OUT-OF-PLANE PROPAGATION AND DEFECT GUIDING OF ELASTIC WAVES IN TWO-DIMENSIONAL PHONONIC BAND-GAP MATERIALS

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Abstract

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 cases of quartz or tungsten rods embedded in an epoxy matrix have been computed. Band-gaps for non-zero values of the wave-vector component parallel to the rods are shown to exist and are investigated. By inserting a nitride aluminum (AlN) rod in the tungsten/epoxy composite, defect modes are found to occur in the band gaps with their eigenvectors being localized inside and around the AlN rod. Such modes can contribute to localize the energy of an external excitation to propagate along the defect rod.

Introduction

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 treatment. For instance, in the case of elastic wave-guides, 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, that 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 a such 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 isotropic and anisotropic structure, that consists of an array of infinitely long parallel square-section rods of quartz (Z-cut) or tungsten embedded in an epoxy matrix. The intersections of the rod axis with the perpendicular plane form a two-dimensional Bravais lattice. To achieve an out-of-plane propagating wave within a confinement in (x,y) plane, we add a defect (AlN rod) which should break the periodicity and induce localized modes in the band gaps. 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 shortly reviewed. The quartz or tungsten-epoxy structures have been chosen because they exhibit absolute band gaps for propagation in the plane perpendicular to the rods. We especially explore the behaviors of band gaps and defect modes as the wave-vector component parallel to the rods increases from zero.

Numerical method

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

$$
\begin{aligned}
T_{ij} &= c_{ijkl}\, u_{k,l} + e_{lij}\, \phi_{,l} \quad , && (2)\\
D_i &= e_{ikl}\, u_{k,l} - \epsilon_{il}\, \phi_{,l} \quad , && (3)\\
\rho \frac{\partial^2 u_j}{\partial t^2} &= T_{ij,i} \quad , && (4)\\
D_{i,i} &= 0 \quad , && (5)
\end{aligned}
$$

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 $\widetilde{\boldsymbol{T}}_i = (\boldsymbol{T}_{i\boldsymbol{k}+\boldsymbol{G}^1}, \ldots, \boldsymbol{T}_{i\boldsymbol{k}+\boldsymbol{G}^N})^T$ and $\widetilde{\boldsymbol{u}} = (\boldsymbol{u}_{\boldsymbol{k}+\boldsymbol{G}^1}, \ldots, \boldsymbol{u}_{\boldsymbol{k}+\boldsymbol{G}^N})^T$, we obtain after some algebra [9] the very compact system

$$
\begin{aligned}
j\, \widetilde{\boldsymbol{T}}_i &= A_{ij}\, \Gamma_j\, \widetilde{\boldsymbol{u}} \qquad (i = 1, 2, 3), && (6)\\
\omega^2 R\, \widetilde{\boldsymbol{u}} &= \Gamma_i\, (j\, \widetilde{\boldsymbol{T}}_i)\,, && (7)
\end{aligned}
$$

and the linear eigenvalue problem

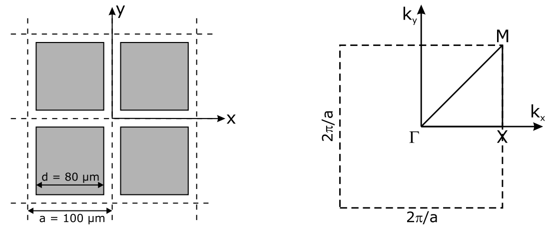
$$
\omega^2 R\, \widetilde{\boldsymbol{u}} = \Gamma_i\, A_{ij}\, \Gamma_j\, \widetilde{\boldsymbol{u}}\,, \tag{8}
$$

where R and A_{ij} are the spectral mass density and material constants 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 $\boldsymbol{k}$. Computations concerning the first studied structure 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 Fig. 2. For higher frequencies, the convergence degrades, although the essential features are conserved.

Computations

Quartz/epoxy composite

Figure 1a displays the cross-section of the first structure considered in this work. The structure consists of



(a) (b)

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

quartz (Z-cut) rods in an epoxy matrix. 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 1b displays the first Brillouin zone associated with the Bravais lattice of Figure 1a.

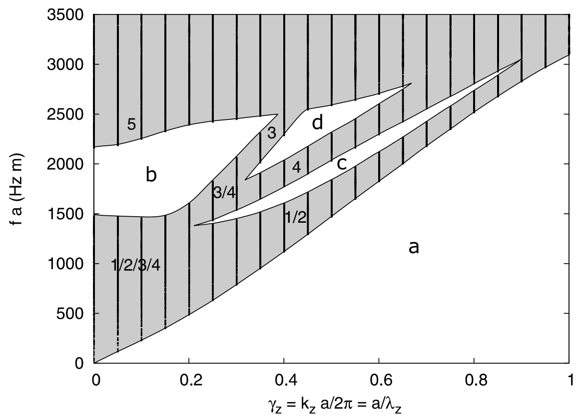


Figure 2: Projection of the phononic band structures in the (k_x, k_y) plane onto the (k_z, f) plane. Numbers indicate the positions of particular branches labeled in Fig. 3. Delimited white regions indicate absolute stop-bands in the (k_x, k_y) plane.

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 quasi-monotonically 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 $M - \Gamma - X - M$ path indicated in Fig. 1b, cal-

Material	Mass density ($\mathrm{kg/m^3}$)	Elastic constants ($10^{10}\mathrm{N/m^2}$)					
	ρ	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{14}
Quartz (SiO_2)	2648	8.674	0.70	1.191	10.72	5.794	-1.791
AlN	3260	34.5	12.5	12	39.5	11.8	-
Tungsten	19300	50	-	-	-	15.13	-
Epoxy	1142	0.7537	-	-	-	0.1482	-

Table 1: Mechanical constants of Quartz (crystal-lattice group 32), AlN,Tungsten and Epoxy. Only the independent constants are given for each material.

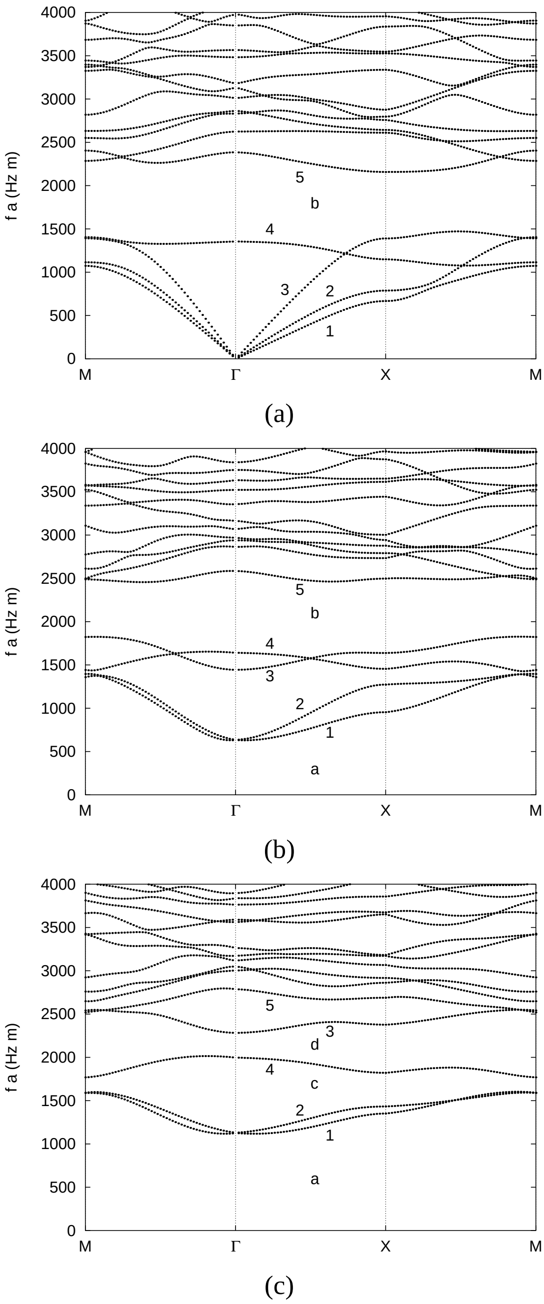


Figure 3: Dispersion curves along the $M-\Gamma-X-M$ path shown in Fig. 1b, for (a) $\gamma_z=0$, (b) $\gamma_z=0.25$, and (c) $\gamma_z=0.4$. The first five branches are numbered in the order of their appearance in the $\gamma_z=0$ dispersion diagram.

culated 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 (k_z, f) plane gives the same result as the projection of all wave-vectors in the first Brillouin zone. The results for $\gamma_z = 0.25$ differ sensitively 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 go to zero anymore as both k_x and k_y tend to zero. In fact, when $\gamma_z \neq 0$ there is a minimum frequency below which no extended solutions exist. 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. Thus, a band-gap below the first band opens up in the phononic band structure for non-zero γ_z, which 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), that vanishes for $\gamma_z \simeq 0.4$, is delimited by the first four branches and the fifth one. Simultaneously, gap (c), that 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), that appears at $\gamma_z \simeq 0.3$, is found between the third and the 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.

Tungsten/epoxy composite with an AlN defect

The second structure consists of tungsten rods in an epoxy matrix with a centered AlN rod. The width of the rods is 45 μm for a period of 100 μm. For computations we define what we call a supercell. It consists of a 3×3 tungsten-rod array, the central rod being replaced with an AlN rod. We have used 18 terms in the series.

As previously, Figure 4 shows the map of the band gaps and defect modes in 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

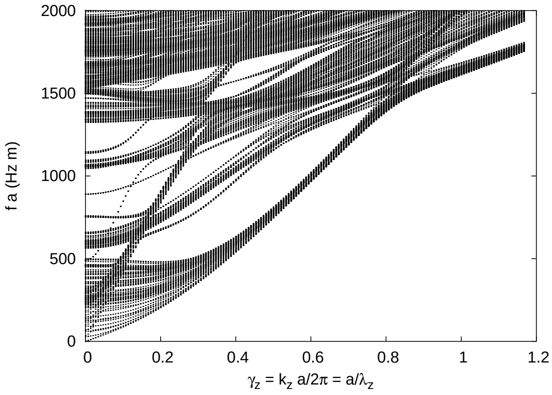


Figure 4: Projection of the phononic band structures in the (k_x, k_y) plane onto the (k_z, f) plane, for the tungsten/epoxy/AlN structure. Delimited white regions indicate absolute stop-bands in the (k_x, k_y) plane. Defect modes appear in these regions.

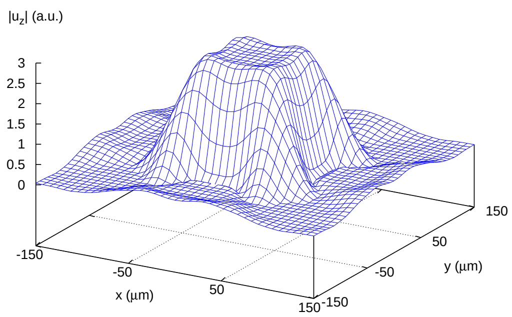


Figure 5: Relative magnitude of displacements of the tungsten/epoxy/AlN structure along the z-axis, for $k_x = k_y = 0$, $\gamma_z = 0.1$, and $f\ a = 848.2$ Hz m.

(k_x, k_y) plane. The branches into the gaps are related to defect modes. It is seen that the structure has several guided modes which go through the different band gaps. If γ_z is held constant, these modes are flat branches in the $(k_x\ , k_y)$ plane. Consequently, their group velocities are zero in the $(x$,$y)$ plane and their excitation leads to the propagation of energy along the rod axis. Figure 5 shows the vibration of one of these modes, for $k_x = k_y = 0$, $\gamma_z = 0.1$, and $f\ a = 848.2$ Hz m. The vibration is localized inside and in the vicinity of the AlN rod and is due to the longitudinal mode of AlN along the z-axis.

Conclusion

In summary, we have computed the phononic band structure of an isotropic and anisotropic infinite square array of parallel quartz or tungsten rods embedded in an epoxy matrix. We have used an extended plane-wave-expansion method that can describe general anisotropic materials. The studied structures possess absolute band-gaps 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 non-zero values of k_z, resulting from the closing of the former gap, and from the opening of other gaps when k_z increases. We have established the occurrence of defect modes by inserting a nitride aluminium (AlN) rod in the tungsten/epoxy composite. These modes are found in the band gaps, with their vibration being localized around the defect sites, therefore being capable of propagating the energy along the defect rods. Finally, this study predicts the possibility of solid-solid phononic fibers guiding elastic waves along the z-axis.

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