Octave Omnidirectional Band Gap in a Three-Dimensional Phononic Crystal

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***Abstract*—We report on the experimental observation of a one-octave-large omnidirectional elastic band gap for longitudinal waves in a three-dimensional phononic crystal consisting of face-centered-cubic arrays of close-packed steel beads in a solid epoxy matrix. The 60% relative width of the band gap is larger than expected based on the contrast in material properties, and is confirmed by band structure diagram and transmission spectra computations. The coupling between shear and longitudinal polarizations is pointed out as a mechanism for enlarging the band gap by comparing with the steel beads in water matrix case.**

I. Introduction

Elastic band gap materials, also termed phononic crystals, are inhomogeneous elastic media composed of 1-, 2-, or 3-D periodic arrays of inclusions embedded in a matrix [1]–[3]. Several classes of phononic crystals exist and differ mainly by the physical nature of the inclusions and of the matrix. Among them, solid/solid, fluid/fluid, and mixed solid/fluid composite systems have received attention. These composite media typically exhibit stop bands in their transmission spectra for which the propagation of sound or vibration is strictly forbidden in all directions. The location and the width of acoustic band-gaps result from the choice of the lattice, of the shape of the inclusions, and of the constitutive materials. It is generally found that the larger the contrast in the value of the elastic constants and/or the mass density of the constitutive materials, the larger the band gaps. Heavy and rigid inclusions embedded inside a light and softer matrix are often a good choice for achieving large band gaps [4].

Because of added theoretical and experimental complexity, 3-D phononic crystals have been studied less than 2-D structures. In the case of 3-D phononic crystals, theoretical studies have revealed the existence of full band gaps in two-component face-centered cubic (fcc) lattices [5], [6]. Planar defects in the form of a plane of impurity spheres in 3-D phononic crystal have also been studied [7]. Experimental studies have been conducted for hexagonal close-packed (hcp) structures of steel spheres in water and three-component composites of coated spheres in a matrix [8].

Manuscript received July 10, 2009; accepted March 4, 2010.

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Digital Object Identifier 10.1109/TUFFC.2010.1592

II. Experimental Setup and Geometrical Parameters

In this work, we discuss experimental and theoretical results on the propagation of ultrasonic waves through a 3-D solid/solid phononic crystal. The crystals used in our experimental consist of close-packed periodic arrays of spherical steel beads embedded in an epoxy matrix. The lattice and the scatterers (apart from their diameter) are essentially the same as in [8], but a solid epoxy matrix (E501, Epotecny, Levallois-Perrit, France) is considered instead of a water matrix. The fcc array was assembled by placing the beads carefully by hand and the layers were stacked vertically in sequence to form slabs with an fcc structure (the [111]-axis is perpendicular to the layers). The beads are very monodisperse and the sphere diameter d is 4 mm $\pm$ 0.05 mm. The thickness of the phononic crystal is equal to 4 periods of the lattice in both the [001] and the [111] directions; thus, there are approximately 9 layers of beads in both directions.

The mass density and the shear and longitudinal velocities for acoustic waves in steel, epoxy, and water are displayed in Table I. The choice of steel and epoxy as the composite materials was originally based on the strong contrast in their densities and elastic constants. Expressed using the acoustic impedance for longitudinal waves, this contrast is approximately 16.4. If instead of epoxy, a water matrix had been used, this contrast would be even higher, approximately 30.5. Surprisingly, as detailed below, we find experimentally that the omnidirectional band gap for longitudinal waves is much larger with the steel/epoxy phononic crystal than with the steel/water one (60% instead of 25% relative bandwidth). As discussed in the next section, we attribute this enlargement of the full band-gap width to the coupling of longitudinal and shear waves inside the solid-epoxy matrix because of the presence of the steel scatterers.

The measurement apparatus is shown in Fig. 1 and is similar to the one we used previously for measurements of 2-D phononic crystals in water [9]–[12]. Ultrasonic pulse propagation through the crystal was measured by placing the crystal between two wide-bandwidth transmitter/receiver acoustic transducers (immersion transducers, Videoscan V301, Panametrics, Waltham, MA). Contact between the transducers and the phononic crystal was obtained using an ultrasonic lubricant. Note that the transducers used are designed to generate longitudinal waves, so only the transmission for longitudinal waves could be measured, and not that for shear waves.

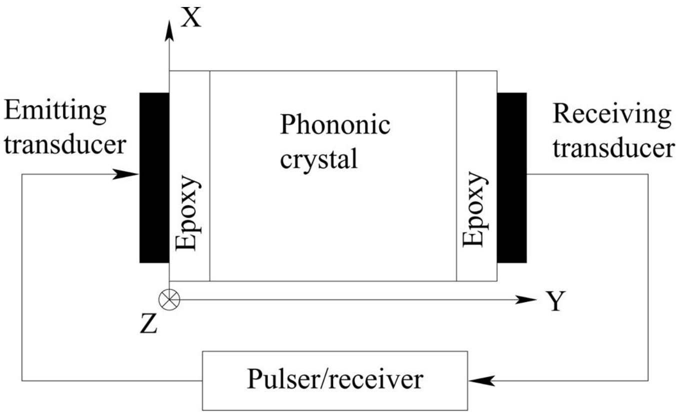

Fig. 1. Experimental set-up used to measure the transmission spectra of phononic crystals using acoustic transducers in acoustical contact with the phononic crystal.

TABLE I. Material Constants of the Phononic Crystal Constituents.

	c_S (m·s^{-1})	c_L (m·s^{-1})	ρ (kg·m^{-3})	Z_L (MRayles)
Steel	3200	5800	7780	45.124
Epoxy	1100	2500	1100	2.75
Water	n.a.	1480	1000	1.48

c_S and c_L are the velocities for shear and longitudinal waves, respectively, ρ is the mass density, and Z_L is the acoustic impedance for longitudinal waves.

III. Experimental and Theoretical Results

The effect of the direction of propagation on the band gaps was first evaluated by performing transmission measurements through the phononic crystals along the [−110], [100], and [111] directions, as shown in Fig. 2. Because of the orientation of the entrance and exit faces of the finite-size phononic crystals, at least two different samples are necessary to measure the transmission along all three directions. The [100] and [111] directions correspond, respectively, to the ΓX and the ΓR directions of the first irreducible Brillouin zone. With the fcc lattice and considering isotropic scatterers and matrix, measurements along the three considered directions are sufficient to evaluate the existence of an omnidirectional band gap for the longitudinal polarization of the wave. The acoustic transmission spectra clearly show a strong attenuation extending from 350 to 650 kHz in the [111] direction, from 260 to 680 kHz in the [100] direction, and from 240 to 680 kHz in the [−110] direction. Overlapping these transmission spectra, we find that an omnidirectional band gap exists for longitudinal waves between 350 and 650 kHz when the three directions are considered jointly; that is more than one octave. The relative bandwidth of the band gap is equal to 60%. However, in the case of the same fcc structure of steel beads in a fluid (water) matrix, in which the contrast of the longitudinal acoustic impedances is enhanced, the relative bandwidth doesn't exceed 25% [8]. Our experimental observation is then in apparent contradiction with two usual beliefs: 1) that the width of the

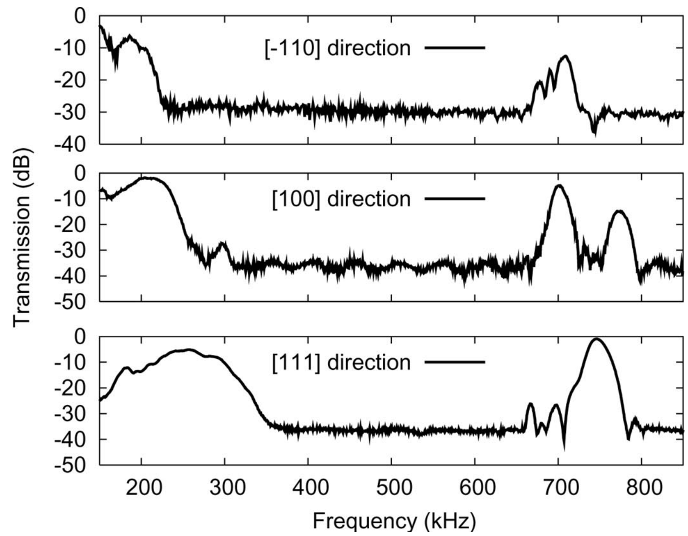

Fig. 2. Experimental transmission power spectra along the [−110], [100], and [111] directions of a phononic crystal composed of 4 periods of a face-centered cubic array of steel beads in epoxy (or 9 layers of beads). An omnidirectional band gap for longitudinal waves extending at least from 350 to 650 kHz is observed.

band gaps of phononic crystals increases with the contrast in the material properties of the two constituents, and 2) that the coupling between shear and longitudinal polarizations should reduce the band-gap opening.

A related effect was observed theoretically by Sigalas and Garcia [13] for a 2-D phononic crystal consisting of aluminum rods in mercury. In that case, they observed that a complete band gap could be found, whereas it was absent if the aluminum rods were replaced by a liquid with an equivalent acoustic impedance. They concluded that shear waves excited in the scatterers were essential in the opening of the band gaps, although they were not present in the matrix material. In our 3-D phononic crystal, there are not only shear waves in the scatterers but also in the solid matrix. Although the transducers we use only generate longitudinal waves, shear waves can appear through diffusion of waves by the scatterers. We propose that this coupling between longitudinal and shear waves strongly enhances the elastic band gaps.

Numerical computations were conducted to understand the phenomena behind the enlarged band gaps. We simulate both the band structure for an infinite periodic crystal and the transmission trough a finite sample composed of a few periods of the phononic crystal structure. In Fig. 3, we first show the band structure of 3-D steel/epoxy phononic crystals computed using the finite element method (FEM). We have here considered two different cases. In Fig. 3(a), the ratio of the beads radius to the period is $r/a = 0.3$. In this case, previously considered by Hsieh *et al.* [14], the beads are not in contact, but are instead separated from each other by a small distance. We notice the existence of a complete (for all polarizations and directions) band gap extending from 300 to 600 kHz with a very large 66% relative bandwith. The lower band gap edge is limited by the folding of the longitudinal branch at the X point, as

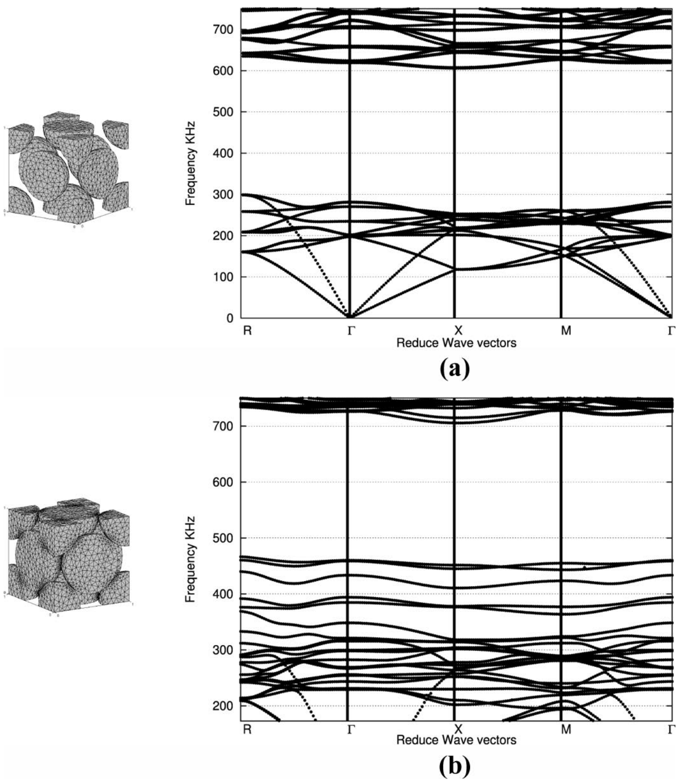

Fig. 3. (left) The lattice arrangement of 3-D face-centered cubic (fcc) lattice phononic crystal with sphere inclusions. (right) Band structure of 3-D fcc lattice phononic crystals composed of spherical steel inclusions in an epoxy matrix, shown for (a) $r/a = 0.3$ and (b) $r/a = 0.35$ (close-packed condition), respectively. Computations are conducted using the finite element method. The considered unit cell is not the elementary unit cell of the fcc lattice, but is rather a cube of length a enclosing a total of 4 beads; this convention introduces some ancillary band foldings but does not change the frequency band gap limits.

shown in [14]. However, because of the practical method of assembly we employ, the beads are in contact in our actual samples where the close-packed condition is reached ($r/a = 0.35$). This contact condition can strongly affect the dispersion, as the band structure in Fig. 3(b) reveals. Indeed, we notice the appearance of several new branches above the previously observed lower band-gap edge. These new branches can be verified to have mostly a shear polarization and they restrict the complete band gap from 450 to 700 kHz. The longitudinal omnidirectional band gap predicted by FEM then still extends from 350 to 700 kHz. This prediction is in accordance with the experimental observations, though the upper band-gap edge is overestimated.

The simulation method we used for finite thickness samples is based on the finite-difference time-domain (FDTD) method that has been proved to be an efficient method for obtaining both the transmission coefficient [15] and the dispersion curves in phononic crystals. FDTD transmission spectra were obtained numerically by discretizing time and space and replacing derivatives by finite differences in the elastic wave equation. We employ a spatial grid with mesh size $\Delta x = \Delta y = \Delta z = 0.2$ mm. The time integration step, Δt, is 10.2 ns. The total propagation time used in our calculations is 1.3 ms. The wave equation is solved using first-order centered finite-difference coefficients for finite thickness samples of 3-D phononic crystals. For the geometrical discretization, the system is composed of three parts along the propagation direction, axis Y. The central region contains the finite-size phononic crystal. This region is sandwiched between two homogeneous epoxy media used for launching and probing elastic waves. The homogeneous epoxy regions have a width of 3 periods, which is enough to consider that their external ends are in the far field for frequencies within the band gap of the phononic crystal. Periodic boundary conditions are applied along both the X and Z direction and Mur's boundary conditions are imposed at the free ends of the homogeneous region along Y direction. A broadband probe wave packet is launched in the first homogeneous epoxy region. The incoming wave is uniform in the XZ plane with a Gaussian time dependence and propagates along the Y axis. The displacements at the source plane are imposed either along the Y direction (for longitudinal waves) or the X direction (for shear waves). The wave displacements are collected at the end of the second homogeneous region and are averaged over the XZ plane. Because of the symmetry of the phononic crystals we consider and of the isotropy of steel and epoxy, the displacements of shear waves along the X and the Z axes are equal.

The effect of shear waves inside the scatterers was first checked independently from shear waves in the matrix by computing the transmission with the shear velocity of epoxy set to zero. Indeed, in this case ($C_t = 0$), only longitudinal waves can propagate in the matrix material, which is similar to the case of a liquid matrix. We found that no omnidirectional band gap could open in such a situation, i.e., directional band gaps exist but do not coincide at any frequency. This result is consistent with the fact that the material constant contrast is larger with water than with epoxy when steel scatterers are considered (see Table I).

Second, the influence of the existence of shear waves in the matrix was evaluated as follows. The following FDTD transmission spectrum matrix for both longitudinal and shear waves was computed,

$$T = \begin{pmatrix} T_{\mathrm{LL}} & T_{\mathrm{LS}} \\ T_{\mathrm{SL}} & T_{\mathrm{SS}} \end{pmatrix}, \tag{1}$$

where the first subscript refers to the polarization of the incoming waves (either longitudinal or shear) and the second subscript refers to the polarization of the output waves. The computed transmission spectra are shown in Fig. 4. The location and the overall shape of the band gaps for longitudinal waves (apparent in T_{LL}) in both directions of propagation compare well with those observed experimentally, although the experimental band gaps appear somewhat wider than the theoretical ones. We observe at this point that the steel beads in the phononic crystal are in contact on a single point, a situation that is difficult to describe with the finite cubic mesh of the FDTD method. This slight discrepancy between the

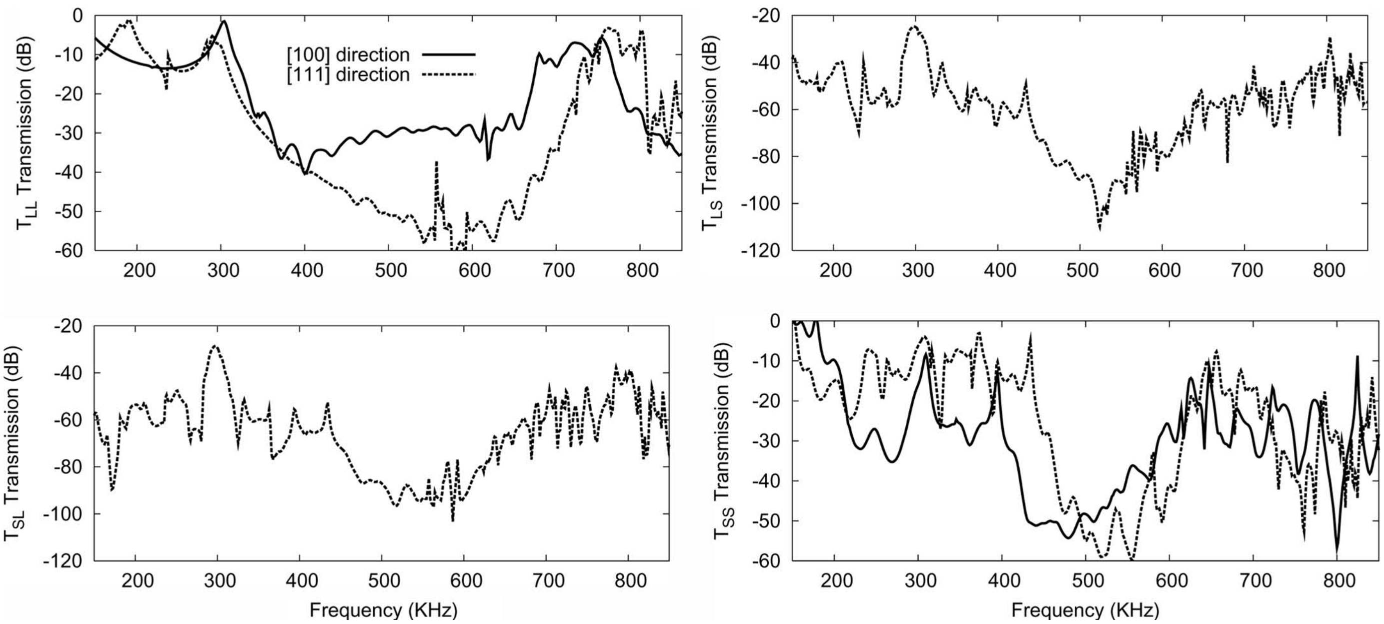

Fig. 4. Theoretical transmission spectra along the [100] (solid line) and the [111] (dashed line) directions of a phononic crystal composed of 4 periods of a face-centered cubic array of steel beads in epoxy. The transmission functions T_{LL}, T_{LS}, T_{SL}, and T_{SS} are shown, where the first subscript refers to the polarization of the incoming waves (either longitudinal or shear) and the second subscript refers to the polarization of the output waves. T_{LS} and T_{SL} for propagation along the [100] direction is vanishingly small.

model and the experimental situation, but also imperfect knowledge of the actual material constants, may explain the observed difference in the band gap widths. Also, this behavior can result from the air bubble (defect) that can occur in the process of solidification of the epoxy. Though they are not compared with experiment here, the computations involving shear waves convey valuable information regarding the influence on band gaps of the coupling between shear and longitudinal waves. The transmission of shear waves as measured by T_{SS} reveals an omnidirectional band gap extending from 450 to 580 kHz, which is entirely contained within the omnidirectional band gap for longitudinal waves. Interestingly, the transmission of longitudinal to shear waves, measured by T_{LS}, and the reverse process, measured by T_{SL}, is weak but non-vanishing along the [111] direction; it is found to be zero to within numerical errors for the [100] direction. They clearly show an even lower transmission at frequencies that are within the longitudinal or the shear complete band gaps.

Based on the previous numerical observations, the physical mechanism we propose to explain the opening of band gaps relies on the coupling of longitudinal and shear waves in the phononic crystal. The waves inside the phononic crystal can be decomposed using the complete basis of propagative and evanescent Bloch waves [16]. Within a band gap, all Bloch waves are evanescent, meaning that their wave vector considered as a complex number acquires a nonzero imaginary part. Though the receiver plane is in the far field of the phononic crystal, and hence does not record the evanescent waves that are present therein, evanescent waves are obviously involved in the properties of wave propagation in the phononic crystal. Furthermore, conversions occur in the phononic crystal between longitudinal and shear waves because of reflection and refraction processes at the steel beads. We stress at this point that the computed transmissions T_{LS} and T_{SL} in Fig. 4 are not representative of the efficiency of these conversions, which should be maximal at angles of incidence on the beads away from zero (the functions T_{LS} and T_{SL} measure these conversions for normal incidence only because the integration along the entrance and exit facets cancels oblique incidence contributions by symmetry). The existence of polarization conversions implies that the polarization of the Bloch waves composing the band structure of the phononic crystal is not pure in general, but may contain a combination of longitudinal and shear components. It is known that when their polarizations are orthogonal, two bands can cross without interacting; however when they are not, the two bands tend to repel and create a pair of evanescent waves around the frequency at which they should have crossed. The strength of the repelling is a measure of the coupling between the two bands, and hence of the width of the frequency band gaps. The net result is a widening of the band gaps as compared with an equivalent phononic crystal supporting only longitudinal or shear waves.

IV. Conclusion

In conclusion, we have investigated experimentally and theoretically the existence of a large omnidirectional elastic band gap for longitudinal waves in a three-dimensional phononic crystal consisting of a face-centered-cubic array of close-packed steel beads in an epoxy matrix. A 60% relative bandwidth omnidirectional band gap is observed in transmission, covering an octave. A band structure diagram and transmission spectra computations are found to be in good agreement with the measurements for longitudinal waves and provide additional information on the propagation of shear waves. We have observed numerically the importance of the coupling between shear and longitudinal components of the polarization for enlarging the band gap by comparing to the equivalent steel/water phononic crystal structure supporting only longitudinal waves and not showing an omnidirectional band gap. A possible explanation for band gap opening was suggested based on the creation of evanescent Bloch waves through polarization coupling between longitudinal and shear waves. In this light, the anisotropy induced by the crystal structure can be viewed as beneficial for band gap formation.

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Authors' photographs and biographies were not available at time of publication.