conclusions

In this paper, an AGA-IFPWEM methodology is proposed for the topology optimization of 2D PnCs in order to establish broad band gap frequency regions. Three numerical examples are introduced to verify the effectiveness, efficiency and convergence of the proposed method.

The improved fast plane wave expansion method (IFPWEM) is introduced to the band structure analysis. Based on the Lauren inverse theorem, by eliminating the jump discontinuity points on the interfacial material boundaries, the continuity of the boundaries is improved and the formulation of the eigenproblem has been revised. The number of wave vectors used for the band structure analysis also decreases from 625 to 81. Compared to the FPWEM model, the IFPWEM model with fewer wave vectors can obtain the same calculation accuracy and much greater computational time. The AGA, which can generate an optimal unit cell design in the first few iterative steps, also decreases the overall iteration time required for convergence, and improves the optimization efficiency. This illustrates the strengths of the proposed AGA-IFPWEM methodology for the topology optimization of PnCs. It should also be noted that although the AGA-IFPWEM model was only applied to 2D PnCs optimization cases in this paper, the method can be easily expanded and applied to 2D PnCs with multi-fields coupling materials [37–41] or 3D PnCs.

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References


