Transmission and dispersion relations of perfect and defect-containing waveguide structures in phononic band gap materials

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By using a combination of finite difference time domain (FDTD) and plane wave expansion (PWE) methods, we study the propagation of acoustic waves through waveguide structures in phononic band gap crystals composed of solid constituents. We investigate transmission through perfect linear waveguides, waveguides containing a resonant cavity, or waveguides coupled with a side branch resonator such as a cavity or a stub. A linear guide can support one or several modes falling in the absolute band gap of the phononic crystal. It can be made monomode over a large frequency range of the band gap by varying the width of the guide. The transmission through a guide containing a cavity can be made very selective and reduced to narrow peaks associated with some of the eigenmodes of the cavity. The effect of a side branch resonator is to induce zeros of transmission in the spectrum of the perfect guide that appear as narrow dips with frequencies depending upon the shape of the resonator and its coupling with the guide. We find perfect correspondences between the peaks in the transmission spectrum of a waveguide containing a cavity and the dips in the transmission of a cavity side coupled waveguide. Finally, when a gap exists in the spectrum of the perfect guide, a stub can also permit selective transmission of frequency in this gap. The results are discussed in relation with the symmetry of the modes associated with a linear guide or with a cavity.

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I. INTRODUCTION

In recent years, a great deal of work has been devoted to the study of propagation of elastic and acoustic waves in inhomogeneous media. More specifically, a lot of attention has been focused onto elastic wave propagation in acoustic band gap (ABG) materials, the so-called phononic crystals. These inhomogeneous materials are periodic repetitions of inclusions in some different host material. 1-3 A variety of materials constitute the inclusions or the matrix including gases, liquids or solids. Similarly to the photonic band gap materials⁴ where the propagation of light is prohibited in some frequency range, these elastic periodic composites can exhibit large acoustic band gaps where the propagation of phonons is forbidden. A phononic crystal can, therefore, behave like a perfect mirror for the propagation of vibrations in some frequency range and may have potential applications in transducer technology, filtering, and guidance of acoustic waves. Several two and three-dimensional phononic crystals made of either solid or fluid constituents, exhibiting a large contrast between their elastic properties, have been investigated. The existence of absolute band gaps was predicted theoretically and observed experimentally.⁵⁻⁹ Localized modes associated with point and linear defects 10 have also been studied including the transmitivity through a linear guide.11

Manipulation of light in waveguides inside photonic crystals allows low loss transmission through sharp bends, filtering or wavelength division multiplexing. ^{12–15} The coupling of a waveguide with resonant cavities can alter drastically

the transmission spectrum and may found useful applications. ^{16–18} In the present paper, inspired by waveguides in photonic crystals, we investigate the propagation of acoustic waves through perfect and defect-containing waveguide structures created inside a phononic crystal composed of solid constituents.

In straight linear waveguides, constructed by removing rows of inclusions in the periodic lattice of the phononic crystal, the number and dispersion of the modes can be adjusted by varying the width of the guide. In particular, the guide can be made monomode over a large frequency range of the phononic band gap. The cut-off frequency of the guided modes can also be selected. Different modes can be excited to participate to transmission depending on whether the initially incident wave is longitudinal or transverse.

Considering fluid/fluid and solid/fluid phononic crystals, we have shown in a recent paper¹⁹ that the transmittance through the waveguide can be significantly altered by attaching to it a side branch resonator (or stub), namely zeros of transmission occur in the spectrum. The results are in qualitative agreement with modellistic calculations. 20 In this paper, we consider waveguides that incorporate in their structure a resonant cavity, either within the waveguide or at its side. Resonant cavities within the linear guide provide a means of limiting the transmitted modes to those of the cavity. On the other hand, grafting a side branch containing a cavity to a perfect linear waveguide leads to the introduction of zeros of transmissions at precise frequencies corresponding to the eigenmodes of the cavity. Thus, we can demonstrate that the notches in the transmittance obtained in the latter case coincide with the peaks obtained in the former

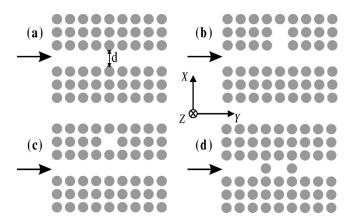


FIG. 1. Cross sections of the phononic crystals for the geometries considered in this paper. (a) A perfect linear waveguide of width, d. (b) A stub attached vertically to the waveguide. (c) A side-coupled waveguide cavity. (d) A cavity inside the linear waveguide.

case. Let us mention that such zeros of transmission can be widened into a gap if a periodic set of side branches are grafted along the guide.²⁰ Thus, from the point of view of applications, such resonators may serve as a building element for the design of specific functions such as filtering or add/drop multiplexing.

In Sec. II, we briefly present both the methods of calculation and the geometrical models studied in this paper. Section III is devoted to the discussion of the dispersion curves and transmittance for linear waveguides without defect. The effect of incorporating cavities inside or at the side of the waveguide is discussed in Sec. IV. A summary of the results is presented in Sec. V.

II. GEOMETRICAL MODELS AND METHODS OF CALCULATION

We consider a solid/solid 2D phononic crystal composed of steel cylinders in epoxy. The physical parameters characterizing the acoustic properties of the constitutive materials are the longitudinal, c_ℓ and transverse, c_t , speeds of sound as well as the mass density ρ . We take $c_\ell = 5825$ m/s, $c_t = 3226$ m/s, $\rho = 7780$ kg/m³ for steel, and $c_\ell = 2569$ m/s, $c_t = 1139$ m/s, $\rho = 1142$ kg/m³ for epoxy. The inclusions have the cylindrical symmetry and are arranged periodically on a square lattice. The parameters specifying the geometry of the crystal are the lattice parameter, a, and the radius of the inclusion, r. The filling fraction of the composite medium is defined as the ratio $\beta = \pi r^2/a^2$. Throughout this paper we assume a = 9 mm and r = 3.5 mm (or $\beta = 0.475$). This insures that the phononic crystal displays a large band gap extending from 85 to 200 kHz.

Figure 1 displays the cross sections of the phononic crystal for the geometries considered in this paper. Simple linear waveguides of different width, d, are created in the phononic crystal by removing one or several rows of cylinders along the Y direction of the square array [Fig. 1(a)]. Stubs of varying lengths and widths can be obtained by removing cylinders in the direction X perpendicular to the waveguide [Fig.

1(b)]. A cavity can be inserted at the side of the waveguide [Fig. 1(c)]. The coupling between the cavity and the waveguide can be modified by changing their separation, although in this work we limit ourselves to a separation of one unit cell. Resonating cavities can also be built out of two basic cylindrical inclusions inserted within the waveguide [Fig. 1(d)].

We study the transmission through the above structures as well as dispersion relations of the perfect waveguide and of an isolated cavity. Our calculations of the dispersion relations and transmitivity are performed by a combination of the plane wave expansion (PWE) method² and of the finite difference time domain (FDTD) method.^{21,22} With the PWE method, taking advantage of the periodicity of ABGs, the elastic wave equation is rewritten in Fourier space and reduced to a simple eigenvalue problem, thus yielding the acoustic band structure of the system. The FDTD method solves the elastic wave equation by discretizing time and space and replacing derivatives by finite differences. It permits the calculation of acoustic transmission spectrum of finite size phononic crystals. It provides also a complementary method for calculating the dispersion relations. These methods, and in particular the FDTD method, have been demonstrated to yield results in very good accord with experiments.5

III. DISPERSION RELATIONS AND TRANSMISSIONS OF LINEAR WAVEGUIDES

In solid/solid 2D phononic crystal, by limiting the wave propagation to the plane XY perpendicular to the cylinders, the propagation modes decouple in the Z modes (with elastic displacement u parallel to the Z direction) and in the XY modes (with u in the plane XY). In this paper, we focus on XY modes. The band structure of the XY modes of the perfect phononic crystal considered in this paper possesses a wide absolute band gap extending from 85 to 200 kHz. This result is obtained from a calculation of the band structure by means of the PWE method using 882 wave vectors of the reciprocal space. It is also confirmed in the transmission spectra of the phononic crystal calculated by the FDTD method along two high symmetry axes of the Brillouin zone.

In this section, we investigate the properties of a phononic crystal containing a simple straight waveguide. As a basis for further discussions, we first consider a guide simply built by removing one row of cylindrical inclusions along the Y direction. This is analogous to the examples considered in Refs. 11 and 19. The width d of the guide, defined by the distance between neighboring cylinders on both sides of the guide, equals d = 11 mm [Fig. 1(a)]. Figure 2(a) reports its band structure. The band gap of the perfect phononic crystal is delimited by the two thick horizontal lines. In order to perform this calculation, a supercell of 5 periods is repeated periodically in the X direction. This means that the waveguide is repeated every 5 periods in the *X* direction. The band structure is calculated with 1586 vectors of the reciprocal space. The dispersion curves appearing inside the gap of the perfect phononic crystal are related to localized modes associated with the linear waveguide. The number and dispersion

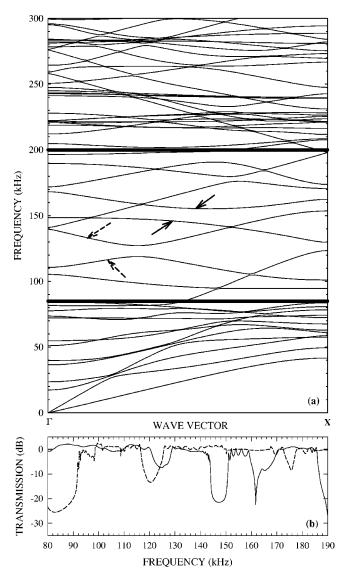


FIG. 2. (a) Band structure of the XY modes of propagation of a phononic crystal containing a linear waveguide along the Y direction as in Fig. 1(a). The calculation is performed by considering a super-cell of five periods along the X direction. The waveguide width is d=11 mm. The band gap of the perfect phononic crystal is delimited by the two thick horizontal lines. The filled arrows indicate two symmetrical dispersion curves that anticross each other giving rise to the dip in the transmission spectrum around 145 kHz. The dashed arrows indicate two antisymmetrical branches that anticross each other giving rise to the dip in the transmission spectrum around 120 kHz. (b) Transmission through the waveguide for two polarizations of the incident wave, longitudinal (solid line) or transverse (dashed line).

of the localized modes can be understood, and qualitatively explained, by considering the propagation of elastic waves in a classical linear guide with rigid boundary conditions for which the dispersion relations can be derived analytically.²³ Indeed this analogy is possible since the displacement field of a wave propagating along the guide in the phononic crystal remains almost confined inside the guide and only penetrates weakly around the steel cylinders situated on both sides of the guide. The main difference between the guide in

the phononic crystal and the classical one is that the former has rough instead of planar walls. The roughness of the walls results from the periodicity of a of the inclusion that bound them along the Y direction. Therefore, for comparison, the dispersion curves of a guide with planar walls should be essentially folded back into a reduced Brillouin zone of dimension π/a . The numerous localized branches inside the gap of the phononic crystal [Fig. 2(a)] are the result of this folding and the resulting interaction between branches that cross each other. The results of Fig. 2(a) resemble qualitatively those of Ref. 11 dealing also with a solid/solid composite, constituted by Pb cylinders in epoxy. On the other hand, in the case of the solid/fluid composite (steel cylinders in water) studied in Ref. 19, the number of localized branches in the band gap is much smaller because the matrix is now constituted by a fluid that can only support compressional waves, but not shear waves.

Like in a classical guide, the vibrational modes of the phononic crystal waveguide can be distinguished according to their symmetric or antisymmetric character with respect to the plane cutting through its middle. Consequently, these modes can be excited with an incident wave of appropriate symmetry. Using the FDTD method, we have calculated [see Fig. 2(b)] the transmission through the guide as a function of the frequency, the probing signal being initially of either longitudinal or transverse polarization. Indeed, as discussed below, these waves are respectively symmetrical or antisymmetrical with respect to the symmetry plane. To calculate the transmission coefficient by FDTD method, we construct a sample in three parts along the Y direction, a central region containing the finite phononic crystal sandwiched between two homogeneous regions. A traveling wave packet is launched in the first homogeneous part and it propagates in the direction of increasing Y along the whole sample. Periodic boundary conditions are applied in the X direction and absorbing Mur's boundary conditions are imposed at the free ends of the homogeneous regions along the Y direction. The incoming signal is a sinusoidal wave of frequency f_0 =400 kHz weighted by a Gaussian profile and propagates along the Y direction. In Fourier space, this signal varies smoothly and weakly in the interval $(0, f_0)$. The amplitude of the input signal does not depend on X; it is directed along the Y direction (resp. X direction) when the input signal is of longitudinal (resp. transverse) polarization. Thus, the incident probing signal is either symmetrical or anti-symmetrical with respect to the mirror plane of the guide. The transmittance is obtained by averaging the displacement field at the guide's exit along a line normal to its axis, followed by a Fourier transformation and by normalizing to the same quantity calculated for the incoming wave packet in the absence of the phononic crystal. It should be pointed out that, with this definition, the transmission can exceed one. Depending on whether the input signal is of longitudinal or transverse polarization, the average is taken over the Y component or the X component of the displacement field.

With an incident wave of longitudinal polarization, the transmittance [Fig. 2(a)] in the frequency range corresponding to the gap of the phononic crystal takes on a value near 1 except for the secondary gaps appearing respectively around 125 kHz, 145 kHz, and 170 kHz. The first dip around 125

kHz results from the folding of the symmetrical branches at the Brillouin zone boundary. The second dip at 145 kHz is associated with the anticrossing between two symmetrical branches marked by arrows in Fig. 2(a). In this example, the length of the guide is taken to be $\ell=15a$. The attenuation of the transmitted signal in these secondary gaps is significantly dependent upon the length of the waveguide. Decreasing this length will result in the weakening of the dips. For instance, the dip at 125 kHz will become very small for a length $\ell=7a$ of the guide, whereas the dip at 145 kHz is less affected by this length. It is likely that this effect is due to the large flat part of the two dispersion curves that anticross each other.

Finally, launching a probing signal of transverse polarization [dashed curve in Fig. 2(b)] yields high transmittance from 93 kHz where the antisymmetric modes of the waveguide start to exist. This transmission spectrum displays a dip in the frequency interval [118–125] kHz due to the anticrossing between two antisymmetric branches [indicated by dashed arrows in Fig. 2(a)].

Now, we investigate another example dealing with a case that has not been mentioned in the literature, namely the possibility of decreasing the number of dispersion curves (and even leading to a monomode regime) by narrowing the width of the waveguide. Indeed, similarly to the case of a classical linear guide, the cut-off frequency of the guided modes in the phononic crystal can be increased by decreasing the width of the guide. This operation can be performed by assuming that the cylindrical inclusions on both sides of the waveguide are separated by a distance smaller than the period a. Decreasing the thickness of the guide will have, at the same time, the effect of reducing the number of the guided mode branches that appears in the gap of the phononic crystal. As a consequence, the guide can even be made monomode over a large frequency range. This effect is sketched in Figs. 3, where we present the band structure of the guided modes (calculated by means of the PWE method) and the corresponding transmission coefficients for a narrow waveguide of width d = 6.5 mm. One notices the existence of a small (secondary) gap around 150 kHz at the edge of the Brillouin zone, between two symmetric branches. This gap gives rise to a dip in the transmission spectrum. This dip becomes less pronounced when decreasing the length of the waveguide. On the other hand, the dispersion curves display two almost flat antisymmetric branches around 140 kHz, and therefore the transmission with a probing signal of transverse polarization mainly extends over the limited frequency domain of [130–147] kHz.

On the contrary, increasing the width of the guide (for instance by removing two or several row of cylinders along the *Y* direction) will increase the number of localized mode branches in the band gap of the phononic crystal and the transmission becomes mainly multimode.

IV. WAVEGUIDES CONTAINING A CAVITY OR SIDE-COUPLED WITH A CAVITY

We now turn to the behavior of a defect cavity in the phononic crystal. The cavity is simply obtained by removing

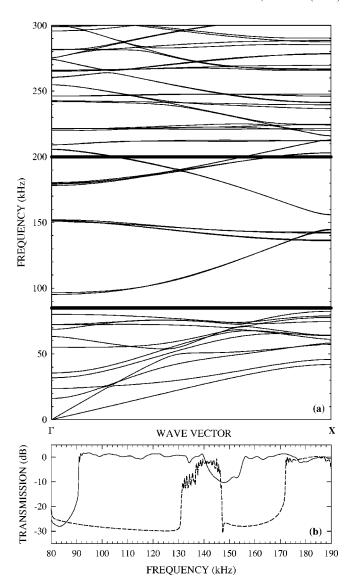


FIG. 3. Same as in Fig. 2, but the width of the waveguide is taken to be d=6.5 mm instead of d=11 mm in Fig. 2.

one cylindrical inclusion thus creating a vacant lattice site. The band structure of such a system is calculated with the PWE method for a super cell of 3×3 cylinders with one vacancy in its center. The number of reciprocal lattice vectors used in the calculation is 2738. The band structure reported in Fig. 4 shows the stop band of the phononic crystal containing several nearly flat bands. These flat bands are representative of the vibrational modes characteristic of the cavity. Let us notice that the cavity possesses two perpendicular symmetry axes X and Y. Thus, its eigenmodes can be labeled according to their symmetry with respect to these axes as SS, AS, SA, and AA, where S and A, respectively, stand for symmetric and antisymmetric (for instance SS means symmetric with respect to both X and Y axes). Using the FDTD method, we have created excitations inside the cavity having each of the four above symmetries. The characteristic frequencies of the cavity, falling in the band gap of the phononic crystal, coincide with those obtained by the PWE method (Fig. 4) within a few percent. In Fig. 5, we

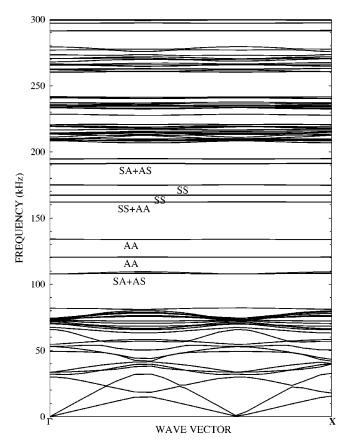


FIG. 4. Band structure of the XY modes in a phononic crystal containing a square cavity obtained by removing one cylinder. The calculation is performed by using a supercell 3×3 . The symmetry of the cavity modes with respect to the X and Y axes are indicated by the letters S and A, where S and A stand for symmetric and antisymmetric, respectively (for instance SS means symmetric with respect to both X and Y axes).

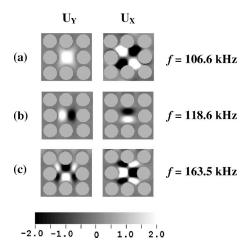


FIG. 5. Map of the components U_X and U_Y of some of the eigenvectors of the cavity modes shown in Fig. 5. f stands for the frequency of each eigenmode. These maps were obtained by using an incident probing signal of either longitudinal polarization [(a) and (c)] or transverse polarization (b).

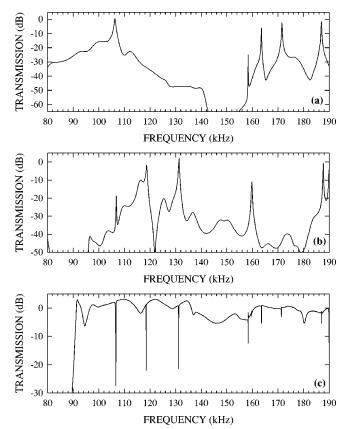


FIG. 6. (a) and (b) Transmittance through a cavity containing waveguide such as in Fig. 1(d). In these figures the polarization of the incident wave is, respectively, longitudinal or transverse and the width of the cavity is d=11 mm. (c) Transmittance through a waveguide coupled to a cavity along its side as illustrated in Fig. 1(d). The width of the waveguide is taken here to be d=6.5 mm to insure the monomode behavior of the propagation in a wide frequency range of the phononic crystal band gap.

give a map of the eigenvectors for some of the cavity modes. These maps are obtained by exciting with an incident probe an eigenmode of the cavity, contained inside a waveguide. We shall again refer to this point in connection with the explanation of transmission spectra shown in Fig. 6.

The eigenmodes of the cavity can be used advantageously to induce either narrow passing bands within the stop band of the phononic crystal or very narrow stopping bands in the pass band of a waveguide. To that effect we consider (i) a waveguide with a side-branch resonator constituted by a cavity [Fig. 1(c)], and (ii) a waveguide in the phononic crystal containing a single cavity [Fig. 1(d)]. Indeed, a single cavity incorporated into the waveguide may limit the transmission mainly to the frequencies situated in the neighborhood of the eigenfrequencies of the cavity. On the contrary, a side-coupled waveguide cavity is expected to induce zeros in the transmission spectrum of the perfect waveguide that occur at the characteristic frequencies of the cavity. So, the same cavity can have two opposite effects depending on whether it is incorporated inside or at the side of the waveguide.

In the following examples, the length of the waveguide is chosen to be $\ell = 9a$ as displayed in Fig. 1. Figure 6 summarizes the transmittance of the two systems. The cavity-

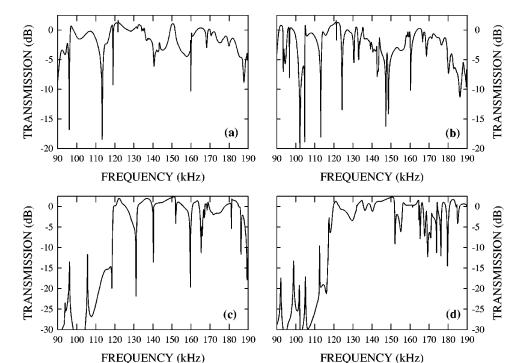


FIG. 7. Transmission through a stubbed waveguide such as in Fig. 1(b). In (a) and (b) the width of the waveguide is d = 6.5 mmand the length of the stub is, respectively, equal to one or two periods of the phononic crystal (i.e., one or two cylinders have been removed perpendicularly to the waveguide). In (c) and (d) the width of the waveguide is only d =4 mm to show the possibility of selective transmission in a frequency range in which the propagation is prohibited along the guide.

containing guide is probed with a longitudinal [Fig. 6(a)] as well as a transverse [Fig. 6(b)] incident wave packet. The longitudinal incident wave is symmetrical with respect to the Y axis and, thus, can probe the eigenmodes of the cavity that have SS and AS symmetries with respect to XY axes. On the other hand, the transverse incident wave can excite eigenmodes of only SA and AA symmetries. This is confirmed by the transmission spectra shown in Figs. 6(a) and 6(b) that are mainly composed of peaks in the vicinity of the characteristic frequencies of the cavity with the appropriate symmetry. It is worthwhile to notice that the maps sketched in Fig. 5 are obtained by using an incident probing signal of either longitudinal polarization [Figs. 5(a) and 5(c)] or transverse polarization [Fig. 5(b)] at the frequencies of the peaks in the transmission spectra of Figs. 6(a) and 6(b). Finally, one can remark that the peaks appearing in the transmission spectra can be made sharper if the isolation of the cavity is increased, for instance by bordering the cavity on each side by two cylindrical inclusions instead of one as was shown in Fig. 1.

In Fig. 6(c), we show the transmittance through the side-coupled waveguide cavity [Fig. 1(c)]. Since this system does not display any particular symmetry, an incident longitudinal wave can probe in principle all the eigenmodes of the cavity. To enhance the zeros of transmission induced by the side branch resonator, we have chosen a linear guide of narrower width than the period, namely d=6.5 mm, to yield monomode guiding character from 90 kHz up to approximately 150 kHz (see Fig. 3). Transmission takes place for most frequencies below 140 kHz but zeros of transmission occur at several frequencies corresponding to the characteristic frequencies of the cavity. It should be mentioned that with a wider guide, for instance of width d=11 mm, the dips in the transmission still exist, but the transmission does not decrease as much as in Fig. 6(c). It is interesting to notice that

the dips in the transmission spectrum of Fig. 6(c) occur exactly at the same frequencies as the peaks in Figs. 6(a) and 6(b).

Finally, we have also investigated the transmission through a stubbed waveguide such as in Fig. 1(b). The results for the transmission spectra are presented in Fig. 7, where we have considered two different lengths of the stub and two different widths of the waveguide, the incident wave being of longitudinal polarization. In Figs. 7(a) and 7(b), the width of the linear guide is chosen to be d = 6.5 mm in order to have a monomode regime over a broad frequency range (see Fig. 3). One can notice that the main effect of the stub is to induce dips, or zeros of transmission, in the spectrum. The existence of such zeros of transmission has been demonstrated in modellistic calculations, ²⁰ especially using perfect boundary conditions on the walls of the guide, and also proved in a numerical simulation of stubbed waveguide in phononic crystals made of fluid/fluid or solid/fluid constituents. 19 The zeros of transmission are associated with the resonance frequencies of the resonators that are attached to the waveguide. However, the number of zeros of transmission for a phononic crystal with a fluid matrix is smaller than that of an all solid phononic crystal, since a fluid can only support compressional waves. In the case of a solid/solid composite considered here, both shear and compressional waves can propagate inside the waveguide and resonators. As a consequence the transmission spectrum appears to be richer and also more complicated due to this coupling between longitudinal and transverse vibrations in solid materials. The results of Figs. 7 show that the transmission spectra still contain very deep narrow transmissions, as well as some smaller dips. Nevertheless, it is difficult to predict the exact frequencies of the dips, in contrast to the case of phononic crystals in which the background is a fluid material that can support only compressional waves. 19 From a qualitative point of view, the number of such zeros of transmission increases by increasing the length of the stub, as can be seen from a comparison of Figs. 7(a) and 7(b). This is expected since the resonator constituted by the stub can support an increasing number of modes when increasing its length.

In Figs. 7(c) and 7(d), the width of the waveguide is made even smaller, i.e., d=4 mm only. This has the effect of shifting upwards the dispersion curves of the waveguide, leaving the lower part of the phononic crystal band gap (from 80 to 120 kHz) free of modes. In other words, the waves are prohibited from propagating along the waveguide in the above frequency range. In this region, due to the presence of the stub, selective transmission becomes possible by tunnel effect at the frequencies of the modes induced by the stub. One can notice a good correspondence between some of these peaks and the strongest dips in Fig. 7(a). Therefore, the same stub can induce selective transmissions or zeros of transmission depending on whether the propagation is forbidden or allowed through the waveguide.

V. SUMMARY

In this paper, we have investigated for the first time the propagation of acoustic waves through defect-containing waveguide structures in phononic crystals composed of solid constituents. First, we have considered the case of perfect waveguides, mainly to show that the number and dispersion of the localized branches that contribute to transmission can be adjusted by varying the width of the guide. In particular, the guide can be made monomode over a large frequency range of the phononic crystal band gap. Other geometrical structures of the waveguide would be also interesting ^{16,24} for applications such as filtering or demultiplexing, but this is beyond the scope of this paper.

The transmission through the waveguide can be significantly altered by incorporating a cavity inside or at the side of the guide. In a cavity-containing waveguide, the transmission can be limited to narrow frequency domains situated in the vicinity of the characteristic frequencies of the cavity. Depending on their symmetry, different modes can be excited and contribute to transmission when either a longitudinal or a transverse incident wave is launched onto the phononic crystal. The transmission peaks can be made sharper by increasing the isolation of the cavity. In the case of a waveguide with a cavity along its side, the main modification in the transmission as compared to the case of a perfect waveguide is the existence of notches that occur at the characteristic frequencies of the cavity. The dips in the transmission become in general deeper when the propagation along the waveguide is made monomode. Zeros of transmission can also be induced in the transmission spectrum by simply coupling the waveguide to a stub. However, unlike the case of an isolated cavity, it is more difficult to find a simple interpretation of their frequencies, especially in the case of solid/solid composites because the longitudinal and transverse waves are strongly coupled together.

It would be interesting to investigate the above phenomena in more detail for different shapes of the cavities and different strengths of their coupling with the guide, as well as a combination of such defects. A rich variety of situations may occur, especially in view of the fact that the phononic crystal can be composed of both solid and fluid constituents that can support different polarizations of the

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