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Band Structure of Three-dimensional Phononic Crystals

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By using the plane-wave-expansion method, the band structure of three-dimension phononic crystals was calculated, in which the cuboid scatterers were arranged in a host with a face-centered-cubic (FCC) structure. The influences of a few factors such as the component materials, the filling fraction of scatterers and the ratio (R_{HL}) of the scatterer's height to its length on the band-gaps of phononic crystals were investigated. It is found that in the three-dimension solid phononic crystals with FCC structure, the optimum case to obtain band-gaps is to embed high-velocity and high-density scatterers in a low-velocity and low-density host. The maximum value of band-gap can be obtained when the filling fraction is in the middle value. It is also found that the symmetry of the scatterers strongly influences the band-gaps. For $R_{HL} \geq 1$, the width of the band-gap decreases as R_{HL} increases. On the contrary, the width of the band-gap increases with the increase of R_{HL} when R_{HL} is smaller than 1.

Key words: Phononic crystals, Band-gap, Face-centered-cubic (FCC), Plane wave expansion method

I. INTRODUCTION

The periodic composites have attracted a great deal of attentions in recent years [1-10]. It is well known that theoretic basis of the semiconductor is the energy band theory. When the electrons propagate in the periodical potential field, the band structure (i.e. the conduction band and the forbidden band) will form, and the electrons can only move freely in the conduction band. People can design and modulate the band-gaps by adjusting the physical parameter in a semiconductor super lattice, and thus promote the development of the semiconductor science and technology. Earlier in 1960s, it was found that the propagation of light-waves in the periodic dielectric structure is similar to that of electron in the semiconductor. If the wavelength of electromagnetic wave has the same order of magnitude as the periodicity of the dielectric structure, the band structure, called photon band, will appear. The gap between photon bands is called photon band-gap, in which the light wave can not propagate, and the corresponding materials are called photonic crystals. Recently, the similar research has been extended to the propagation of elastic/acoustic waves in the periodic composites called phononic crystals. Because elastic/acoustic wave is a full vector and each component includes three independent parameters, namely, the mass of density, the transverse and longitudinal speed of sound. Thus, the research on phononic crystals is of greater physical significance [1-4].

The research on the band structure of periodic composites and the propagation of elastic (acoustic) waves in different periodic composites is very important. It will help us realize the influences of the different components and the structures of phononic crystals on the band structure and will help us understand the theory of the phononic crystals. These theories will guide us to design new function materials to satisfy our needs.

At present, several methods such as the plane-wave-expansion method [1-7], finite-difference-time-domain method, multiple scattering theory, transfer matrix and variational approach are used to calculate the band structure of phononic crystals. It has been found that band-gaps can be influenced by the following factors [1-7,9]: (i) the ratio of mass density, sound velocity and impedance of the scatterers to those of the host(ii) the geometrical size and the filling fraction of the scatterers and (iii) the topology of the scatterers in the crystal. In this work, the band structure of binary three-dimension (3-D) phononic crystals is calculated by using the plane-wave-expansion method. The band-gaps of 3-D composites which consist of cuboid scatterers (A) arranged in a face-centered-cubic (FCC) structure in host (B) are calculated. Comparisons are made among the bad-gaps of 3-D phononic crystals which are composed of different component materials. The influences of some factors such as the filling fraction of scatterer and the ratio of the scatterer's height to its length on the band structure are investigated.

II. MODEL AND FORMULA

The basic idea of the plane-wave-expansion method is to expand the density and elastic coefficient of mate-

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rial to the superposition of plane wave in reciprocal-lattice vectors space. Then the acoustic wave equation is translated into an eigen equation. By solving this equation, we can get the dispersion relations of the spreading phonon.

The three-dimension phononic crystal is composed of various shapes of scatterers embedded in a host. Regardless of the factor of time, the three-dimension elastic wave equation in a medium with local isotropy can be written as the following:

$$(\lambda+2\mu)\nabla(\nabla\cdot\vec{u})-\mu\nabla\times\nabla\times\vec{u}+\rho\omega^2\vec{u}=0 \quad (1)$$

In a rectangular coordinate system, equation (1) can be rewritten as follows [1,4,7]:

$$\frac{\partial^2 u^i}{\partial t^2}=\frac{1}{\rho}\left\{\frac{\partial}{\partial x_i}\left(\lambda\frac{\partial u^l}{\partial x_l}\right)+\frac{\partial}{\partial x_l}\left[\mu\left(\frac{\partial u^i}{\partial x_l}+\frac{\partial u^l}{\partial x_l}\right)\right]\right\} \quad (2)$$

where $u^i(i=x,y,z)$ are the Cartesian components of the displacement vector $\vec{u}(\vec{r})$, $x_l(l=x,y,z)$ are the Cartesian components of the position vectors $\vec{r}$, $\lambda(\vec{r})$ and $u(\vec{r})$ are Lamé coefficients, $\rho(\vec{r})$ is mass density. λ, μ and $\rho(\vec{r})$ are periodic functions of $\vec{r}$:

$$f(\vec{r}+\vec{R})=f(\vec{r}) \quad (3)$$

In Eq.(3), $\vec{R}=n_1\vec{a}_1+n_2\vec{a}_2+n_3\vec{a}_3$, in which n_1, n_2, n_3 are integers, $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ are crystals lattice basis vector. $f(\vec{r})$ stands for $\lambda(\vec{r})$, $\mu(\vec{r})$ or $\rho^{-1}(\vec{r})$. Owing to its periodicity, it can be expanded in a 3-D Fourier series:

$$f(\vec{r})=\sum_{\vec{G}} f_{\vec{G}}e^{i\vec{G}\cdot\vec{r}} \quad (4)$$

The summation extends over all the reciprocal vectors $\vec{G}$, which is defined by the following relation: $\vec{G}=m_1\vec{b}_1+m_2\vec{b}_2+m_3\vec{b}_3$, in which m_1, m_2 and m_3 are integers, $\vec{b}_1$, $\vec{b}_2$ and $\vec{b}_3$ are reciprocal lattice basis vectors. They can be defined as follows:

$$\begin{aligned}\vec{b}_1&=\frac{2\pi(\vec{a}_2\times\vec{a}_3)}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}\\ \vec{b}_2&=\frac{2\pi(\vec{a}_3\times\vec{a}_1)}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}\\ \vec{b}_3&=\frac{2\pi(\vec{a}_1\times\vec{a}_2)}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}\end{aligned} \quad (5)$$

Reciprocal vector $\vec{G}$ is a periodic function with the same periodicity as the phononic crystals. Owing to the common periodicity of all the coefficients in Eq.(3) and (4), its eigenvalues, according to the Bloch's theorem, can be written as the follows:

$$\vec{u}(\vec{r})=e^{i\vec{K}\cdot\vec{r}}\vec{u}_{\vec{K}}(\vec{r}) \quad (6)$$

where $\vec{K}$ is a 3-D Bloch vector which is restricted within the first Brillouin zone (BZ) (Fig.1), and $\vec{u}_K(\vec{r})$ is a periodic function of $\vec{r}$ just like λ, μ and ρ. $\vec{u}_K(\vec{r})$ can also be expanded into Fourier series according to Eq.(4). Thus, we have,

$$\vec{u}(\vec{r})=\sum_{\vec{G}}\vec{u}_{\vec{K}+\vec{G}}e^{i(\vec{K}+\vec{G})\cdot\vec{r}} \quad (7)$$

Substituting Eq.(4)(with $f=\lambda$, μ, ρ^{-1}) and Eq.(7) into Eq.(2), we can obtain:

$$\begin{aligned}\omega^2 u^i_{\vec{K}+\vec{G}} \;=\; &\sum_{\vec{G}'}\Big\{\sum_{l,\vec{G}''}\rho^{-1}_{\vec{G}-\vec{G}''}\Big[\lambda_{\vec{G}''-\vec{G}'}(\vec{K}+\vec{G}')_l\\ &\Big(\vec{K}+\vec{G}'')_i+\mu_{\vec{G}''-\vec{G}'}(\vec{K}+\vec{G}')_i(\vec{K}+\vec{G}'')_l\Big]\\ &\times u^l_{\vec{K}+\vec{G}'}+\sum_{\vec{G}''}\Big[\rho^{-1}_{\vec{G}-\vec{G}''}\mu_{\vec{G}''-\vec{G}'}\\ &\times\sum_j(\vec{K}+\vec{G}')_j(\vec{K}+\vec{G}'')_j\Big]u^i_{\vec{K}+\vec{G}'}\Big\}\end{aligned} \quad (8)$$

In this work, we have investigated the binary 3-D phononic crystals, in which every unit cell is composed of two materials. One is the scatterer and the other is the host. They are labeled with A and B respectively. Thus material $A(B)$ can be characterized by the parameters $\rho_A(\rho_B)$, $\mu_A(\mu_B)$ and $\lambda_A(\lambda_B)$. We specified the occupancy ration of the volume of each material by F (for A) and $1-F$(for B) respectively. The Fourier coefficients in Eq.(4) now take a particularly simple form and can be written as,

$$f_{\vec{G}}=\frac{1}{V}\int f(\vec{r})\exp(-i\vec{G}\cdot\vec{r})\mathrm{d}^3\vec{r} \quad (9)$$

The integration covers the unit cell, V is the volume of the unit cell. We define a structure function $P(\vec{G})$, and

$$P(\vec{G})=\frac{1}{V}\int\exp(-i\vec{G}\cdot\vec{r})\mathrm{d}^3\vec{r} \quad (10)$$

where the integration only covers the volume of scatterers A. It is found that the form of the structure function $P(\vec{G})$ does not depend on the type of the Bravais lattice, but on the geometry of scatterers A only. Now Eq.(9) can be written as:

$$f(\vec{G}) = f_AF+f_B(1-F)\equiv\overline{f} \qquad (\vec{G}=0) \quad (11)$$

$$f(\vec{G}) = (f_A-f_B)P(\vec{G})=\Delta fP(\vec{G}) \quad (\vec{G}\neq 0) \quad (12)$$

If the scatterers are cuboids with l_1 in length, l_2 in width and l_3 in height, we can write the structure function $P(\vec{G})$ as the following,

$$P(\vec{G})=F\frac{\sin(G_xl_1/2)}{G_xl_1/2}\frac{\sin(G_yl_2/2)}{G_yl_2/2}\frac{\sin(G_zl_3/2)}{G_zl_3/2} \quad (13)$$

By using Eqs.(11) and (12), it is not difficult to rewrite Eq.(8) in the form of a standard eigenvalue equation. If the infinite series in Eqs.(4) and (7) are approximated by a sum of M reciprocal vectors, Eq.(8) can be reduced to a $3M \times 3M$ matrix eigenvalue equation about $3M$ unknown coefficients $u^i_{\overrightarrow{K}+\overrightarrow{G}}(i = x, y, z)$. This equation can be solved by a numerical method and the desired precision can be achieved by increasing the value of M. To a given wave vector $\overrightarrow{K}$ in the first BZ, an infinite number of eigenvalues can be obtained, every of which is characterized by a natural number n. The corresponding eigen frequency is $\omega_{K,n}$. Let $\overrightarrow{K}$ scan the irreducible BZ, we can get the band structure by solving the eigenvalue equation. The value of $\overrightarrow{K}$ is usually focused on the middle and edge of the first BZ. We illustrate the first BZ of 3-D face-centered-cube lattice in Fig.1, in which $\overrightarrow{K}$ is varied along straight segments UL-$L\Gamma$-ΓX-XW-WK.

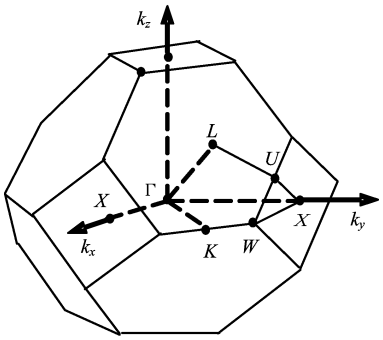

FIG. 1 Frist Brillouin-zone of three-dimensional face-center-cube lattic(FCC)

III. NUMERICAL RESULTS

Firstly, we have calculated the band gaps of a 3-D periodic system which is composed of an Au cuboid scatterer embedded in Epoxy with FCC structure. The corresponding physical parameters are listed in Table I. In our calculation, m_1, m_2 and m_3 are permitted to take the integer values between -3 and $+3$. Then Eq.(8) become a 1029×1029 matrix elements, thus, a very good convergence can be obtained. When $\overrightarrow{K}$ varies along the high symmetric straight segments of the first BZ, we can obtain a series curves of $\overrightarrow{K}$ *vs.* $\omega_{K,n}$. The band structure for a=4.0 cm, F=0.3 and l_1=l_2, l_3=1.1l_1 is shown in Fig.2(a), where the abscissa stands for the dimensionless Bloch wave vector of high-symmetry points in the first BZ and the ordinate stands for normalized frequency $\Omega = \omega a/(2\pi C_t)$, in which a is the lattice constant, ω is the angular frequency and C_t is the transverse velocities in the host. In the lowest 25 bands, we found a relative band-gap which located between the sixth and the seventh band. The normalized frequency of the mid-gap is $\Omega_g \approx 1.41$, the value of gap/mid-gap frequency is $\Delta\Omega/\Omega_g = 0.4565$, and the value of the normalized gap width is $\Delta\Omega = 0.6437$.

TABLE I The main physical parameters of the materials

Material	$\rho/(10^3\mathrm{kg/m}^3)$	$C_l/(\mathrm{m/s})$	$C_t/(\mathrm{m/s})$
Epoxy	1.85	2830	1160
Si	2.33	8950	5359
Au	19.5	3360	1240
Pb	11.4	2158	860

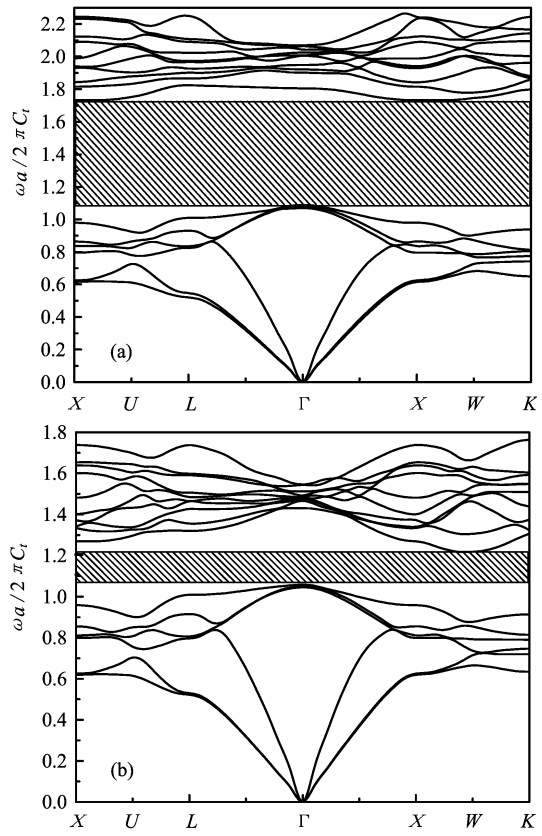

FIG. 2 Elastic wave band structure of three-dimension system with FCC lattice. (a) The case of Au cuboid embeded in epoxy host. (b) The case of Pb cuboid embedded in epoxy host. The ratio of scatterer's height to length is 1.1/1, the filling fraction of scatterer is 0.3, the lattice constants is 4.0 cm.

We changed the material of the scatterers by substituting Pb for Au (namely Pb/epoxy system). Pb cuboids are arranged periodically in an FCC lattice within an Epoxy host and the other parameters are fixed. The calculated results of the band structure are shown in Fig.2(b). It is found that a band-gap also appears between the sixth and the seventh band, and the parameters of the band-gap are Ω_g=1.13, $\Delta\Omega/\Omega_g$=0.148 and $\Delta\Omega$=0.168. If we substitute silicon for Epoxy (Au/Si system) and keep the other parameters the same as Au/Epoxy system mentioned above, no band-gap appears.

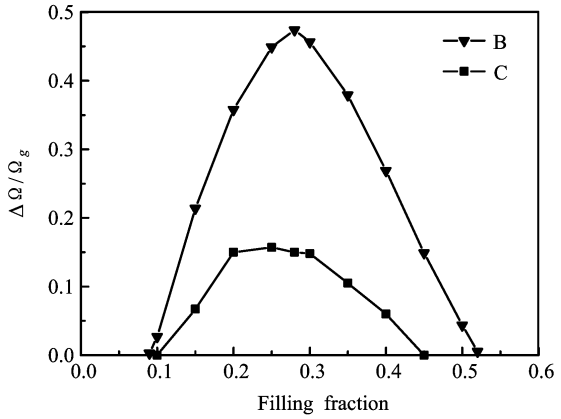

FIG. 3 The relative width of the gap, $\Delta\Omega/\Omega_g$ versus the filling fraction of the scatterer. B and C curves correspond to Au/epoxy and Pb/epoxy system.

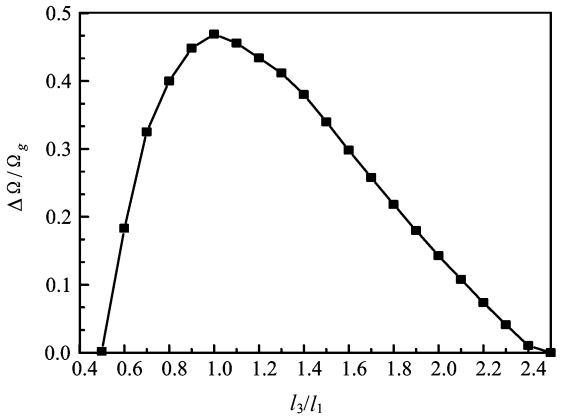

FIG. 4 The relative width of the gap, $\Delta\Omega/\Omega_g$, versus the ratio of scatterer's height to length for Au/epoxy system.

The influence of the filling fraction of the scatterers on phononic band-gaps was also studied. The relation between the band-gap width $\Delta\Omega/\Omega_g$ and the filling fraction F is shown in Fig.3. The curve marked B (or C) represents Au (or Pb) cuboid embedded in the Epoxy host with a FCC structure. It is found that the Au/Epoxy system always produces a larger gap than that of the Pb/Epoxy system for any filling fraction. It is remarkable that a complete gap opens up over a large range of filling fraction ($0.08 \leq F \leq 0.53$) in case B. The range of filling fraction is $0.09 \leq F \leq 0.45$ for us to obtain a gap in case C. The largest gap in both cases corresponds to the middle-filling fraction $F \approx 0.28$.

In addition, we choose the Au/epoxy system to investigate the influence of the ratio of cuboid scatterers' height to its length (l_3/l_1) on gap width. Let $R_{HL}=l_3/l_1$, the dependence of $\Delta\Omega/\Omega_g$ on R_{HL} is showed in Fig.4. It shows that the maximum value of $\Delta\Omega/\Omega_g$ appears when $R_{HL}=1$, and the gap disappears on the condition of $R_{HL}<0.4$ and $R_{HL}>2.5$. When $0.4<R_{HL}<1$, the gap-width increases rapidly with the increase of R_{HL}, while on the condition of $1<R_{HL}<2.5$, the gap-width decreases slowly with the increase of R_{HL}.

IV. CONCLUSIONS

By using the plane-wave-expansion method, we calculated the band structure of the binary three-dimensional solid phononic crystals consisting of cuboid scatterers embedded in a host. The scatterers are arranged in face-centered-cubic structure. Several factors, which help to obtain band-gaps and influence on the properties of band-gaps are investigated. The results show (i) Scatterers with High-velocity and high-density embedded in a host with low-velocity, and low-density provide an optimum situation to obtain large band-gaps. (ii) The symmetry of scatterers has a great influence on the band-gaps. For example, cube scatterers are more favorable than cuboid scatterers for band-gaps. The higher the symmetry of scatterers, the easier the appearance of band-gaps. (iii) The widest gap can be obtained when the filling fraction is in the middle value. If we choose appropriate physical parameters of the composites, we can obtain wider band-gaps.

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