PHYSICAL REVIEW E **67**, 065602(R) (2003)

Out-of-plane propagation of elastic waves in two-dimensional phononic band-gap materials

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(Received 7 March 2003; published 26 June 2003)

We have used a plane-wave-expansion model to study the out-of-plane propagation of elastic waves in a two-dimensional phononic band-gap material. The case of quartz rods embedded in an epoxy matrix has been computed. Band gaps for nonzero values of the wave-vector component parallel to the rods are shown to exist and are investigated. For wavelengths smaller than the period of the structure, modes are found that are localized in the epoxy intersites, and propagate perpendicularly to the plane of the structure.

DOI: 10.1103/PhysRevE.67.065602 PACS number(s): 43.20.+g, 43.40.+s, 46.40.Cd, 63.20.−e

Acoustic band-gap materials [1–5], also called phononic crystals, are receiving increasing attention as potential candidates for the design of passive components dedicated to signal processing. For instance, in the case of elastic waveguides, bulk localized states have been predicted [6,7], and surface states as well as localization phenomena have been calculated and observed in linear and point defects [8]. Acoustic band-gap materials are composite elastic media, constituted of two- or three-dimensional periodic repetitions of different solids or fluids, which exhibit stop bands in the spectrum of transmission of elastic waves. The existence, location, and width of acoustic band gaps in the transmission spectrum result from a large contrast in the value of the elastic constants and/or mass density of the constitutive materials.

In most theoretical and experimental studies of two-dimensional structures, elastic waves have been assumed to propagate in the plane perpendicular to cylinders. In this case, for isotropic media, the out-of-plane-polarized $[u_z(x,y)]$ and the in-plane-polarized $[u_x(x,y),u_y(x,y)]$ elastic waves are decoupled. It has been found that in some cases, these phononic band structures display gaps that exist for all incidences of plane acoustic waves scattered by the structure. In general, band gaps for in-plane polarizations do not overlap band gaps for out-of-plane polarizations in the same structure. Of particular interest has been the search for periodic two-dimensional isotropic structures that possess band gaps common to waves of both polarizations. These have come to be called absolute band gaps.

However, these band structures remain unexplored in the case of out-of-plane propagation. In particular, it might be of interest, for technological applications of such a two-dimensional periodic structure that displays an absolute band gap in its phononic band structure for in-plane propagation, to know the extent to which acoustic waves can propagate out of plane while an absolute band gap can still be seen in the corresponding band structure. Also, the possibility of guiding waves propagating perpendicularly to the plane of the structure can be revealed by such an analysis.

In this paper, we theoretically study the propagation of acoustic waves in a two-dimensional periodic anisotropic structure, which consists of an array of infinitely long parallel square-section rods of quartz (Z cut) embedded in an epoxy matrix. The intersections of the rod axis with the perpendicular plane form a two-dimensional Bravais lattice. Numerical calculations are performed using a plane-wave-expansion method, which was originally developed for 1-3 connectivity piezoelectric composites [9] and is here adapted to anisotropic solid-solid phononic band-gap materials. This method is first briefly reviewed. The quartz-epoxy structure has been chosen because it exhibits an absolute band gap for propagation in the plane perpendicular to the rods. We especially explore how this gap closes up and other absolute gaps appear as the wave-vector component parallel to the rods increases from zero.

The plane-wave-expansion method of Ref. [9] is applied to the study of two-dimensional periodic band-gap structures as follows. According to the Bloch-Floquet theorem, any field $h(\boldsymbol{r},t)$ in a periodic structure can be expanded as the infinite series,

$$h(\boldsymbol{r},t)=\sum_{\boldsymbol{G}} h_{\boldsymbol{k}+\boldsymbol{G}}\exp[j(\omega t-\boldsymbol{k}\cdot\boldsymbol{r}-\boldsymbol{G}\cdot\boldsymbol{r})], \quad (1)$$

where $\boldsymbol{k}$ is the wave vector and $\boldsymbol{G}$ are the vectors of the reciprocal lattice. Here the field h represents either the displacements u_i, the stresses T_{ij}, the electric potential ϕ, or the electric displacement D_i, with i and j running from 1 to 3. The mechanical, piezoelectric, and dielectric constants, and the mass density are expanded as Fourier series over the reciprocal lattice. Considering the usual constitutive relations of piezoelectricity together with the fundamental equation of dynamics and Poisson's equation for insulating media,

$$T_{ij}=c_{ijkl}u_{k,l}+e_{lij}\phi_{,l}, \quad (2)$$

$$D_i=e_{ikl}u_{k,l}-\epsilon_{il}\phi_{,l}, \quad (3)$$

TABLE I. Material constants of quartz (crystal-lattice group 32) and epoxy. Only the independent constants are given for each material.

Material	Mass density (kg/m^3) ρ	Elastic constants (10^{10} N/m^2) c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{14}	Piezoelectric constants (C/m^2) e_{11}	e_{14}	Dielectric constants (10^{-11} F/m) ε_{11}^S	ε_{33}^S
Quartz (SiO_2)	2648	8.674	0.70	1.191	10.72	5.794	−1.791	0.171	−0.0406	3.92	4.103
Epoxy	1142	0.7537				0.1482				3.8	

$$\rho \frac{\partial^2 u_j}{\partial t^2} = T_{ij,i}, \tag{4}$$

$$D_{i,i} = 0, \tag{5}$$

we define a generalized displacement vector $\boldsymbol{u} = (u_1, u_2, u_3, \phi)^T$ and generalized stress vectors $\boldsymbol{T}_i = (T_{i1}, T_{i2}, T_{i3}, D_i)^T$. Assuming N terms in the expansions, and considering the following vector notation $\tilde{\boldsymbol{T}}_i = (\boldsymbol{T}_{i\boldsymbol{k}+\boldsymbol{G}^1}, \ldots, \boldsymbol{T}_{i\boldsymbol{k}+\boldsymbol{G}^N})^T$ and $\tilde{\boldsymbol{u}} = (\boldsymbol{u}_{\boldsymbol{k}+\boldsymbol{G}^1}, \ldots, \boldsymbol{u}_{\boldsymbol{k}+\boldsymbol{G}^N})^T$, we obtain after some algebra [9] the very compact system

$$j\,\tilde{\boldsymbol{T}}_i = A_{ij}\Gamma_j \tilde{\boldsymbol{u}} \quad (i = 1,2,3), \tag{6}$$

$$\omega^2 R\,\tilde{\boldsymbol{u}} = \Gamma_i (j\,\tilde{\boldsymbol{T}}_i), \tag{7}$$

and the linear eigenvalue problem

$$\omega^2 R\,\tilde{\boldsymbol{u}} = \Gamma_i A_{ij} \Gamma_j \tilde{\boldsymbol{u}}, \tag{8}$$

where R and A_{ij} are the spectral mass density and material constant matrices, respectively. The diagonal matrices Γ_i contain the components of the wave vector and of the reciprocal-lattice vectors. We use the orthogonality properties of the expansions to separate the independent spectral unknowns and set up the algebraic system. The modes of the periodic structures are obtained by solving the eigenvalue problem (8) for ω as a function of the wave vector $\boldsymbol{k}$. All computations in this study have been performed considering 100 terms (10×10) $\boldsymbol{G}$ in each of the Fourier and Bloch-Floquet series, resulting in a 400×400 eigenvalue problem. It was verified, by using more reciprocal-lattice vectors, that the convergence is better than a few per cent for the first band gaps shown in Figs. 2 and 3. For higher frequencies, as considered in Fig. 4, the convergence degrades, although the essential features are conserved.

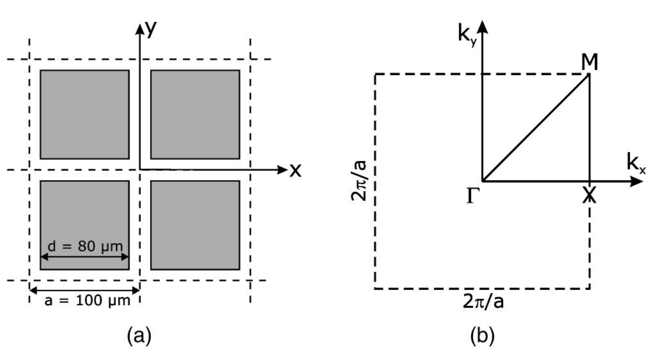

FIG. 1. (a) Cross section of a biperiodic solid-solid phononic band-gap material, consisting of quartz rods in epoxy. (b) First Brillouin zone in the (k_x, k_y) plane.

Figure 1(a) displays the cross section of the structure considered in this work. The structure consists of quartz (Z cut) rods in an epoxy matrix (see material constants in Table I). The inclusions are arranged periodically on a square lattice and are assumed to have a square cross section so that the filling fraction $(d/a)^2$ is 0.64. For instance, the width d of the inclusions is 80 μm, with a lattice parameter a equal to 100 μm. Figure 1(b) displays the first Brillouin zone associated with the Bravais lattice of Fig. 1(a).

Figure 2 shows the projected band structures in the (k_x, k_y) plane onto the reduced frequency fa, normalized-wave-vector, γ_z, plane, with $\gamma_z = k_z a/2\pi$. The white regions indicate absolute band gaps in the (k_x, k_y) plane. The width of the low-frequency band gap, labeled (a) in Fig. 2, is seen to increase quasimonotonically from zero with increasing γ_z. When γ_z increases, the width of gap (b) that exists from $fa = 1500$ Hz m to $fa = 2200$ Hz m initially increases until $\gamma_z \simeq 0.15$, then decreases and vanishes at $\gamma_z \simeq 0.4$. Gap (c) appears at $\gamma_z \simeq 0.2$ and vanishes at $\gamma_z \simeq 0.9$, while gap (d) exists from $\gamma_z \simeq 0.3$ to $\gamma_z \simeq 0.65$.

In order to understand better the evolution of these gaps, Fig. 3 displays the phononic band structures in the first Brillouin zone for the high symmetry axis, i.e., along the

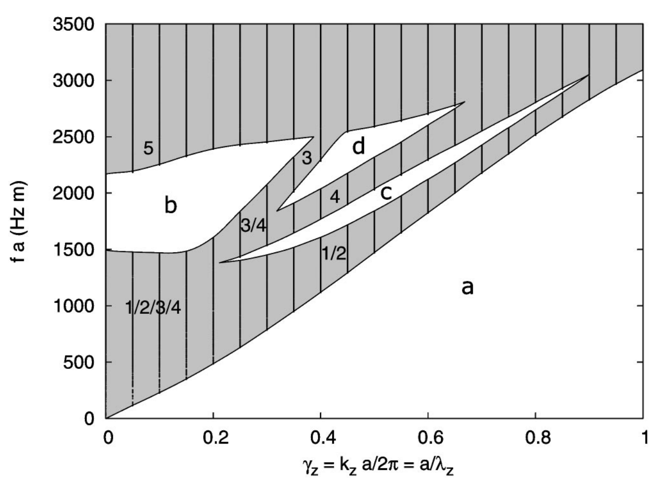

FIG. 2. Projection of the phononic band structures in the (k_x, k_y) plane onto the (k_z, f) plane. Numbers indicate the positions of particular branches labeled in Fig. 3. Delimited white regions indicate absolute stop bands in the (k_x, k_y) plane.

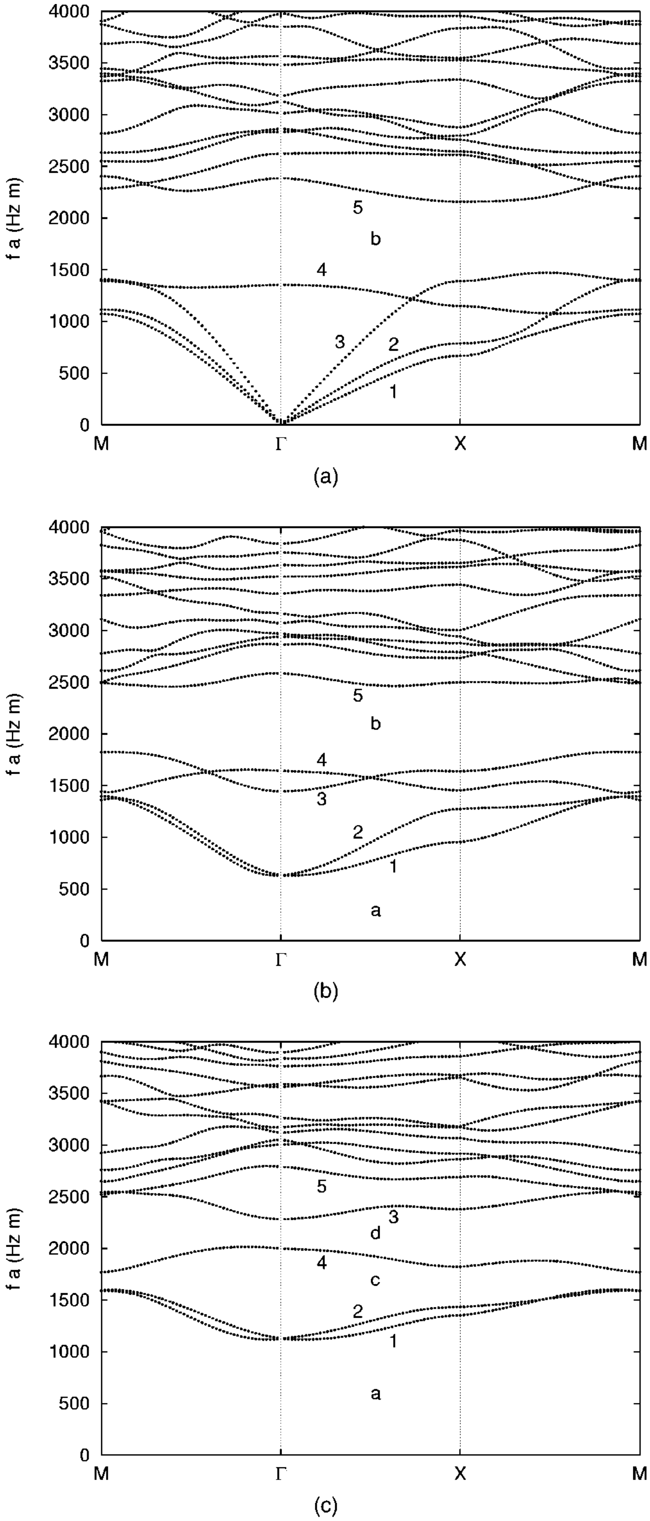

FIG. 3. Dispersion curves along the M-Γ-X-M path shown in Fig. 1(b), for (a) $\gamma_z = 0$, (b) $\gamma_z = 0.25$, and (c) $\gamma_z = 0.4$. The first five branches are numbered in the order of their appearance in the $\gamma_z = 0$ dispersion diagram.

M-Γ-X-M path indicated in Fig. 1(b), calculated when the normalized wave vector $\gamma_z = k_z a/2\pi$ equals 0, 0.25, and 0.4, respectively. Indeed, we have verified by numerical computation that the projection of such dispersion curves onto the

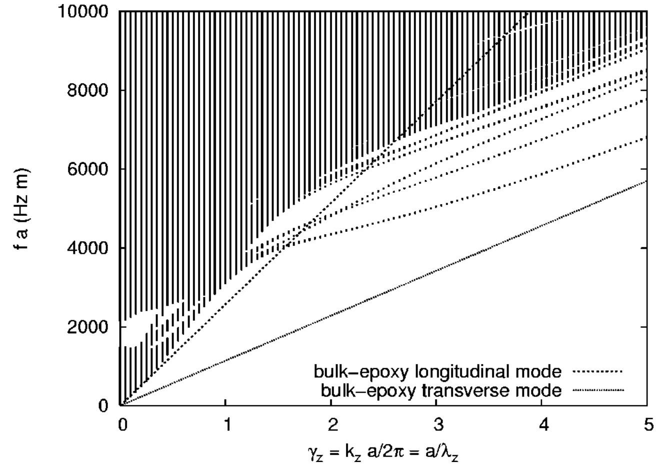

FIG. 4. Same as Fig. 2 but for an enlarged range of k_z values. Bulk-epoxy longitudinal and transverse modes are indicated.

(k_z, f) plane gives the same result as their projection for all wave vectors in the first Brillouin zone. The results for $\gamma_z = 0.25$ differ significantly from those for $\gamma_z = 0$. The most striking difference is that the dispersion curves for the lowest-frequency branches, in the case $\gamma_z = 0.25$, do not tend to zero anymore as both k_x and k_y tend to zero. Thus, a band gap below the first band opens up in the phononic band structure for nonzero γ_z, whose width increases as γ_z increases.

In Fig. 3, the first five branches were numbered in order to follow their evolution with increasing γ_z. It can be seen that gap (b), which vanishes for $\gamma_z \simeq 0.4$, is delimited by the first four branches and the fifth one. Simultaneously, gap (c), which appears from $\gamma_z \simeq 0.2$, is delimited by the first two branches and the fourth, since the third branch is now found at higher frequencies. Gap (d), which appears at $\gamma_z \simeq 0.3$, is found between the third and fourth branches. In fact, the third and fourth branches cross each other as γ_z increases from 0, so that the third branch is found at higher frequencies than the fourth one when γ_z is larger than 0.3. Consequently, the three apparent gaps (a)–(c) can be considered as a unique gap traversed by two acoustic modes.

Figure 4 is the same as Fig. 2 with an enlarged range of γ_z. It can be observed that for $\gamma_z > 1$, i.e., when the wavelength λ_z along the z axis is smaller than the period of the structure, some quasilinear branches appear that are separated by gaps. If γ_z is held constant, these modes are flat branches in the (k_x, k_y) plane. Consequently, their group velocities $(\partial\omega/\partial k_x, \partial\omega/\partial k_y)$ are zero in the (x,y) plane, and energy propagates along the rod axes. It has been verified by plotting their modal distribution that energy is localized in the epoxy matrix. Moreover, these branches seem to have an asymptotic behavior, i.e., they tend to the branch of the bulk-epoxy transverse mode. Figure 4 also illustrates a property of the existence of gap (a), as labeled in Fig. 2. There are no allowed states from zero up to a certain frequency when k_z is greater than zero. This is because the slowest wave in the structure is the bulk-epoxy transverse mode, irrespective of the values of k_x and k_y. Then gap (a) always exists, and extends at least over the triangle below the bulk-epoxy transverse-mode line shown in Fig. 4.

An interesting feature of phononic band structures is that not only does the band gap in anisotropic media gradually closes up as γ_z increases from zero, but other gaps open up for nonzero values of γ_z. Also, the frequencies of the lower and upper limits of those gaps shift to higher values as γ_z increases. Consequently, the frequency filtering characteristics of two-dimensional phononic structures can be modified by varying γ_z away from zero. This property can be useful for technological applications of periodic structures, but also implies that accurate alignment of the wave vector of the elastic waves is required. An immediate application of this study concerns waveguiding in the plane of such periodic structures when some defaults are added or dropped. Even if the wave-vector component along the z axis is not exactly zero, the elastic wave is still guided since the band gap still exists. The theory presented also accounts for solid-solid phononic crystal fibers, for which propagation is along the normal to the periodic plane.

In summary, we have computed the phononic band structure of an anisotropic infinite square array of parallel quartz rods embedded in an epoxy matrix. We have used an extended plane-wave-expansion method that can describe general anisotropic materials. The studied structure possesses an absolute band gap in the plane perpendicular to the rods, i.e., for all polarizations of elastic waves propagating in the plane of the structure. We have demonstrated the existence of band gaps for nonzero values of k_z, resulting from the closing of the former gap, and from the opening of other gaps when k_z increases. For wavelengths smaller than the period of the structure, modes appear that are localized in the matrix intersites in the plane of the structure, and propagate perpendicular to it. Finally, this study predicts the possibility of solid-solid phononic fibers to guide elastic waves along the z axis.

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