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Anisotropy of homogenized phononic crystals with anisotropic material

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Abstract – The anisotropy of elastic waves propagating in two-dimension phononic crystals with cubic crystal material was theoretically investigated in the long wavelength limit. The anisotropy can be tuned efficiently by either rotating the crystalline orientation of the material or changing the filling fraction. It can even disappear at a given orientation and filling fraction. The pure vibration mode direction and the pure propagation mode direction can be efficiently tuned to a desired direction deviating from the symmetric plane of the phononic crystal lattice. These results will be useful in manipulating the anisotropy of a homogenized composite and dealing with a PC with anisotropic material.

Introduction. – Elastic waves propagating in an anisotropic medium are much more complex than those in an isotropic medium [1–10]. In order to calculate the elastic constants the pure vibration mode directions (PVMDs) of the crystal should be carefully identified. In addition, the pure propagation mode directions (PPMDs) of the crystal need also to be identified for designing the acoustoelectronic and acousto-optic devices because the energy flow vectors are not always collinear with the wave propagation vectors. Because of these directional dependent properties, the phononic crystal (PC) composed of anisotropic material has attracted attention in recent years [11–15]. It was shown that the band gaps can be tuned by rotating the orientation of anisotropic filler material and mode coupling may occur due to the anisotropy of host material.

At low frequencies, where the dispersion relation is linear, the PC can be equivalent to be a homogenized medium [16–26]. In this frequency range, the PC may have numerous applications in new acoustic refractive devices, such as acoustic lenses [19–21]. Recently, the anisotropy of the effective velocities of the elastic waves in the PC with isotropic material has been studied [24–26]. It has been pointed that the anisotropy of the effective velocities can be influenced by the filling fraction and the structure of the PC lattice. However, to our knowledge, the anisotropy of the homogenized PC composed of anisotropic material has not been studied up to now. Due to the directional dependent properties, it is hoped that the anisotropy of the homogenized PC can be tuned by the material anisotropy.

In this paper the anisotropy of two-dimension (2D) square lattice PCs with cubic crystal material was theoretically investigated in the long wavelength limit. Effective velocities, polarization vectors and power flow angles of the homogenized plane elastic waves were analyzed using the plane wave expansion (PWE) method. It is shown that these properties can be tuned efficiently by either rotating the crystalline orientation or changing the filling fraction. The anisotropy can be magnified or even degenerated to isotropy at the given orientation and the filling fraction. Moreover, the PVMD and PPMD of the homogenized composite can be efficiently tuned to a desired direction deviating from symmetric planes of the PC lattice, which cannot be realized for PCs with isotropic material. These results will be useful in manipulating the anisotropy of a homogenized composite and dealing with a PC with anisotropic material.

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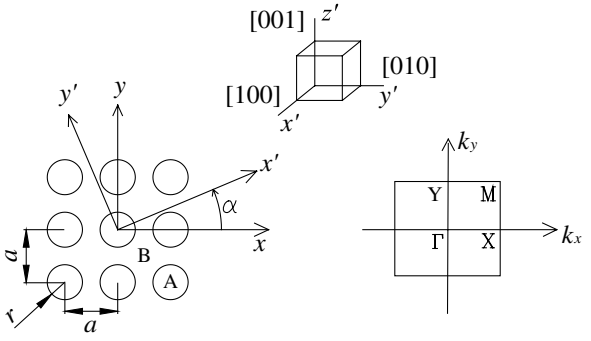

Fig. 1: The rotation angle of the cubic crystal material orientation and the first Brillouin zone. The inset indicates the material coordinate system $x'y'z'$ along the main axes of the cubic crystal material.

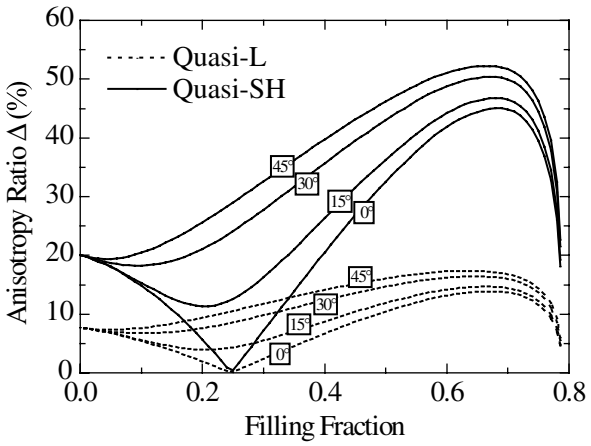

Fig. 2: The anisotropy ratio $\Delta = (c_e^{max} - c_e^{min})/c_e^{max}$ (where c_e is the effective velocity of the Quasi-L mode or Quasi-SH mode) of the quasilongitude mode and quasishear mode for the rotation angle $\alpha = 0°$, 15°, 30°, 45°, with filling fraction f changing from 0 to $\pi/4$.

Formulation. – The PC investigated in this paper is composed of square lattice isotropic epoxy cylinders (A) embedded in the single crystalline silicon (B) (cubic crystal) as shown in fig. 1. The lattice constant is a, and the radius of the cylinder is r. The PC coordinate system xyz and the material coordinate system $x'y'z'$ are set with the z-axis and the z'-axis parallel to the cylinder axis as shown in fig. 1. When rotating the main crystalline axes of the material about the z-axis with angle α, the elastic matrix $\mathbf{C}$ referred to the PC coordinate system can be obtained by the rotational transformation $\mathbf{C} = \mathbf{M} \times \mathbf{C}' \times \mathbf{M}^{\mathrm{T}}$, where $\mathbf{C}'$ is the elastic matrix referred to the material coordinate system. $\mathbf{M}$ is the Bond stress transformation matrix derived from the rotation transformation matrix [6].

For 2D PCs with the square lattice composed of cubic crystal material, a pure out-plane (SV) mode and two mixed in-plane modes, *i.e.* the quasilongitude (Quasi-L) mode and the quasishear (Quasi-SH) mode, propagate in the plane of periodicity [11,13,24]. Because the SV mode is little anisotropic and is not influenced by the rotation of the crystalline orientation of the material, only mixed modes were considered.

The general eigenvalue problem for calculating the effective velocities and polarized vectors of the mixed modes was derived by the PWE method in the long wavelength limit following refs. [22–24]. The displacement vector $u(\mathbf{r}) = (u_x(\mathbf{r}), u_y(\mathbf{r}))$ can be expanded as

$$u(\mathbf{r}) \approx u_0 e^{i\mathbf{k}\cdot\mathbf{r}} + \sum_{\mathbf{G}\neq 0} u_{\mathbf{k}+\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}, \tag{1}$$

where $\mathbf{r} = (x, y)$ is the position vector, $u_0 = (u_{x0}, u_{y0})$ is the $\mathbf{G} = 0$ term of the Fourier coefficients of the displacement vector, $\mathbf{k} = (k_x, k_y)$ is the Bloch vector and $\mathbf{G} = (G_x, G_y)$ is the reciprocal lattice vector. If the wavelength is much larger than the lattice constant, the inhomogeneous medium behaves like a homogeneous one and the Bloch waves are reduced to plane waves with polarization vector u_0 [22,23]. In order to directly obtain the polarization vector, an eigenvalue problem different from the references was derived by eliminating $u_{\mathbf{k}+\mathbf{G}}$ as

$$k^2 \mathbf{S} u_0 = \omega^2 \mathbf{R}_0 u_0, \tag{2}$$

where both $\mathbf{S}$ and $\mathbf{R}_0$ are second-order symmetric matrices. The larger and smaller eigenvalues correspond to the effective velocity of the Quasi-L mode and Quasi-SH mode, respectively. And the corresponding two eigenvectors are the polarization vectors of the Quasi-L mode and Quasi-SH mode, respectively.

In order to guarantee convergence 225 plane waves were used in the numerical calculation. Parameters of materials are $\rho_{\mathrm{Si}} = 2331\,\mathrm{kg/m^3}$, $C'_{11\mathrm{Si}} = 165.78\,\mathrm{GPa}$, $C'_{12\mathrm{Si}} = 63.94\,\mathrm{GPa}$, $C'_{44\mathrm{Si}} = 79.62\,\mathrm{GPa}$, $\rho_{\mathrm{epoxy}} = 1142\,\mathrm{kg/m^3}$, $C'_{11\mathrm{epoxy}} = 7.54\,\mathrm{GPa}$, $C'_{44\mathrm{epoxy}} = 1.48\,\mathrm{GPa}$ [27]. Due to the symmetry of the PC lattice and the material, α is changed from 0° to 45°. From the calculation, it is found that the z-axis which is the fourfold axis of both the PC square lattice and the cubic crystal material is also the fourfold axis of the composite's slowness curve, so only the propagation direction from 0° to 90° was considered here, *i.e.* from the ΓX direction to the ΓY direction in the first Brillouin zone as shown in fig. 1.

Velocities anisotropy. – The anisotropy of the effective velocities is characterized by the anisotropy ratio $\Delta = (c_e^{max} - c_e^{min})/c_e^{max}$, where c_e is the effective velocity of Quasi-L mode or Quasi-SH mode [24]. Figure 2 gives the anisotropy ratio of the Quasi-L mode and the Quasi-SH mode for the rotation angle $\alpha = 0°$, 15°, 30°, 45°, with filling fraction f changing from 0 to $\pi/4$. It can be seen that the anisotropy of the Quasi-SH mode is larger than that of the Quasi-L mode. Compared with $f = 0$, for each nonzero filling fraction, anisotropy ratios of both modes increase with the rotation. When the [100] crystalline axis of the material is parallel to the [10] axis of the PC lattice

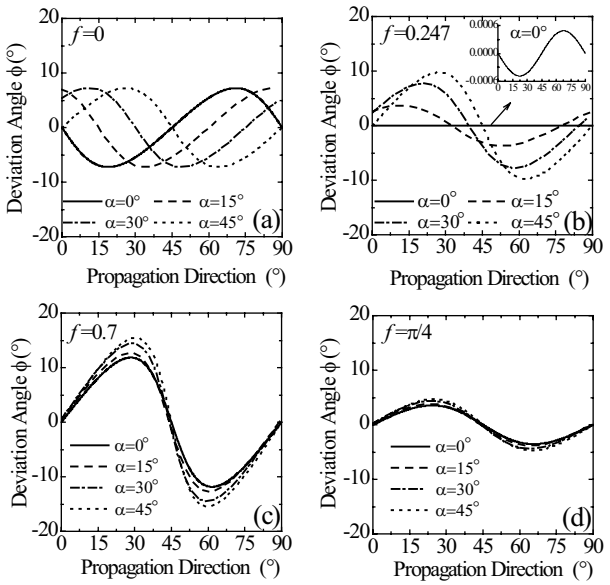

Fig. 3: Deviation angles with different rotation angles and different propagation directions: $f = 0$ (a), $f = 0.247$ (b), $f = 0.7$ (c), $f = \pi/4$ (d). The inset in (b) plots the deviation angle when $f = 0.247$ and $\alpha = 0°$, which shows that the effective velocities are nearly isotropic.

($\alpha = 0°$), the anisotropy ratios of both modes are lowest. When the [100] axis of the material is parallel to the [11] axis of the PC lattice ($\alpha = 45°$), the anisotropy ratios are largest.

From fig. 2 it can also be noted that the effect of the filling fraction on the anisotropy ratio is different for different rotation angles. The most striking feature is that there is a critical value of the filling fraction $f_{cr} = 0.247$ for which the minimum anisotropy ratio of both modes is nearly zero when $\alpha = 0°$. But this is not true for other rotation angles. It is worth noting that the anisotropy can be tuned in a large region by modifying the filling fraction and the crystalline orientation. For the Quasi-SH mode, the anisotropy ratio varies from 0 to above 52%, for the Quasi-L mode, it varies from 0 to above 17%. Moreover, when $f = f_{cr}$ and $\alpha = 0°$, both modes' anisotropy ratios approach zero, the effective velocities are nearly isotropy.

Deviation angle and PVMD. – Because of the orthogonality of the polarization vectors of the Quasi-L mode and the Quasi-SH mode, only the polarization of the Quasi-L mode was considered here. The deviation angle ϕ which is the deviation of the polarization of the Quasi-L mode from the propagation direction was obtained by $\phi = \arcsin((\mathbf{I_u} \times \mathbf{I_k})_3)$, where $\mathbf{I_u}$ is the unit polarization vector, $\mathbf{I_k}$ is unit propagation vector, the subscript 3 indicates the z-direction component. When ϕ is zero, the propagation direction is PVMD.

Figure 3 shows the deviation angles for different rotation angle α as a function of the propagation direction with filling fraction $f = 0$, 0.247, 0.7, $\pi/4$, respectively. For each nonzero f the maximum value of the deviation angle increases with α increasing as shown in fig. 3(b), (c), (d) which is different from the case $f = 0$. When $f = 0.247$ and $\alpha = 0°$, the deviation angle approaches zero, as shown in fig. 3(b). Again, it is proved that the effective velocities are nearly isotropic as the inset in fig. 3(b). The maximum deviation angle can reach above 15° when $f = 0.7$ and $\alpha = 45°$ as in fig. 3(c). Figure 3(d) shows that, when $f = \pi/4$, the deviation angle will be influenced only a little by the rotation angle. These behaviours lead us to conclude that the polarization vector will be changed by changing the crystalline orientation of the material or the filling fraction.

There are two kinds of PVMDs when the propagation direction changes from 0° to 90°. For simplification, the PVMDs analyzed here were chosen as follows: when the propagation direction changes from 0° to the PVMD, the deviation angle changes from negative to zero. It can be seen that when $f = 0$ and 0.247, PVMDs rotate from 45° to 90° monotonously with α which is different from the case when $f = 0.7$ and $\pi/4$. For nonzero f, PVMDs will be influenced by both the periodic structure and the anisotropy of the anisotropic material. It has been shown that there is a critical value of the filling fraction f_{cr} for which the homogenized composite is isotropic when $\alpha = 0°$. When $f < f_{cr}$, the material anisotropy plays the main role in the changes of the PVMDs; the PVMDs can follow the rotation of the material, and change from 45° to 90°. However, when $f > f_{cr}$, the effects of the periodic structure play the main role; as a result the PVMDs will be influenced weakly by the rotation. When $\alpha = 0°$ or 45° as the [100] crystalline axis of the material is collinear with the [10] or [11] axis of the PC lattice, the PVMDs are also in the direction of [10] or [11] axis and will not be influenced by the filling fraction. But when the [100] axis of the material deviates from the [10] or [11] axis as $\alpha = 15°$ and 30°, the PVMDs will be tuned by the filling fraction. It is concluded that the PVMDs can be tuned efficiently by changing the orientation of the material or the filling fraction. The PVMDs can deviate from the symmetric direction of the PC lattice and the material simultaneously.

Power flow angle and PPMD. – The unit energy flux vector $\mathbf{I_e}$ is coincident with the unit normal vector $\mathbf{N}$ of the slowness curve for no dissipation medium [6–8]. The power flow angle can be got by $\theta = \arcsin((\mathbf{N} \times \mathbf{I_k})_3)$, $\mathbf{N}$ can be derived from the slowness curve as in ref. [8]. When $\theta = 0°$ the propagation direction is the PPMD. Power flow angles for $f = 0$, 0.247, 0.7 and $\pi/4$ are shown in fig. 4. It is noted that for each filling fraction the maximum power flow angle of the Quasi-SH mode is larger than that of the Quasi-L mode. This is due to the fact that the Quasi-SH mode has larger anisotropy than the Quasi-L mode as shown above. In addition, the zero power flow angles of the Quasi-L mode and the Quasi-SH mode are in the same propagation directions. Furthermore, for both modes the PPMDs are coincident with the PVMDs as compared with

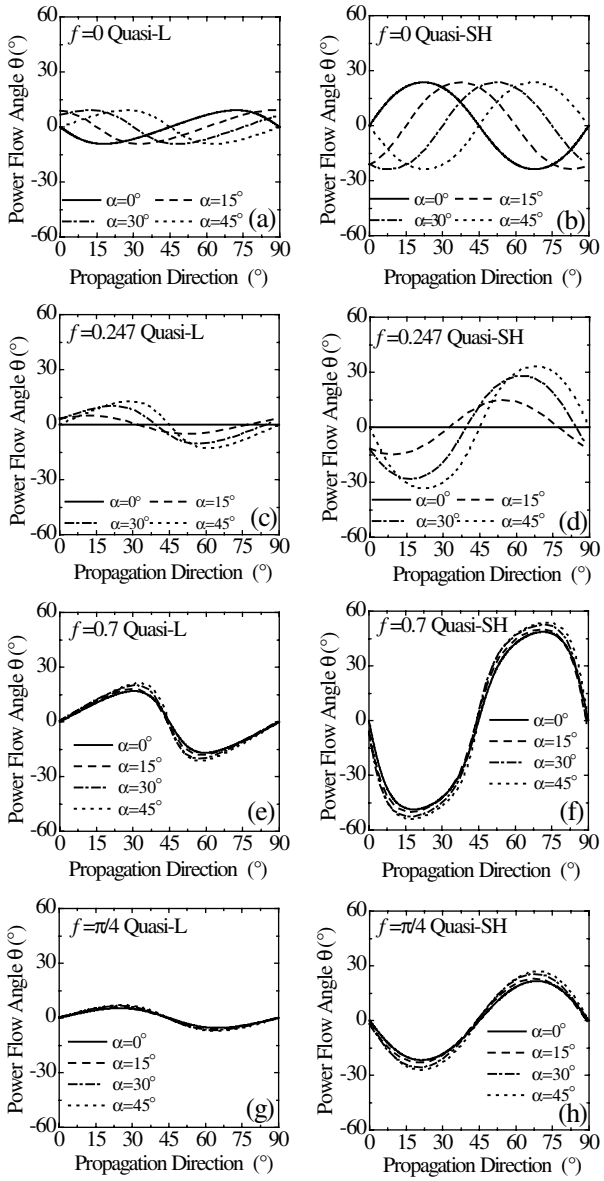

Fig. 4: The power flow angles *vs.* different rotation angles and propagation directions for the Quasi-L mode and the Quasi-SH mode, respectively, with $f = 0$, 0.247, 0.7 and $\pi/4$.

fig. 3. Generally the PPMD is not always coincident with the PVMD in the anisotropic material for the Quasi-SH mode [5,7]. For the Quasi-L mode, however, the PPMD is collinear with PVMD [5,7]. Due to the coincidence of the PPMD between the Quasi-SH and the Quasi-L mode here, the PPMD is also collinear with the PVMD for the Quasi-SH mode. Thus, the PPMD for the two modes will behave in the same way as the PVMD for different rotation angles α and different filling fractions *f*.

Conclusion. – In summary, the anisotropy of mixed modes in phononic crystals with square lattice epoxy cylinders embedded in single crystalline silicon were theoretically investigated by using the PWE method in the long wavelength limit. It is found that: by changing the filling fraction and the crystalline orientation of the material, 1) the anisotropy of effective velocities can be tuned in a large range; it can even approach to isotropy for the given filling fraction and the crystalline orientation; 2) the polarization vector and the energy flow vector (or the deviation angle and the power flow angle) can be changed; 3) the pure vibration mode direction and the pure propagation mode direction can be tuned to deviate simultaneously from the symmetric direction of the PC lattice and the material.

Through the theoretical investigation, an effective method was provided to obtain the desired anisotropy of the homogenized composite which is useful in designing acoustoelectronic and acousto-optic devices. These results can also propose the guidance for the calculation of the effective elastic constants of the PC with anisotropic material, in which case the pure vibration mode direction and pure propagation mode direction may not be collinear with the symmetric direction of the Brillouin zone.

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