Complete band gaps in two-dimensional phononic crystal slabs

A. Khelif,[1] B. Aoubiza,[2] S. Mohammadi,[3] A. Adibi,[3] and V. Laude[1]
[1]*Institut FEMTO-ST, CNRS UMR 6174, Université de Franche-Comté, Besançon, France*
[2]*Laboratoire de Mathématiques de Besançon, CNRS UMR 6623, Université de Franche-Comté, Besançon, France*
[3]*School of Electrical and Computer Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332, USA*
(Received 12 July 2006; published 17 October 2006)

The propagation of acoustic waves in a phononic crystal slab consisting of piezoelectric inclusions placed periodically in an isotropic host material is analyzed. Numerical examples are obtained for a square lattice of quartz cylinders embedded in an epoxy matrix. It is found that several complete band gaps with a variable bandwidth exist for elastic waves of any polarization and incidence. In addition to the filling fraction, it is found that a key parameter for the existence and the width of these complete band gaps is the ratio of the slab thickness, d, to the lattice period, a. Especially, we have explored how these absolute band gaps close up as the parameter d/a increases. Significantly, it is observed that the band gaps of a phononic crystal slab are distinct from those of bulk acoustic waves propagating in the plane of an infinite two-dimensional phononic crystal with the same composition. The band gaps of the slab are strongly affected by the presence of cutoff frequency modes that cannot be excited in infinite media.

DOI: 10.1103/PhysRevE.74.046610 PACS number(s): 43.20.+g, 43.35.+d, 77.65.Dq

The propagation of elastic waves in inhomogeneous media has attracted much attention over the last years. Recently, there has been a growing interest in a special type of inhomogeneous material, the so-called phononic crystal, whose elastic coefficients vary periodically in space [1,2]. The interest in these materials arises mainly from the possibility of having frequency regions, known as absolute phononic gaps, over which there can be no propagation of elastic waves, whatever their polarization and wave vector [3]. In addition to their ability to behave like perfect mirrors, these structures can prove particularly useful for applications requiring a spatial confinement of acoustic waves and can hence be used as acoustic filters or very efficient waveguides. All these functions can be achieved in a very tight space of the order of some acoustic wavelengths [4–10]. At the same time, the use of elastic waves in piezoelectric slabs (which are often referred to as Lamb waves or plate modes in the literature) is important in a variety of applications, including physical, chemical, and biological sensors. Lamb waves and plate modes can also be used for high-frequency applications, such as radio-frequency filters [11].

The purpose of this paper is to investigate theoretically the propagation of elastic waves in the slab geometry with a periodic variation of material constants in the plane, a structure to which we refer to as a phononic crystal slab. Such a structure has for example been studied experimentally by Zhang *et al.* [12]. These authors have identified directional band gaps for slab or plate modes, though they term these modes surface acoustic waves. We note that surface acoustic waves exist in principle on semi-infinite media, or at least on slabs much thicker than the surface wave penetration depth. Directional [13] and complete [14] band gaps for surface acoustic waves have been observed experimentally. In models, phononic crystals are generally considered infinite or semi-infinite, whereas actual phononic crystals in experiments are obviously of finite size, with the slab geometry being the simplest and most widespread. It should not be taken for granted that band structures and band gaps are identical in the slab and infinite phononic crystal cases. Indeed, we show in the following that they can differ significantly.

The system considered in the computations to follow is a square lattice of finite quartz cylinders (with their c crystallographic axis aligned along the principal axis of the cylinder) embedded in an epoxy host material, as depicted in Fig. 1. The choice of quartz and epoxy as the composite materials is based on the strong contrast between their mass densities and phase velocities, as usual when complete band gaps are sought. In addition, the piezoelectricity of quartz makes it possible to generate and detect waves within the composite material. As an example this property is exploited in piezocomposite acoustic transducers. It should be noted however, that piezoelectricity is not essential for the results we obtain. In particular, it has only a faint influence on band structures, which are mostly determined by elastic material constants. Band structure calculations are performed by using the finite element method with periodic boundary conditions [14]. We show the existence of several full band gaps with a variable bandwidth for acoustic waves of any polarization and incidence. These band gaps are markedly different from those of an equivalent two-dimensional phononic crystal, i.e., a phononic crystal slab for which the thickness would be allowed to go to infinity. We especially discuss the role of the

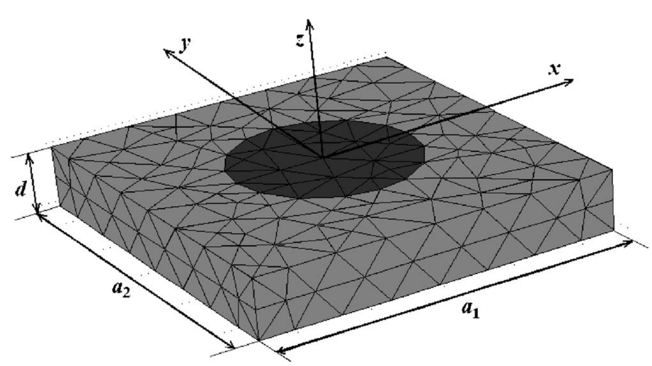

FIG. 1. Illustration of a unit cell structure.

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

Material	Mass Density (kg/m^2)	Elastic constants (10^{10} N/m^2)						Piezoelectric Constants (C/m^2)		Dielectric Constants (10^{-11} F/m)	
	ρ	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{14}	e_{11}	e_{14}	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	

ratio of the slab thickness to the lattice period as a key parameter for the opening and the closing of the band gaps.

The geometry of a square lattice phononic crystal slab is depicted in Fig. 1. The phononic crystal is assumed to be infinite and arranged periodically in the x and y directions. The structure has a finite size in the z direction. The whole domain is split into successive unit cells, consisting of a single cylinder of quartz surrounded by the epoxy matrix (see material constants in Table I). The inclusions are assumed to have a circular cross section so that the filling fraction is $F=\pi r^2/a^2=0.5$, where r is the radius of the inclusion and a is the pitch of the structure. Each unit cell is indexed by (m,p). The unit cell is meshed and divided into finite elements connected by nodes as shown in Fig. 1 where d denotes the thickness of the slab and a_1 and a_2 are the pitches of the array ($a_1=a_2=a$ for the square lattice). According to the Bloch-Floquet theorem, all fields obey a periodicity law, yielding for instance the following relation between the mechanical displacements u_i for nodes lying on the boundary of the unit cell:

$$u_i(x+ma_1,y+pa_2,z)=u_i(x,y,z)\exp[-j(k_x ma_1)] \times \exp[-j(k_y pa_2)], \quad (1)$$

where k_x and k_y are the components of the Bloch wave vectors in the x and y directions, respectively. Considering the periodical boundary conditions above allows us to reduce the model to a single unit cell which can be meshed using finite elements. A mechanical displacement and electrical potential finite element scheme is used. Considering a monochromatic variation of mechanical and electrical fields with a time dependence in $\exp(j\omega t)$ where ω is the angular frequency, the general piezoelectric problem with no external applied force can be written

$$\begin{bmatrix} K_{uu}-\omega^2 M_{uu} & K_{u\phi}, \\ K_{\phi u}, & K_{\phi\phi} \end{bmatrix} \begin{pmatrix} u \\ \phi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad (2)$$

where K_{uu} and M_{uu} are the stiffness and mass matrices of the purely elastic part of the problem, $K_{u\phi}$ are $K_{\phi u}$ are piezoelectric-coupling matrices, and $K_{\phi\phi}$ accounts for the purely dielectric problem. u and ϕ represent, respectively, all displacements and electrical potential at the nodes of the mesh, gathered together in vector form. As the angular frequency ω is a periodical function of the wave vector, the problem can be reduced to the first Brillouin zone. The dispersion curves are eventually built by varying the wave vector on the first Brillouin zone for a given propagation direction. The full band structure is then deduced using symmetries.

The quartz-epoxy structure with a filling fraction $F=0.5$ has been chosen for illustrations because it exhibits a clear complete band gap for bulk waves propagating in the plane of an infinite phononic crystal. Indeed, Fig. 2 displays the phononic band structure along the high symmetry axes of the first Brillouin zone, i.e., along the Γ-X-M-K-Γ path depicted in Fig. 2. The plot shows the variation of eigenfrequencies with the Floquet wave vector taken along the boundaries of the first irreducible Brillouin zone. We observe in the low frequency region the existence of two complete elastic band gaps, within which the vibration and propagation of waves of any polarization and incidence are forbidden. The first band gap extends from $fa=1100$ to 1200 m/s while the second band gap extends from 1350 to 1800 m/s, where f is the wave frequency ($\omega=2\pi f$). The two band gaps are separated by a quasiflat single mode, the group velocity of which is very small.

Let us now consider the effect of the finite thickness on the band structure of a square-lattice phononic crystal slab. To evaluate the effect of this single parameter, d, the filling fraction will remain the same in the following as in the infinite phononic crystal case of Fig. 2, i.e., $F=0.5$. As it is well known that all band gap properties scale with the lattice pitch, a, it is sufficient to study the influence of the thickness to lattice pitch ratio, d/a. From a computational point of view, it should be noticed that the band structure in Fig. 2 is obtained from a two-dimensional mesh of the plane of the infinite phononic crystal, with all three components of the

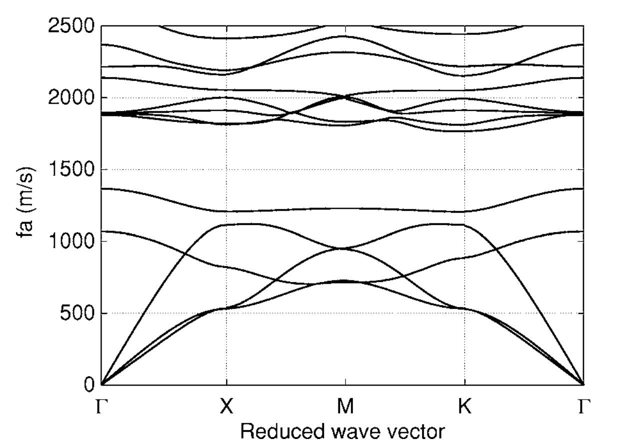

FIG. 2. Band structure of a square-lattice two-dimensional infinite phononic crystal of quartz cylinders in epoxy, computed for waves propagating in the plane of the crystal. The product of the frequency, f, times the lattice pitch, a, is plotted against the reduced wave vector taken along the Γ-X-M-K-Γ path of the first irreducible Brillouin zone. The filling fraction is 0.5.

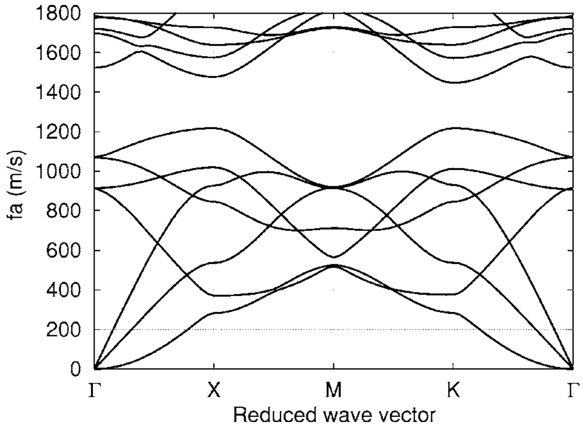

FIG. 3. Band structure of a square-lattice two-dimensional phononic crystal slab of quartz cylinders in epoxy. The filling fraction is 0.5 and the thickness to lattice pitch ratio, d/a, equals 0.3.

mechanical displacements taken into account. In the case of phononic crystals slabs, a three-dimensional mesh is used, with all three components of the mechanical displacements again taken into account. In addition, traction-free boundary conditions are enforced on both the upper and lower side of the slab.

Figures 3–6 display the bands structures for four different values of d/a, i.e., 0.3, 0.5, 1.0, and 1.3, respectively. In all four figures, the vertical axis is the frequency pitch product, fa, and the horizontal axis is the reduced wave vector taken along the Γ-X-M-K-Γ path of the first irreducible Brillouin zone. In Fig. 3, $d/a=0.3$ and we find one complete band gap between the seventh and the eighth bands. This complete band gap extends from $fa=1200$ m/s to 1450 m/s, and the relative bandwith $\delta f/f_m$ equals 18.8%. As a first observation, the band structure clearly differs from the infinite phononic crystal case. In Fig. 4, $d/a=0.5$, the complete band gap extend from $fa=1320$ m/s to 1634 m/s and the relative bandwith increases to 21.3%. This demonstrates that the band gaps are quite sensitive to the thickness to lattice pitch ratio, d/a, and that this parameter can be tuned to obtain larger relative bandwidths. For higher thickness to lattice pitch ratios, we observe the existence of two complete band gaps. Indeed when the thickness equals the pitch, as shown in Fig. 5, we observe the opening of two complete band gaps extending from $fa=1070$ to 1140 m/s and from 1325 to 1483 m/s, respectively. The higher complete band gap closes for $d/a=1.3$, as shown in Fig. 6. This closing is caused by the appearance of a new mode around $fa=1300$ m/s. This is the first slab mode with a cutoff-frequency, as we discuss below. It is worth noting that the low frequency band gap will also be affected by the same mode when the thickness to lattice pitch ratio is increased, and will eventually close.

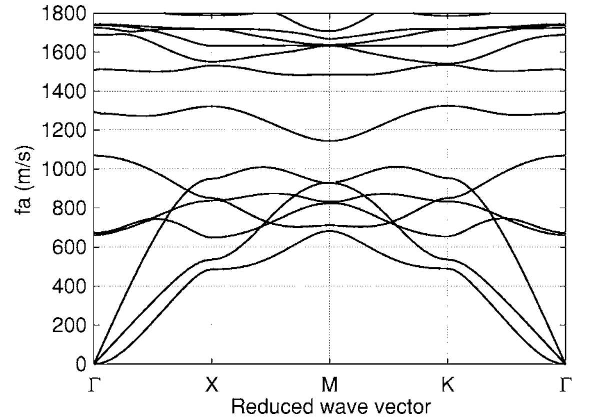

FIG. 5. Band structure of a square-lattice two-dimensional phononic crystal slab of quartz cylinders in epoxy. The filling fraction is 0.5 and the thickness to lattice pitch ratio, d/a, equals 1.0.

It is well known that the uniform slab has three bands starting from $\omega=0$, two of which have a sagittal polarization while the third has a transverse polarization, whereas higher bands have cutoff frequencies. Higher bands with cutoff frequencies are intimately linked to the boundary conditions on both surfaces of the slab. They are thus a manifestation of the finite thickness of the slab and they do not occur in infinite media. Therefore, when we deal with the low frequency region of the phononic crystal slab, it is sufficient to take into account the lowest three bands, and of course their folding caused by periodicity. In particular, this treatment is justified for phononic crystal slabs whose thickness is small enough

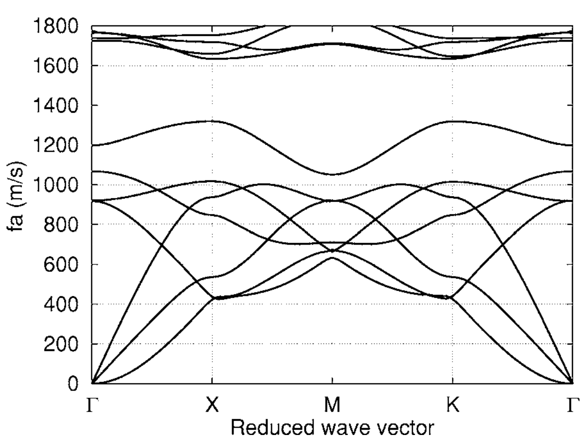

FIG. 4. Band structure of a square-lattice two-dimensional phononic crystal slab of quartz cylinders in epoxy. The filling fraction is 0.5 and the thickness to lattice pitch ratio, d/a, equals 0.5.

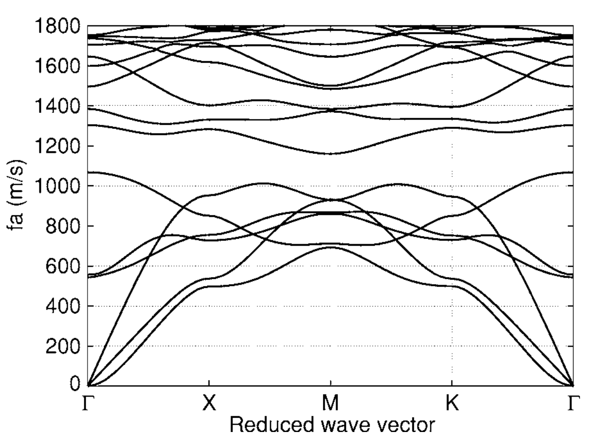

FIG. 6. Band structure of a square-lattice two-dimensional phononic crystal slab of quartz cylinders in epoxy. The filling fraction is 0.5 and the thickness to lattice pitch ratio, d/a, equals 1.3.

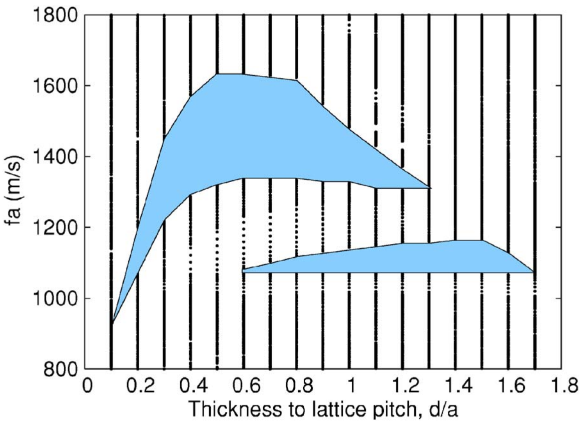

FIG. 7. (Color online) Complete band gap frequencies as a function of the thickness to lattice pitch ratio d/a for the quartz/epoxy square-lattice phononic crystal slab with a filling fraction of 0.5.

with respect to the pitch of lattice, in which case the cutoff frequencies are much higher than the band gap frequencies. However, when the thickness of the slab is comparable or larger than the pitch of the structure, higher order modes should clearly be taken into account.

A gap map showing the dependence of complete band gap frequencies with the thickness to lattice pitch ratio d/a is shown in Fig. 7. It is plotted for the quartz/epoxy square-lattice phononic crystal slab with a filling fraction of 0.5. The first complete band gap opens at the ratio $d/a=0.2$ and closes for a value of 1.3. The maximum width of the complete band gap appears at $d/a=0.5$. The second complete band gap exists in the domain $0.7<d/a<1.6$ and reaches a maximum band gap width around $d/a=1.5$. Its closing is due to the appearance of a higher order slab mode. As a general rule, when increasing the ratio d/a the cutoff frequencies of higher order modes of the equivalent homogeneous slab will decrease and eventually close the band gaps. This means that when the ratio d/a is small, the creation of complete band gaps is a consequence of the folding of the first three bands at low frequency only. But the opening of complete band gaps becomes more difficult as the ratio d/a gets larger. For values of d/a larger than two we did not observe the existence of any complete band gap. It should be noted that in practice the computation of thick slabs becomes more and more difficult as the mesh size increases.

It might appear surprising that the complete band gaps of the phononic crystal slab close as d/a goes to infinity, whereas they remain open for an infinite phononic crystal with the same structure. In fact, the infinite case is not obtained as a limiting process as the thickness of the slab goes to infinity, as it might be tempting to believe. When d/a increases, higher order slab modes appear continously; they eventually become infinitely many as d/a tends to infinity. At the same time, their cutoff frequencies go to zero. In the infinite medium case, the number of partial waves is fixed (eight for a homogeneous piezoelectric plate). The reason is that higher order slab modes require boundary conditions on both surfaces to be defined, whereas these boundary conditions are replaced by radiation conditions at infinity in the infinite case. In practice, any phononic crystal sample is of finite size, for instance with the slab geometry. The idealization used in models to turn a finite phononic crystal into an infinite one relies on the assumption that higher order slab modes cannot be excited in practice, in which case only a limited number of bands should be kept in the band structure, i.e., those bands that do not depend on the boundary conditions at the surfaces. As an example, phononic crystal slabs with a triangular lattice of air holes in epoxy on a glass substrate were recently investigated experimentally using Brillouin light scattering [15]. These phononic crystal slabs had a thickness to lattice pitch ratio $d/a=4.4$. In Ref. [15] it was assumed that the band structure for Brillouin phonons is given by that of bulk elastic waves propagating in the plane of the phononic crystal. However, at least the upper surface influences the propagation of Brillouin phonons in the slab, and the above approximation must be taken with caution.

We have here examined the propagation of elastic waves in a phononic crystal slab consisting of piezoelectric inclusions placed periodically in a host material. Our system is composed of a square lattice of quartz cylinders embedded in an epoxy matrix. We found two complete bandgaps with a variable bandwidth for a filling fraction of 50%. In addition to the three parameters that influence the formation of band gaps in phononic crystals—the lattice symmetry, the filling fraction, and the contrast between the physical parameters of the constituents—we find that the thickness to lattice pitch ratio, d/a, plays a crucial role in the opening of complete band gaps. Indeed, this parameter conditions the cutoff frequencies of higher order modes of the slab and hence the closing of the complete band gaps as the thickness increases. Significantly, the band structure of a phononic crystal differs from that of the infinite phononic crystal with the same geometry and composition.

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