Study of improved plane wave expansion method on phononic crystal

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An improved plane wave expansion method (IPWEM) is deduced by the combination of a dynamic differential equation, the Bloch theory and Fourier expansion. The IPWEM is proposed to improve the convergence of the conventional plane wave expansion method (CPWEM) in dealing with large band gaps in phononic crystals. The IPWEM is supported by the experiments: bend waves transmitting through a 2D phononic crystal. The numerical simulations show that the IPWEM has better prediction precision and higher efficiency compared to the CPWEM, in searching for large band gaps in phononic crystals.

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1. Introduction

The study of phononic crystals has become more and more important with their increasing usages in acoustic engineering applications [1]. Phononic crystals are considered idea materials for making acoustic frequency filters owing to its periodic, heterogeneous structures [2] and the possibility of having phononic band gaps. Based on the relevant experimental research and theoretical modeling, phononic crystals have been successfully designed as high efficiency waveguides [3, 4] and frequency demultipliers [5, 6] in the past decade.

The existence of band gaps in periodic materials has been studied extensively; theoretically and experimentally [1, 7-9]. Among those, conventional plane wave expansion method [10, 11] and finite difference time domain method [12] are two of the popular conventional theoretical modeling.

The conventional plane wave expansion method (CPWEM) expands material parameters in reciprocal vectors based on its lattice structure, and the resulted dynamic differential equation is transformed to algebraic eigen-value equations with the utilization of the Bloch theory. The CPWEM has been widely adopted in theoretical predictions and calculations of phononic band gaps in many kinds of phononic crystals due to the simplicities of its theoretical assumptions. The agreement between CPWEM and experimental research seems to be excellent in locating the band gaps [13].

With the understanding that large acoustic band gaps in materials with periodic structure is a large contrast in their physical properties of the inclusions and the host material, many researches of phononic crystals have focused on the search for large band gaps in their periodic structures [14]. Even though the CPWEM works well in most of the studies, it shows poor convergences dealing with large differences between elastic parameters of inclusion and matrix where the Gibbs phenomena becomes obvious; the otherwise piecewise continuously differentiable periodic function has a jump discontinuity at the interface of the materials [15].

In this paper, the CPWEM is modified mathematically as an improved plane wave expansion method (IPWEM) with the attempts to force the overshoot of the Fourier series to die out sooner to increase the piecewise continuity of the CPWEM. The theoretical model is created by the association of a dynamic differential equation, Bloch theory, and the Fourier expansion. The advantages of the IPWEM over the CPWEM are verified through the interpretations of experimental simulations using a phononic crystal thin plate with cylindrical inclusions of Al_2O_3 embedded periodically in the epoxy matrix.

2. Improved plane wave expansion method

The dynamic differential equation of heterogeneous thin plate with uniform thickness h can be expressed as following general form [16]:

$$-a\frac{\partial^2 w}{\partial y^2}=\frac{\partial^2}{\partial x^2}\left(D\frac{\partial^2 w}{\partial x^2}\right)+b\frac{\partial^2 w}{\partial y^2}+2\frac{\partial^2}{\partial x\partial y}+g\frac{\partial^2 w}{\partial x\partial y}+\frac{\partial^2}{\partial y^2}D\frac{\partial^2 w}{\partial y^2}+\frac{\partial^2 w}{\partial x^2} \tag{1}$$

where w is the transverse displacement in the direction z, $D = Eh^3/12(1-n^2)$ is the bending rigidity in which E is the Young's modulus and u is the Poisson's ratio, $a = rh$, $b = Dn$, $g = D(1-n)$. All of these variables are periodic functions of position vector $\boldsymbol{r} = (x, y)$, so the unified form of these material parameters can be given as $M(\boldsymbol{r})$.

According to Bloch theory, the displacement fields in the phononic crystal thin plate can be written in the following form:

$$w(\boldsymbol{r}, t) = \exp[\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r} - wt)]w_k(\boldsymbol{r}) \tag{2}$$

where $\boldsymbol{k}$ is the wave vector limited in the first Brilliouin zone. $w_k(\boldsymbol{r})$ is a periodic function with the spatial periodicity of material parameters:

$$w_k(\boldsymbol{r}) = \sum_{\boldsymbol{G}1} \exp(\mathrm{i}\boldsymbol{G}_1\cdot\boldsymbol{r})W_{\boldsymbol{G}1} \tag{3}$$

where $\boldsymbol{G1} = 2p(n_1/a, n_2/a)$ is the two-dimensional reciprocal lattice with $n_1, n_2 = 0, \pm 1, \pm 2, \mathrm{L}, \pm n$ and $W_{\boldsymbol{G}1}$ is the corresponding Fourier coefficient.

$M(\boldsymbol{r})$ can also be rewritten by Fourier series:

$$M(\boldsymbol{r}) = \sum_{G2} \exp(\mathrm{i}\boldsymbol{G}_2\cdot\boldsymbol{r})M_{\boldsymbol{G}2} \tag{4}$$

where $M_{\boldsymbol{G}2}$ is the corresponding Fourier coefficient under the two-dimensional reciprocal lattice $\boldsymbol{G}2$ with

$$M_{\boldsymbol{G}2} = \begin{cases} fM_{\mathrm{I}} + (1-f)M_{\mathrm{M}} & \boldsymbol{G}2 = 0 \\ (M_{\mathrm{I}} - M_{\mathrm{M}})P_{\boldsymbol{G}2} & \boldsymbol{G}2 \neq 0 \end{cases} \tag{5}$$

where $f = pr_0^2/a^2$ is the filling fraction of the inclusions which is defined as the ratio between the sectional area of a cylinder inclusion and a unit cell, and M_{I}, M_{M} are material parameters of inclusion and matrix. $P_{\boldsymbol{G}2}$ is the structure factor which is defined as $P_{G2} = \int_A \exp(\mathrm{i}\boldsymbol{G}\cdot\boldsymbol{r})\mathrm{d}r^2/S$. Taking the two-dimensional phononic crystal which circular inclusions embedded in matrix with square lattice for example, $P_{\boldsymbol{G}2} = 2fJ_1(|\boldsymbol{G}2|r_0)/(|\boldsymbol{G}2|r_0)$ where f is the volume fraction of inclusion, $J_1(\cdot)$ is first order Bessel function of the first kind, and $|\boldsymbol{G}2|$ is the modulus of reciprocal vector $\boldsymbol{G}2$, and r_0 is the radius of inclusion.

Substituting Eqs. (2)-(5) into Eqs. (1), we have the following eigen-value equation:

$$\begin{aligned} & w^2 \sum_{\boldsymbol{G}1} a_{\boldsymbol{G}3-\boldsymbol{G}1}W_{\boldsymbol{G}1} \\ &= \sum_{\boldsymbol{G}1} (\boldsymbol{k}+\boldsymbol{G}1)_x^2 (\boldsymbol{k}+\boldsymbol{G}3)_x^2 D_{\boldsymbol{G}3-\boldsymbol{G}1}W_{\boldsymbol{G}1} \\ &+ \sum_{\boldsymbol{G}1} (\boldsymbol{k}+\boldsymbol{G}1)_y^2 (\boldsymbol{k}+\boldsymbol{G}3)_x^2 b_{\boldsymbol{G}3-\boldsymbol{G}1}W_{\boldsymbol{G}1} \\ &+ 2\sum_{\boldsymbol{G}1} (\boldsymbol{k}+\boldsymbol{G}1)_x (\boldsymbol{k}+\boldsymbol{G}1)_y (\boldsymbol{k}+\boldsymbol{G}3)_x \\ &(\boldsymbol{k}+\boldsymbol{G}3)_y g_{\boldsymbol{G}3-\boldsymbol{G}1}W_{\boldsymbol{G}1} \\ &+ \sum_{\boldsymbol{G}1} (\boldsymbol{k}+\boldsymbol{G}1)_y^2 (\boldsymbol{k}+\boldsymbol{G}3)_y^2 D_{\boldsymbol{G}3-\boldsymbol{G}1}W_{\boldsymbol{G}1} \\ &+ \sum_{\boldsymbol{G}1} (\boldsymbol{k}+\boldsymbol{G}1)_x^2 (\boldsymbol{k}+\boldsymbol{G}3)_y^2 b_{\boldsymbol{G}3-\boldsymbol{G}1}W_{\boldsymbol{G}1} \end{aligned} \tag{6}$$

where $\boldsymbol{G}3 = \boldsymbol{G}1 + \boldsymbol{G}2$. Eqs. (6) is an infinite-order eigen-value problem, so the Fourier series need to be truncated to finite items if we want to solve the problem numerically. Usually, finite reciprocal vectors near the origin are chosen. The more reciprocal vectors we choose, the closer the numerical result to the true value. When n inclusions are selected in half axis direction which means $(2n+1)^2$ reciprocal vectors are chosen, we can obtain $(2n+1)^2 \times (2n+1)^2$ order matrix equation from Eqs. (6) written in the standard eigen-value equation as:

$$w^2\boldsymbol{P}\boldsymbol{W} = \boldsymbol{Q}\boldsymbol{W} \tag{7}$$

where $\boldsymbol{P}$ and $\boldsymbol{Q}$ are $(2n+1)^2 \times (2n+1)^2$ order matrixes, and $\boldsymbol{W}$ is $(2n+1)^2$ order array. The elements of $\boldsymbol{P}$, $\boldsymbol{W}$ and $\boldsymbol{Q}$ are:

$$P_{ij} = \begin{cases} a & \boldsymbol{G}_3^{(i)} - \boldsymbol{G}_1^{(j)} = 0 \\ 0 & \boldsymbol{G}_3^{(i)} - \boldsymbol{G}_1^{(j)} \neq 0 \end{cases} \tag{8}$$

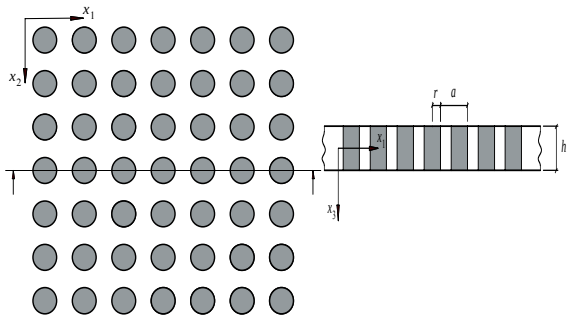
$$W_j = W_{G_1^{(j)}} \tag{9}$$

$$\begin{aligned} Q_{ij} &= (\boldsymbol{k}+\boldsymbol{G}_1^{(j)})_x^2 (\boldsymbol{k}+\boldsymbol{G}_3^{(i)})_x^2 [D]_{\boldsymbol{G}_3^{(i)}-\boldsymbol{G}_1^{(j)}} \\ &+ (\boldsymbol{k}+\boldsymbol{G}_1^{(j)})_y^2 (k+\boldsymbol{G}_3^{(i)})_x^2 [b]_{\boldsymbol{G}_3^{(i)}-\boldsymbol{G}_1^{(j)}} \\ &+ 2(\boldsymbol{k}+\boldsymbol{G}_1^{(j)})_x (\boldsymbol{k}+\boldsymbol{G}_1^{(j)})_y (\boldsymbol{k}+\boldsymbol{G}_3^{(i)})_x \\ &(\boldsymbol{k}+\boldsymbol{G}_3^{(i)})_y [g]_{\boldsymbol{G}_3^{(i)}-\boldsymbol{G}_1^{(j)}} \\ &+ (\boldsymbol{k}+\boldsymbol{G}_1^{(j)})_y^2 (\boldsymbol{k}+\boldsymbol{G}_3^{(i)})_y^2 [D]_{\boldsymbol{G}_3^{(i)}-\boldsymbol{G}_1^{(j)}} \\ &+ (\boldsymbol{k}+\boldsymbol{G}_1^{(j)})_x^2 (\boldsymbol{k}+\boldsymbol{G}_3^{(i)})_y^2 [b]_{\boldsymbol{G}_3^{(i)}-\boldsymbol{G}_1^{(j)}} \end{aligned} \tag{10}$$

where $\boldsymbol{G1}^{(j)}$ is the reciprocal vector in the $\boldsymbol{G1}$ reciprocal vector space with index j, $\boldsymbol{G3}^{(i)}$ is the reciprocal vector in the $\boldsymbol{G3}$ reciprocal vector space with index i. W_{G1} is the eigen-displacement coefficient in the $\boldsymbol{G1}$ reciprocal vector space with index j.

3. Numerical calibration of IPWEM and CPWEM

In order to study the difference between IPWEM and CPWEM, we consider bending waves propagating in a phononic crystal thin plate with cylindrical inclusions of Al_2O_3 embedded periodically in the epoxy matrix (Fig. 1). Inclusions are arranged square lattice with lattice constant a = 0.02 m. The radius of the inclusion is r = 0.006 mm, and thickness of the plate is h = 0.002 mm. Material parameters of inclusion and matrix are shown in Table 1.



(a) Top view (b) Cross section

Fig. 1. Phononic crystal thin plate with square lattice.

Table 1. Material parameters of inclusion and matrix.

	Density r /(kg/m^3)	Young's modulus E /(GPa)	Poisson's ratio n
Inclusion (Al_2O_3)	3970	396.4	0.24
Matrix (Epoxy)	1180	4.35	0.378

When we choose n = 25 (2601 plane waves), the first 10 bands calculated by IPWEM and CPWEM are shown in Fig. 2, which continual line is the numerical simulation of CPWEM and dashed line is the result of IPWEM. $W = \omega a / c_t$ is the normalized frequency which c_t = 1160 m/s is the transverse wave velocity in epoxy. The results show that two methods agree well in low frequencies (1-4 bands), but they don't agree well in high frequencies (5-10 bands). Moreover, the results of CPWEM are always lower than the results of IPWEM either in low frequencies or high frequencies.

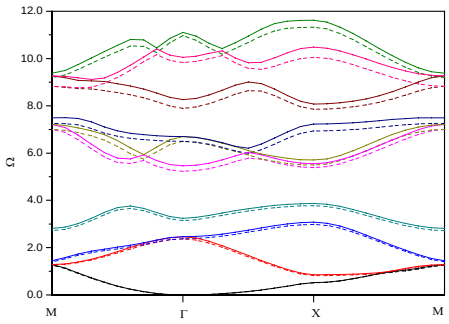
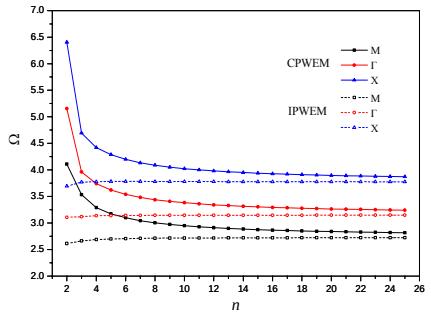
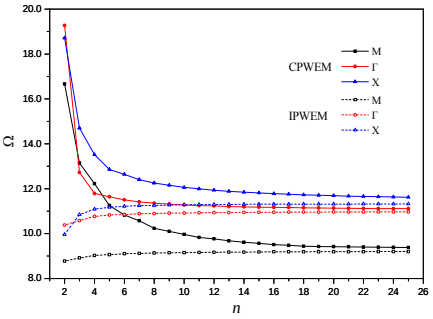


Fig. 2. Band structure of phononic crystal thin plate.



(a) Fourth order eigen-frequencies



(b) Tenth order eigen-frequencies

Fig. 3. The trend of eigen-frequencies calculated with varied plane waves of the highly symmetric points.

Then vary numbers of plane wave are chosen (n = 2,3,L ,25) and we calculate the band structure by IPWEM and CPWEM respectively. The trend of fourth and tenth eigen-frequencies at the highly symmetric points M, G and C are shown in Fig. 3. We can draw the following conclusions:

a. The eigen-frequencies calculated by CPWEM always converge to real value downward, while the eigen-frequencies calculated by IPWEM always converge to real value upward. This means, if same numbers of plane wave are chosen, the results of CPWEM are always bigger than real value and the results of IPWEM, and the results of IPWEM are always smaller than real value and the results of CPWEM.

b. IPWEM converges faster than CPWEM either in high frequencies or in low frequencies. The frequencies by IPWEM are converged when $n \geq 4$ in low frequencies and $n \geq 8$ in high frequencies. Meanwhile, the results of CPWEM are still not converged even when $n > 20$.

c. Low-order frequencies converge faster than high-order frequencies either by IPWEM or CPWEM.

Above all, the results show that IPWEM has good convergency in both low frequencies and high frequencies because of the appropriate choice for P_{ij}. Therefore, eigen-value functions are piecewise smooth and continuous at the interface of inclusion and matrix.

4. Conclusions

An improved plane wave expansion method (IPWEN) is proposed and theoretically deduced. The IPWEM is proved to effectively improve the convergence of the CPWEM at the material interface. The calculations and interpretations of experimental simulations by both methods lead to the following conclusions:

a. The IPWEM shows better convergence at the interface of inclusion and matrix, and therefore, provides better prediction precisions on the existence of large acoustic band gaps. The progresses are directly related to the better piecewise smoothness and continuity of the eigen-value functions presented in the IPWEM;

b. The IPWEM is especially suitable for searching large acoustic band gaps in phononic crystals for its ability of mathematically reducing or eliminating the Gibbs phenomena in their periodic structures. For that reason, the IPWEM is expected to be widely used in studies of periodic materials which have large contrast in physical properties between the inclusions and the matrix in future researches.

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