Three-Dimensional Phononic Band Gap Calculations Using the FDTD Method and a PC Cluster System

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Abstract—This paper aims at studying the band gap phenomena of three-dimensional phononic crystals using the finite difference time domain (FDTD) method and a PC cluster system. In the paper, Bloch's theorem is applied to the wave equation and to the boundary conditions of the periodic structure. We calculate the variations of displacements and take discrete Fourier transform to acquire the resonances of the structures. Then, the dispersion relations of the bulk acoustic wave can be obtained and the band gaps are predicted accordingly. On the other hand, because of larger data calculation in three-dimensional phononic crystals, we introduce the PC cluster system and parallel FDTD programs written with respect to the architecture of a PC cluster system. Finally, we discuss the numerical calculation of two-dimensional and three-dimensional phononic crystals consisting of steel/epoxy and draw conclusions regarding the band gap phenomena between these phononic crystals.

I. INTRODUCTION

THERE has been research pertaining to artificial crystals starting with photonic crystals since the 1980s. A photonic crystal is a periodic arrangement of dielectric materials that an electromagnetic (EM) wave of a specific frequency range is forbidden to pass through—the so-called band gap phenomenon of the photonic crystal. Owing to the analogy of EM waves and acoustic waves, the band gap phenomenon also exists in phononic crystals, the periodic arrangement of elastic materials. The band gap phenomenon may potentially find many engineering applications, such as in acoustic wave filters, the acoustic waveguide, and acoustic resonators, which enhance the necessity to develop a fast and efficient wave propagation theory for the phononic crystal.

Theoretical analyses on the band gaps of phononic crystals have been conducted during the last 15 years. For research in band gaps of bulk acoustic wave (BAW) modes of phononic structures, the mixed and transverse polarization modes have been carried out using the plane wave expansion (PWE) method [1]–[7]. The PWE method is also adopted to study level repulsions of bulk acoustic waves in composite materials [8]. The phononic struc-

tures considered in the aforementioned studies include two-dimensional (2D) solid/air, solid/solid, and solid/fluid structures. It is worth noting that in conducting the acoustic waves in the solid/fluid structure, a modified PWE method was used [4]–[7]. In addition to the band gap analyses of bulk modes in 2D phononic structures, there is some literature on the investigation of band gaps of surface acoustic waves (SAW) [9]–[11]. More detailed studies of temperature effects of surface wave band gaps and electromechanical coupling coefficient in a piezoelectric phononic crystal are also reported [12], [13]. Instead of the PWE method, the multiple scattering theory (MST) has been applied to study the band gaps of bulk wave properties in three-dimensional (3D) periodic acoustic composites and the band structure of a phononic crystal consisting of complex and frequency-dependent Lamé coefficients [14]–[17]. With regard to the numerical simulation of band gaps in phononic structures, the finite difference time domain (FDTD) method was applied to interpret the experimental data of 2D systems consisting of cylinders of fluids (Hg, air, and oil) inserted periodically in a finite slab of aluminum host [18]. It was also used to calculate the periodic solid-solid, solid-liquid, and solid-vacuum composites [19]. The coupling characteristics of localized phonons in photonic crystal fibers and analyses of mode coupling in joined parallel phononic crystal waveguides using the FDTD method are reported in [20], [21].

In these studies, most phononic crystals were 2D structures; some 3D phononic crystals are reported. The 3D structures include the simple cubic (SC), body-centered cubic (BCC), and face-centered cubic (FCC) lattices consisting of water/mercury (liquid-liquid) [22], mercury/aluminum (liquid-solid) [23], and steel/polyester (solid-solid) [24], [25]. In these 3D phononic crystals, the band gaps were evaluated by both the MST and the PWE methods. However, the MST method has a limitation of calculating with overlap scatters, and the PWE method encounters convergence problems when the phononic crystal has a large elastic mismatch. The FDTD method is very suitable for dealing with different geometric structures and for handling the convergence problem but requires considerable calculation.

The purpose of the present study was to develop a parallel FDTD method and a PC cluster system to handle and accelerate the calculation of band gap phenomenon of the phononic crystal in 3D cases. By using a heterogeneous FDTD formulation, the material property and the

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geometric shape can be changed easily and the formulation can be employed to study the band gap phenomenon in different geometric shapes, material properties, and design patterns. We adopted the message passing interface (MPI) to write the parallel FDTD program in order to accelerate the whole computational speed in the PC cluster system. Owing to the high-speed computation of the FDTD method and the PC cluster system, calculations of 3D phononic crystal can be achieved quickly.

II. THE FINITE DIFFERENCE TIME DOMAIN (FDTD) METHOD

Whether the FDTD method or the PWE method is used, the BAW theory of phononic crystal is based on the same physical concept. In this paper, the periodic boundary using Bloch's theorem is used to describe the periodic arrangement of the phononic crystal. The principle of FDTD is mentioned in this section.

A. Equation of the Wave Propagation

According to the theory of elasticity, all the elastic materials are considered in the linear elastic range. Equation of motion and constitutive law with the anisotropic and inhomogeneous material can be expressed as [26]:

$$\rho \ddot{u}_i = \tau_{ij,j} + \rho f_i, \quad (1)$$

$$\tau_{ij} = C_{ijkl} \varepsilon_{kl}, \quad (2)$$

where ρ is the density of materials, u_i is the displacement, τ_{ij} is the stress, f_i is body force, C_{ijkl} is elastic constant, and ε_{kl} is strain. Eq. (1) and (2) describe the behavior of an infinitesimal element of an anisotropic material, and they can apply to the inhomogeneous structure. Therefore, the FDTD method based on (1) and (2) is suitable to analyze the phononic crystal by arranging the density and elastic constant periodically.

In this FDTD method, the displacement and stress variables in materials are used as the bases to describe the equation of motion and constitutive law, and further to develop the difference equations. To cooperate with the staggered grids adopted in the following difference equation, the anisotropy of elastic material is limited. An orthotropic material with nine independent elastic constants is allowed in the program. The matrix form of the elasticity constant using an abbreviated notation is

$$C_{IJ} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{21} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{31} & C_{32} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}, \quad (3)$$

where the subscripts 1, 2, 3, 4, 5, and 6 of material constant C represent xx , yy , zz , yz , xz , and xy , respectively.

From (1), (2), and (3), we can derive the 3D wave equation in which the displacement and stress are regarded as the variables; thus the nine equations of wave equations in matrix form are

$$\begin{bmatrix} \ddot{u}_1 \\ \ddot{u}_2 \\ \ddot{u}_3 \end{bmatrix} = \frac{1}{\rho} \begin{bmatrix} \tau_{11} & \tau_{12} & \tau_{13} \\ \tau_{21} & \tau_{22} & \tau_{23} \\ \tau_{31} & \tau_{32} & \tau_{33} \end{bmatrix} \begin{bmatrix} \partial_1 \\ \partial_2 \\ \partial_3 \end{bmatrix} + \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}, \quad (4)$$

$$\begin{bmatrix} \tau_{11} \\ \tau_{22} \\ \tau_{33} \\ \tau_{23} \\ \tau_{13} \\ \tau_{12} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{21} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{31} & C_{32} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix} \begin{bmatrix} \partial_1 u_1 \\ \partial_2 u_2 \\ \partial_3 u_3 \\ \partial_2 u_3 + \partial_3 u_2 \\ \partial_1 u_3 + \partial_3 u_1 \\ \partial_1 u_2 + \partial_2 u_1 \end{bmatrix}. \quad (5)$$

In (4) and (5), the subscript numbers 1, 2, and 3 of displacement u and stress τ denote the components along the x , y , and z directions in the Cartesian coordinate, respectively, and the symbol ∂_i represents the partial differential in direction i .

Then we use the second-order center difference equation and the first-order center difference equation to approximate the second-order differential equation and the first-order differential equation, respectively. Therefore we define the first-order center difference equation in space first as:

$$\begin{aligned} D_1 [M(i, j, k, l)] &= \frac{1}{\Delta x_1} \left[M\left(i + \frac{1}{2}, j, k, l\right) - M\left(i - \frac{1}{2}, j, k, l\right) \right] \\ D_2 [M(i, j, k, l)] &= \frac{1}{\Delta x_2} \left[M\left(i, j + \frac{1}{2}, k, l\right) - M\left(i, j - \frac{1}{2}, k, l\right) \right] \\ D_3 [M(i, j, k, l)] &= \frac{1}{\Delta x_3} \left[M\left(i, j, k + \frac{1}{2}, l\right) - M\left(i, j, k - \frac{1}{2}, l\right) \right]. \end{aligned} \quad (6)$$

In (6) and the following formulas, the i , j , and k inside the bracket represent the position index of the x , y , and z directions, respectively, and the symbol l is the index of time step. The Δx_i , where $i = 1, 2$, and 3 , represents the distance of two nearby discrete grids in the x , y , and z directions. By replacing the second-order differential in time with the second-order center difference in time, we have

$$\frac{\partial^2}{\partial t^2} [M(i, j, k, l)] = \frac{1}{(\Delta t)^2} \left[M\left(i, j, k, l + \frac{1}{2}\right) - 2M(i, j, k, l) + M\left(i, j, k, l - \frac{1}{2}\right) \right]. \quad (7)$$

After the discrete procedure, we have the difference equation of the displacement and stress (8)–(16) (see next two pages).

In (8)–(16), the symbol U_i and T_{ij} are the discrete displacement and stress components, respectively, with

$$\begin{aligned}
U_1\left(i + \frac{1}{2}, j, k, l + \frac{1}{2}\right) &= 2U_1\left(1 + \frac{1}{2}, j, k, l\right) - U_1\left(i + \frac{1}{2}, j, k, l - \frac{1}{2}\right) \\
&+ \frac{(\Delta t)^2}{\rho\left(i + \frac{1}{2}, j, k\right)} \left\{ D_1 \left[T_{11}\left(i + \frac{1}{2}, j, k, l\right) \right] + D_2 \left[T_{12}\left(i + \frac{1}{2}, j, k, l\right) \right] \right. \\
&\quad \left. + D_3 \left[T_{13}\left(i + \frac{1}{2}, j, k, l\right) \right] \right\} + f_1\left(i + \frac{1}{2}, j, k, l + \frac{1}{2}\right) \quad (8)
\end{aligned}$$

$$\begin{aligned}
U_2\left(i, j + \frac{1}{2}, k, l + \frac{1}{2}\right) &= 2U_2\left(i, j + \frac{1}{2}, k, l\right) - U_2\left(i, j + \frac{1}{2}, k, l - \frac{1}{2}\right) \\
&+ \frac{(\Delta t)^2}{\rho\left(i, j + \frac{1}{2}, k\right)} \left\{ D_1 \left[T_{21}\left(i, j + \frac{1}{2}, k, l\right) \right] + D_2 \left[T_{22}\left(i, j + \frac{1}{2}, k, l\right) \right] \right. \\
&\quad \left. + D_3 \left[T_{23}\left(i, j + \frac{1}{2}, k, l\right) \right] \right\} + f_2\left(i, j + \frac{1}{2}, k, l + \frac{1}{2}\right) \quad (9)
\end{aligned}$$

$$\begin{aligned}
U_3\left(i, j, k + \frac{1}{2}, l + \frac{1}{2}\right) &= 2U_3\left(i, j, k + \frac{1}{2}, l\right) - U_3\left(i, j, k + \frac{1}{2}, l - \frac{1}{2}\right) \\
&+ \frac{(\Delta t)^2}{\rho\left(i, j, k + \frac{1}{2}\right)} \left\{ D_1 \left[T_{31}\left(i, j, k + \frac{1}{2}, l\right) \right] + D_2 \left[T_{32}\left(i, j, k + \frac{1}{2}, l\right) \right] \right. \\
&\quad \left. + D_3 \left[T_{33}\left(i, j, k + \frac{1}{2}, l\right) \right] \right\} + f_3\left(i, j, k + \frac{1}{2}, l + \frac{1}{2}\right) \quad (10)
\end{aligned}$$

$$\begin{aligned}
T_{11}(i, j, k, l + 1) &= C_{11}(i, j, k) \cdot D_1 \left[U_1\left(i, j, k, l + \frac{1}{2}\right) \right] \\
&+ C_{12}(i, j, k) \cdot D_2 \left[U_2\left(i, j, k, l + \frac{1}{2}\right) \right] + C_{13}(i, j, k) \cdot D_3 \left[U_3\left(i, j, k, l + \frac{1}{2}\right) \right] \quad (11)
\end{aligned}$$

$$\begin{aligned}
T_{22}(i, j, k, l + 1) &= C_{21}(i, j, k) \cdot D_1 \left[U_1\left(i, j, k, l + \frac{1}{2}\right) \right] \\
&+ C_{22}(i, j, k) \cdot D_2 \left[U_2\left(i, j, k, l + \frac{1}{2}\right) \right] + C_{23}(i, j, k) \cdot D_3 \left[U_3\left(i, j, k, l + \frac{1}{2}\right) \right] \quad (12)
\end{aligned}$$

$$\begin{aligned}
T_{33}(i, j, k, l + 1) &= C_{31}(i, j, k) \cdot D_1 \left[U_1\left(i, j, k, l + \frac{1}{2}\right) \right] \\
&+ C_{32}(i, j, k) \cdot D_2 \left[U_2\left(i, j, k, l + \frac{1}{2}\right) \right] + C_{33}(i, j, k) \cdot D_3 \left[U_3\left(i, j, k, l + \frac{1}{2}\right) \right] \quad (13)
\end{aligned}$$

$$T_{23} \left(i, j + \frac{1}{2}, k + \frac{1}{2}, l + 1 \right) = C_{44} \left(i, j + \frac{1}{2}, k + \frac{1}{2} \right) \cdot \left\{ D_3 \left[U_2 \left(i, j + \frac{1}{2}, k + \frac{1}{2}, l + \frac{1}{2} \right) \right] + D_2 \left[U_3 \left(i, j + \frac{1}{2}, k + \frac{1}{2}, l + \frac{1}{2} \right) \right] \right\} \quad (14)$$

$$T_{13} \left(i + \frac{1}{2}, j, k + \frac{1}{2}, l + 1 \right) = C_{55} \left(i + \frac{1}{2}, j, k + \frac{1}{2} \right) \cdot \left\{ D_3 \left[U_1 \left(i + \frac{1}{2}, j, k + \frac{1}{2}, l + \frac{1}{2} \right) \right] + D_1 \left[U_3 \left(i + \frac{1}{2}, j, k + \frac{1}{2}, l + \frac{1}{2} \right) \right] \right\} \quad (15)$$

$$T_{12} \left(i + \frac{1}{2}, j + \frac{1}{2}, k, l + 1 \right) = C_{66} \left(i + \frac{1}{2}, j + \frac{1}{2}, k \right) \cdot \left\{ D_2 \left[U_1 \left(i + \frac{1}{2}, j + \frac{1}{2}, k, l + \frac{1}{2} \right) \right] + D_1 \left[U_2 \left(i + \frac{1}{2}, j + \frac{1}{2}, k, l + \frac{1}{2} \right) \right] \right\} \quad (16)$$

Fig. 1. The unit of the grids in the FDTD method.

$i, j = 1 \sim 3$. The positions of the staggered grids are defined by these discrete wave equations. Fig. 1 shows the unit of the staggered grids in the calculation of the FDTD method, and the relationship between the displacement grids and the stress grids.

B. Boundary and Initial Conditions

To calculate the dispersion curves of phononic crystals, the periodic boundary condition of FDTD is developed. Because of the periodicity of phononic crystals, we applied Bloch's theorem to fulfill the boundary condition. The periodic boundary condition satisfying Bloch's theorem is promoted by Tanaka *et al.* in [19] for 2D phononic crystal cases. In the present article, we deal with 3D phononic crystals based on the same principle. According to Bloch's theorem, the displacement and stress components in the periodic structure can be expressed in a periodic function as follows:

$$U_i(\mathbf{x}, t) = e^{i\mathbf{k} \cdot \mathbf{x}} \bar{U}_i(\mathbf{x}, t), \quad (17)$$

$$T_{ij}(\mathbf{x}, t) = e^{i\mathbf{k} \cdot \mathbf{x}} \bar{T}_{ij}(\mathbf{x}, t), \quad (18)$$

where $\mathbf{k} = (k_1, k_2, k_3)$ is a wave vector, and $\bar{U}_i$ and $\bar{T}_{ij}$ are periodic functions which satisfy the following relation:

$$\bar{U}_i(\mathbf{x} + \mathbf{a}, t) = \bar{U}_i(\mathbf{x}, t), \quad (19)$$

$$\bar{T}_{ij}(\mathbf{x} + \mathbf{a}, t) = \bar{T}_{ij}(\mathbf{x}, t), \quad (20)$$

where $\mathbf{a}$ is a lattice translation vector with the components a_1, a_2 , and a_3 of each direction.

In [19], the equation of motion (1) and constitutive law (2) are translated to solve the periodic functions $\bar{U}_i$ and $\bar{T}_{ij}$ and to apply the periodic boundary conditions (19) and (20). Alternatively, we develop the FDTD in U_i and T_{ij} , and therefore the periodic boundary conditions are derived as:

$$U_i(\mathbf{x} + \mathbf{a}, t) = e^{i\mathbf{k} \cdot \mathbf{a}} U_i(\mathbf{x}, t), \quad (21)$$

$$T_{ij}(\mathbf{x} + \mathbf{a}, t) = e^{i\mathbf{k} \cdot \mathbf{a}} T_{ij}(\mathbf{x}, t). \quad (22)$$

Expanding (21) and (22), we have the discrete forms of the surface normal to the X, Y, and Z axes:

Normal to the X axis:

$$\begin{aligned} U_1 \left(-\frac{1}{2}, j, k, l \right) &= e^{ik_1 a_1} U_1 \left(a_1 - \frac{1}{2}, j, k, l \right) \\ U_2 \left(0, j + \frac{1}{2}, k, l \right) &= e^{ik_1 a_1} U_2 \left(a_1, j + \frac{1}{2}, k, l \right) \\ U_3 \left(0, j, k + \frac{1}{2}, l \right) &= e^{ik_1 a_1} U_3 \left(a_1, j, k + \frac{1}{2}, l \right) \end{aligned} \quad (23)$$

$$\begin{aligned} T_{11}(0, j, k, l) &= e^{ik_1 a_1} T_{11}(a_1, j, k, l) \\ T_{12} \left(-\frac{1}{2}, j + \frac{1}{2}, k, l \right) &= e^{ik_1 a_1} T_{12} \left(a_1 - \frac{1}{2}, j + \frac{1}{2}, k, l \right) \\ T_{13} \left(-\frac{1}{2}, j, k + \frac{1}{2}, l \right) &= e^{ik_1 a_1} T_{13} \left(a_1 - \frac{1}{2}, j, k + \frac{1}{2}, l \right). \end{aligned}$$

Normal to the Y axis:

$$\begin{aligned}
 U_1 \left(i + \frac{1}{2}, 0, k, l \right) &= e^{ik_2 a_2} U_1 \left(i + \frac{1}{2}, a_2, k, l \right) \\
 U_2 \left(i, -\frac{1}{2}, k, l \right) &= e^{ik_2 a_2} U_2 \left(i, a_2 - \frac{1}{2}, k, l \right) \\
 U_3 \left(i, 0, k + \frac{1}{2}, l \right) &= e^{ik_2 a_2} U_3 \left(i, a_2, k + \frac{1}{2}, l \right) \\
 T_{12} \left(i + \frac{1}{2}, -\frac{1}{2}, k, l \right) &= e^{ik_2 a_2} T_{12} \left(i + \frac{1}{2}, a_2 - \frac{1}{2}, k, l \right) \\
 T_{22}(i, 0, k, l) &= e^{ik_2 a_2} T_{22}(i, a_2, k, l) \\
 T_{23} \left(i, -\frac{1}{2}, k + \frac{1}{2}, l \right) &= e^{ik_2 a_2} T_{23} \left(i, a_2 - \frac{1}{2}, k + \frac{1}{2}, l \right).
 \end{aligned} \tag{24}$$

Normal to the Z axis:

$$\begin{aligned}
 U_1 \left(i + \frac{1}{2}, j, 0, l \right) &= e^{ik_3 a_3} U_1 \left(i + \frac{1}{2}, j, a_3, l \right) \\
 U_2 \left(i, j + \frac{1}{2}, 0, l \right) &= e^{ik_3 a_3} U_2 \left(i, j + \frac{1}{2}, a_3, l \right) \\
 U_3 \left(i, j, -\frac{1}{2}, l \right) &= e^{ik_3 a_3} U_3 \left(i, j, a_3 - \frac{1}{2}, l \right) \\
 T_{13} \left(i + \frac{1}{2}, j, -\frac{1}{2}, l \right) &= e^{ik_3 a_3} T_{13} \left(i + \frac{1}{2}, j, a_3 - \frac{1}{2}, l \right) \\
 T_{23} \left(i, j + \frac{1}{2}, -\frac{1}{2}, l \right) &= e^{ik_3 a_3} T_{23} \left(i, j + \frac{1}{2}, a_3 - \frac{1}{2}, l \right) \\
 T_{33}(i, j, 0, l) &= e^{ik_3 a_3} T_{33}(i, j, a_3, l).
 \end{aligned} \tag{25}$$

After setting up the periodic boundaries, we need to define the initial condition for the calculation. Because the periodic structure needs to be vibrated in this method, we provide a small disturbance in a random position of the structure for the setting of the initial condition, and we have the initial disturbance which is set in any grid of the unit cell

$$U_i(x_1, x_2, x_3) = \delta_{x_1, x} \delta_{x_2, y} \delta_{x_3, z}, \tag{26}$$

where δ is a delta function and (x_1, x_2, x_3) is the random point which excites a wide-band signal in the unit cell at the initial time step $l = 0$. Thus, all possible wave modes are transported inside the phononic crystal under consideration, and then the signal is expanded into a time Fourier series; this permits the finding of the information about possible types of waves.

Before the calculation is started, the specific wave number in the first Brillouin zone needs to be defined for the boundary condition. During the calculation, the variation of the displacement must be recorded while time increases. After obtaining a sufficiently large number of displacement data, we Fourier-transformed the variation of the displacement into the frequency space. Then the resonant frequencies of the periodic structure can be obtained. The resonant points are the existing peaks in the frequency spectra; they identified the eigenfrequencies of the phononic crystal for a given wave vector.

Fig. 2. The hardware architecture of a PC cluster system.

III. PARALLEL COMPUTING IN THE PC CLUSTER SYSTEM

The traditional supercomputer no longer satisfies the demands of large scientific computing in that the hardware has met the bottleneck of design and the price of a supercomputer is too expensive to be afforded by general research institutions. So the PC cluster system is becoming the most popular high-efficiency computation machine in scientific and technologic fields nowadays. In this study, because of the high-speed computation and low cost of the PC cluster system, the complex research of 3D phononic crystals can be calculated and discussed by saving much of the CPU computation time.

As Fig. 2 shows, the PC cluster consists of several PCs with different operating systems and different hardware architectures. PCs are connected with each other by external network devices, such as network cards based on Ethernet. Thus the PCs in the system can use the messages passing around to communicate with each other. Therefore the whole system of PCs can be regarded as a complete parallel machine.

The parallel model of the PC cluster is SPMD (single program multiple data). In the model of SPMD, the parallelism is controlled by the programs, not the CPU instructions. The controller of the system sends the program to every computational node involved in the calculation, and commands every PC to do the task. In the parallel computing of the PC cluster system, we adopt MPICH [27], a high-performance portable implementation of the standard MPI, to parallel the program. MPICH offers many kinds of parallel ways in the library so that the programmer can easily pass the message from one of the computers to the others by simply calling the function offered from the library.

In this paper, we accelerate the calculation speed by paralleling the program. Among several kinds of parallel

Fig. 3. Parallel model—working queue.

methods for calculation, such as dividing the calculation time or space, here we propose the method of dividing the calculation by wave vectors. Unlike dividing the calculation by time or space, which requires numbers of data exchanging, by calculating different wave vectors around the irreducible part of the first Brillouin zone, there are fewer messages passing in PC cluster system so that the computation can achieve higher performance. There is no message passing, data exchanging, and synchronization between the calculations with different wave vectors. Therefore, dividing the computation by the wave vector is expected to obtain higher performance in PC cluster system.

In this parallel method, as Fig. 3 shows, the working queue is created to store all the wave vectors of the whole computation in the server before the calculation. Then the client sends the request to the server for the jobs asked for in the calculation. If the working queue in the server is not empty, the new job will be sent to the client. After receiving the reply from the server, the client can do the calculation with the specific wave vector. Then the client can iterate the job requesting process until the working queue is empty. Therefore the whole computation is finished completely.

Using this kind of parallel method, the whole computation can save more calculation time by increasing numbers of CPUs. Because the numbers of CPUs in calculation are increased, jobs dispatched to each node are also reduced. And in this method there is no message passing between the clients and fewer data exchanging between the client and the server. Thus the total waiting time is spent mostly in the calculation and just a little in the waiting for message passing. Therefore this parallel method is very suitable for use in the FDTD study of phononic crystals.

Fig. 4. (a) A 2D phononic crystal with square lattice arrangement; (b) The irreducible part of the first Brillouin zone.

IV. EXAMPLES OF PHONONIC BAND GAP CALCULATIONS (2D AND 3D)

In this section, the above-mentioned BAW theory of a phononic crystal using the FDTD method is employed to discuss phononic band gaps with different crystal structures. The results for 2D and 3D phononic crystals are presented, including 2D cases with square lattice arrangement, and 3D cases with SC lattice, BCC lattice, and FCC lattice arrangements. In all of the numerical calculations of phononic crystals, the background and filling materials chosen are epoxy and steel. These materials are well-known for the study of the property of both acoustic band gaps and total band gaps [21], [28]. Thus it is convenient to choose them for demonstrating the results of 2D and 3D phononic crystals in this study. The density and the elastic constants C_{11} and C_{44} of epoxy are assumed as 1180 kg/m³, 7.61 GPa, and 1.59 GPa, respectively, and those for steel are 7780 kg/m³, 264 GPa, and 81 GPa. To proceed with the calculation of the FDTD method, the phononic crystals are created by assigning the material constants of corresponding positions according to the shape of inclusions. In this study, although the phononic crystals are formed with isotropic background and filling materials, the anisotropic lattice structures demonstrate the anisotropic property of wave propagation, as shown below.

A. Two-Dimensional Phononic Crystals

In this subsection, we consider a 2D steel/epoxy phononic crystal with square lattice arrangement as shown in Fig. 4(a). The unit cell of the square lattice phononic crystal can be chosen as either the square with a full inclusion inside or a square with four quarters of the inclusion. In this study, we adopt the former one for simplicity. The first Brillouin zone of the phononic crystal in square arrangement is shown in Fig. 4(b). Owing to the symmetry of the material and lattice, the irreducible part of the first Brillouin zone is an isosceles right triangle. Therefore we calculate the dispersion relations for a BAW along the boundary of the irreducible part of the first Brillouin zone. The symbols Γ , X , and M in Fig. 4(b) denote the vertexes

Fig. 5. Dispersion relation of a circular inclusion phononic crystal with square lattice arrangement.

of the first Brillouin zone of square-arrayed phononic crystals.

First, we discuss the band gap phenomena of a phononic crystal with circular inclusion. The radii of the cylinder are 9 and 15 grids while the lattice constant is 30 and 50 grids. The filling fraction of the 2D phononic crystal is defined as the ratio of the cross-section areas of the inclusion and the unit cell. Therefore, the filling fraction f is 0.283 for these cases. To verify the result of the FDTD method, the dispersion relation is also calculated by the PWE method. There are 1681 reciprocal lattice vectors (RLV) for the PWE method while each unit cell is divided into 30 by 30 and 50 by 50 grids for the FDTD method. The dispersion curves are shown in Fig. 5, where the lines with solid triangle symbols “▲” represent the results of the PWE method and the lines with hollow circle “○” and hollow rhombus “◇” symbols represent those of the FDTD method. The dispersion relation shows the allowed elastic wave modes inside the phononic crystal. The vertical axis is the normalized frequency $\Omega = \omega a / C_t$ and the horizontal axis is the reduced wave vector defined as ka / π , where ω is the angular frequency, k the wave vector, a lattice constant, and C_t the transverse wave velocity of the background material.

As Fig. 5 shows, the results show good agreement between the PWE and the FDTD methods. The PWE method shows the total band gap from the normalized frequency 4.07 to 6.79, and the FDTD method shows the band gap from $\Omega = 4.08$ to 6.67 and 4.05 to 6.67 for 30×30 and 50×50 grids per unit cell, respectively. The dispersion curves match each other in the lower frequency range and show slight differences in higher frequency range. The possible reason is that the presentation of the inclusion shape is limited by the orthogonal grids system. Therefore, the

resonance frequencies of higher eigenmodes change slightly when the phononic crystal unit cell is defined by more grids. Basically, the result of the FDTD method with the unit cell divided into 30×30 grids shows very high agreement with that for 50×50 grids, but the calculation time is less than half that of the latter. It is also worth indicating that the numbers of reciprocal lattice vectors (RLV) affect the accuracy of dispersion curves. The PWE work shows that with the larger number of RLV, the dispersion curves shift to a lower value. With the results, the FDTD method is verified and the division of the unit cell is also discussed for the trade-off of accuracy and efficiency.

Second, Fig. 6 shows the results of 2D phononic crystals with a square lattice arrangement but the inclusion is a square rod. Although the orthogonal discrete grids may limit accuracy of the inclusion shapes, the FDTD method is very convenient to study the phononic crystals with a different inclusion shape. The square inclusions are defined by designating the material constants in the corresponding grids, and furthermore the square inclusions are orientated in different directions, such as 0, 15, 30, and 45 degrees with respect to the X-axis. These cases have an equal filling fraction, but the apparent band gaps change due to the orientation of square inclusions. Fig. 6(a) shows the results of 2D phononic crystals whose filling fraction is 0.27. The filling fraction is approximately equal to, but smaller than, that in Fig. 5. The hollow rhombus “◇” symbols of the 0 degree orientation case, for example, represent a total band gap width of 2.58, with a normalized frequency from 3.97 to 6.55. Meanwhile, Fig. 6(b) shows the dispersion curves of the phononic crystals with filling fraction 0.36, and thus the length of the side of square rod is 30 grids, equal to the diameter of the circle in Fig. 5. A total band gap of the 0 degree orientation case appears to have a normalized frequency from 3.73 to 7.67 and the width of the band gap is 3.94. The other symbols, hollow circle, triangle, and square, represent the cases with orientation 15, 30, and 45 degrees, respectively, and the band gaps are included in Fig. 6(c).

When the filling fractions are equal, we find the total band gap widths of the phononic crystal with the square inclusion in the square lattice arrangement approximately equal to that with the circular inclusion, but the interval changes to a higher frequency range with the increase of the orientation angle. In addition, if a general radius is defined as the vertical distance from the center of the geometric shape to the boundary such as the half length of a square side and the radius of a circle, then the cases of equal general radius show that the crystal with the square rod inclusion exhibits a wider total band gap.

B. Three-Dimensional Phononic Crystals

By replacing the material constant of each grid, the FDTD method is appropriate to study the 3D phononic crystals. We analyze three types of 3D phononic crystals in this subsection, including SC lattice, BCC lattice, and FCC lattice arrangements. Due to the considerable com-

Fig. 6. Dispersion relation of a square inclusion phononic crystal with different orientations: (a) The case of filling fraction 0.27; (b) The case of filling fraction 0.36; (c) The distribution of total band gaps.

Fig. 7. A 3D simple cubic lattice phononic crystal with a sphere inclusion: (a) Lattice arrangement and the first Brillouin zone; (b) Dispersion relation.

putation of 3D cases, we introduce the PC cluster system for the numerical work. In addition, the unit cell of the 3D phononic crystal is divided into $30 \times 30 \times 30$ grids. It is believed that the accuracy is good enough from the study of the 2D cases in the previous subsection. The time step is chosen as $0.002a/C_t$ to satisfy the convergence condition of the FDTD method in wave propagation, and the calculation is with the time evolution of 100,000 time steps.

Fig. 7(a) shows the unit cell of the 3D phononic crystal with a sphere inclusion in the SC lattice arrangement. The first Brillouin zone of an SC lattice is also shown in the figure. Due to the symmetric property of geometry and material, the irreducible part is a tetrahedron with corners labeled Γ , X, M, and R. The radius of the sphere is 9 grids, and thus the filling fraction of this SC phononic crystal is 0.113. The dispersion relation for a BAW in the first Brillouin zone is represented in Fig. 7(b) and a total band gap is observed from a normalized frequency of 4.68 to 4.90 with a width of 0.22.

Fig. 8. A 3D simple cubic lattice phononic crystal with a cube inclusion: (a) Lattice arrangement; (b) Dispersion relation.

Next, we replace the sphere inclusion in the SC lattice with a cube inclusion, as shown in Fig. 8(a). The length of the cube side equals 16 grids and the filling fraction is 0.152. The dispersion relation is analyzed along the irreducible volume again and a band gap from 4.48 to 5.38 is obtained. The width of the band gap is 0.9, which is wider than that of the sphere inclusion. The band gap becomes larger when the side length of cube inclusion equal 18 grids. Therefore a cube inclusion can create a larger band gap than a sphere one for an equal general radius.

Further, the 3D phononic crystal with a BCC lattice arrangement and its first Brillouin zone are shown in Fig. 9(a). The tips of the irreducible part are labeled Γ , H, N, and P. The radius of the sphere is 9 grids, the same as in the SC case. Since each cubic unit cell in the BCC lattice arrangement contains two spheres, the filling fraction is 0.226. The dispersion curves for a BAW are calculated along the selected direction and shown in Fig. 9(b). A total band gap appears from a normalized frequency of 5.37 to 8.07 and the width is 2.7.

Fig. 9. A 3D body-centered cubic lattice phononic crystal with sphere inclusions: (a) Lattice arrangement and the first Brillouin zone; (b) Dispersion relation.

The final 3D phononic crystal case is the FCC lattice arrangement in Fig. 10(a). The tips of the irreducible part of first Brillouin zone are labeled Γ , X, W, K, L, and U. With the same dimension of the lattice constant and sphere, each cubic unit cell contains four spheres and the filling fraction is 0.452. There is a noticeable total band gap from 6.79 to 14.60 with a width of 7.81.

Thus we find that the 3D phononic crystal with the cube inclusion has a larger band gap than that with the spherical inclusion; this is also true in the 2D case. It is apparent that in the 3D phononic crystal the band gap phenomenon is affected by the geometric shape of the inclusion. Furthermore, the 3D phononic crystals, including SC, BCC, and FCC lattice arrangements, show that the band gap width in the FCC case is larger than those of the BCC and SC cases and that the band gap width of the BCC case is larger than that of the SC case. We can also inspect the phononic band gaps in terms of relative band width $\Delta\omega/\omega_0$, defined as ratio of the band gap to the central frequency of gap. The relative band width values of the SC, BCC, and FCC lattice cases of spherical inclusions are 0.046, 0.40, and 0.73, respectively. So the band gap enlarges as the filling fraction increases, and a high-density package arrangement has a larger band gap in the

Fig. 10. A 3D face-centered cubic lattice phononic crystal with sphere inclusions: (a) Lattice arrangement and the first Brillouin zone; (b) Dispersion relation.

3D phononic crystal. The FCC lattice has a considerable total band gap of its BAW and thus can potentially be applied to the design of 3D waveguides and filters.

V. CONCLUSIONS

This paper proposes a FDTD theory of the BAW in 3D phononic crystals consisting of materials with orthotropic symmetry. The FDTD method is very suitable for dealing with various periodic phononic structures and easily satisfies the convergence condition of materials with large elastic mismatch. With the periodic boundary condition derived from Bloch's theorem, the FDTD method can be used to analyze the dispersion relations of 2D and 3D phononic crystals efficiently. We also develop and execute parallel FDTD programs on a PC cluster system to minimize the calculating time for the 3D structures. The parallel programs are realized by distributing jobs with specific wave vectors, and they have increased our work efficiency many times.

In the discussion of phononic crystals, we generalize the relation between the band gap phenomenon and the geometric shape by extensive study of phononic crystals of different geometric designs. Some band gap characteristics of both 2D and 3D phononic crystals drawn from the aforementioned study are as follows:

1. In the 2D cases of square lattice arrangement, phononic crystals with the square inclusion arrangement have a larger band gap. The range of total band gaps varies with the orientation angle of the square inclusion while the widths do not show obvious differences.
2. The geometric shapes of inclusions in 3D phononic crystals also change the appearance of total band gaps. A cube inclusion creates a larger band gap than a sphere inclusion of equal general radius.
3. The band gaps of 3D phononic crystals with a constant sphere size are calculated for SC, BCC, and FCC lattice arrangements. The largest band gap is obtained in the FCC case and the next largest for the BCC case. This can be understood by the increase of the filling fraction. These analyses are the fundamental steps toward development of further applications. For example, the BCC lattice phononic crystal with real dimensions of the 10-mm lattice constant and the 3-mm spherical radius supports a total band gap from 99.2 kHz to 149.1 kHz. This property can be of use for an acoustic wave filter and further to accordingly design a 3D acoustic waveguide.

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