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ABSOLUTE BAND GAPS IN TWO-DIMENSIONAL PHONONIC CRYSTAL PLATES

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ABSTRACT

The elastic band structures of two-dimensional phononic crystal plates are computed with the help of a super-cell plane wave expansion (PWE) method. These band structures strongly differ from the infinite 2D phononic crystal dispersion curves. In particular, these band structures exhibit surface modes and guided modes. The influence of the constituent materials, of the plate thickness and of the geometry of the array on the band structure is investigated. We focus more specifically on determining the thicknesses of the plate for which absolute forbidden bands exist. Namely, we show that absolute forbidden bands occur in the band structure if the thickness of the plate is of the same order of magnitude as the periodicity of the array of inclusions.

INTRODUCTION

Phononic crystals also named acoustic band gaps materials (ABG), are composite materials made of two or three dimensional periodic distributions of inclusions embedded in a matrix. The periodic structure of these composite materials gives them peculiar properties, in particular the existence, under certain conditions, of absolute acoustic band gaps i.e. forbidden bands that are independent of the direction of propagation of the incident elastic wave [1, 2]. Absolute band gaps confer to these artificial materials potential applications as sound insulators or for the filtering and demultiplexing of acoustic waves [3–5]. Earlier studies of bulk phononic crystals i.e. phononic crystals assumed of infinite extent along the 3 spatial directions, have shown that the bandwidth of the forbidden band depends strongly on the contrast between the physical characteristics (density and elastic moduli) of the inclusions and the matrix, as well as the geometry of the array of inclusions, the inclusion shape and the filling factor of inclusions [1–3]. More recently, various authors have studied theoretically the existence of surface acoustic waves (SAW) localized at the free surface of a semi-infinite two-dimensional phononic crystal [6–9]. For this geometry, the parallel inclusions are of cylindrical shape and the surface con-

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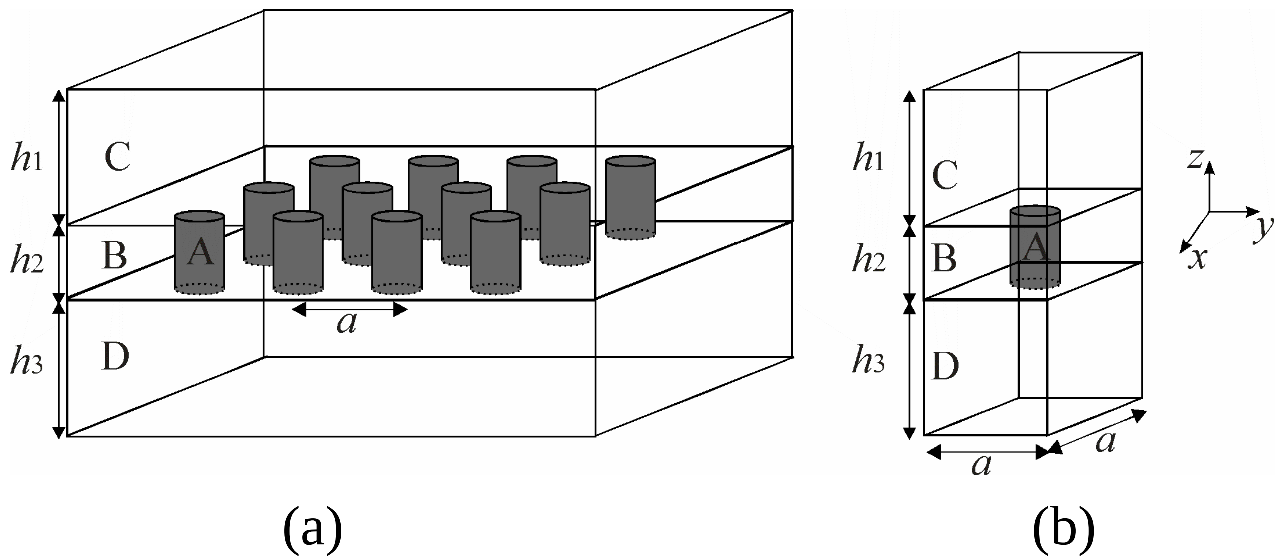

Figure 1. (a) 2D PHONONIC CRYSTAL PLATE SANDWICHED BETWEEN TWO SLABS OF HOMOGENEOUS MATERIALS, (b) 3D SUPER-CELL CONSIDERED IN THE COURSE OF THE PWE COMPUTATIONS.

sidered is perpendicular to their axis. Various arrays of inclusions [6, 7], crystallographic symmetries of the component materials [8], and also the piezoelectricity of one of the constituent [9] were taken into account. In these works, the same method of computation of the SAW band structure was applied. This method is based on the well-known plane wave expansion (PWE) method [1, 2] with SAW explicitly searched as solutions of the Fourier-transformed equation of propagation, exponentially decreasing along the cylinders direction and by imposing the right boundary conditions on the free surface. The same method was also applied for computing the symmetric Lamb modes band structure of two-dimensional phononic crystals plates made of W cylinders in a Si background [10]. The propagation of acoustic waves along a surface parallel to the cylinders in a 2D phononic crystal has also been studied [11]. More recently, the guided elastic waves in a glass plate coated on one side with a periodic monolayer of polymer spheres immersed in water was investigated with the help of the layer-multiple scattering method [12]. On the experimental point of view, high frequency SAW was observed with a pair of interdigital transducers placed on both sides of a thick silicon plate in which a square array of holes was drilled [13]. The existence of gaps for acoustic waves propagating at the surface of an Air/Aluminium 2D phononic crystal plate was shown experimentally through laser ultrasonic measurements [14].

In this paper, we show that the band structure of a 2D phononic crystal plate of finite thickness along the axis of the cylinders exhibits surface modes and guided modes. This band structure strongly differs from the bulk 2D phononic crystal dispersion curves. The influence of the constituent materials, of the plate thickness and of the geometry of the array on the band structure is investigated. We focus especially on determining the thicknesses for which absolute forbidden bands still exist.

This paper is organised as follows. In section II, we present the model and the method of calculation of the acoustic band structure of 2D phononic crystal plates. Several numerical results are then presented in section III. Section IV contains discussion of these results and the main conclusions drawn from this study.

METHOD OF CALCULATION

We calculate the acoustic band structures of 2D phononic crystal plates using a method based on the plane wave expansion (PWE) method. The phononic crystal plate of thickness, h_2, is assumed infinite in the xy plane of the Cartesian coordinates system (O,x,y,z). The phononic crystal is a periodic array of cylindrical inclusions constituted of an isotropic material A embedded in an isotropic elastic matrix B. The cylinders of radius R are parallel to the z direction and the nearest neighbor distance between cylinders is a. In the xy plane, the filling factors are f and $(1-f)$ for materials A and B respectively. The plate is sandwiched between two slabs of thicknesses h_1 and h_3, made of elastic isotropic homogeneous materials C and D (see Fig. 1(a)). In the course of the numerical calculations, one considers the parallelepipedic super-cell depicted in Fig. 1(b). The super-cell of surface, a^2, in the xy plane, and of height ℓ along the z direction with $\ell = h_1 + h_2 + h_3$, contains one, or more, cylinder A of height h_2, surrounded by material B and sandwiched between two plates of thicknesses h_1 and h_3. This super-cell is repeated periodically along the x, y and z directions. We desire medium C to be a low impedance medium (L.I.M.) such as vacuum. Medium D can be either vacuum or a homogeneous material depending on whether one wants to model a phononic crystal plate or a structure made of a phononic crystal plate deposited on a substrate of finite thickness. The triple periodicity along the 3 spatial directions allows one to develop the elastic moduli and the mass density of the constituent materials as Fourier series as $\eta(\vec{r}) = \sum_{\vec{G}} \eta(\vec{G}) \exp(i\vec{G}\vec{r})$ where $\vec{r}$ and $\vec{G}$ are three-dimensional position vectors and reciprocal lattice vectors respectively. The components in the xy plane of the $\vec{G}$ vectors depend on the geometry of the array of inclusions while along the z direction, $G_z = \frac{2\pi}{\ell} n_z$ where n_z is an integer. Moreover, the displacement field satisfies the Bloch theorem and one searches for solutions to the Fourier transformed equation of propagation as harmonic waves of pulsation ω and wave vector $\vec{K}$. The components, in the xy plane, of the $\vec{K}$ vectors are limited to the periphery of the first Brillouin zone of the array while K_z is assumed equal to zero. The choice of the physical parameters characterizing vacuum in the course of the PWE computations is of main importance. Indeed, it is well known that convergence problems occur when considering abruptly a transverse speed of sound for the fluid equals zero in the PWE computations of band structures of solid/fluid composites [11,14]. On the other hand, the super-cell method requires an interaction as low as possible between the vibrational modes of neighboring phononic crystal slabs. Then vacuum must be modeled as a fictitious material where propagation of acoustic waves is forbidden [11]. Vacuum has been modeled by an isotropic L.I.M. with very low density and very high speeds of sound C_ℓ and C_t. More specifically, we choose $\rho = 10^{-4} kg.m^{-3}$ and $C_\ell = C_t = 10^5 m.s^{-1}$. This ensures that the ratio between the elastic moduli of vacuum and those of any other solid material approaches zero. For checking the reliability of these parameters, we have considered the peculiar case of a 2D bulk phononic crystal made of a square array of cylindrical holes drilled in a solid matrix. We computed its PWE band structure by modeling the material inside the holes with our isotropic L.I.M., on one hand. On the other hand, the transmission coefficients along the principal directions of propagation were calculated with the help of the finite difference time domain (FDTD) method and the material inside the holes was explicitly considered as air i.e. $\rho_A = 1.23 kg.m^{-3}$, $C_\ell^A = 340 m.s^{-1}$ and $C_t^A = 0$. Let us recall that the FDTD method allows one to compute accurately transmission coefficients through solid/fluid composite materials by modeling fluids with their real physical characteristics i.e. in particular, a transverse speed of sound equals 0 [15,16]. We observed that the PWE and FDTD results compared quite well. In particular, the domains of low transmission in the transmission coefficients coincided exactly with the absolute band gaps of the band structure. This indicates that in the course of the PWE calculations, these values of the L.I.M. physical characteristics allows one to model air (or vacuum) without numerical difficulties. Moreover we also checked that our super-cell PWE method leads to similar results to those published [6,7,13] for semi-infinite phononic crystals, provided the thickness of the plate is large enough. Finally with our numerical method, computations of dispersion curves of phononic crystal plates with $K_z = 0$ and with any other non vanishing value of K_z, lower than π/ℓ, lead to the same result. This indicates that the homogeneous slab C made of the L.I.M. modeling vacuum rigorously forbids the propagation of acoustic waves in the Z direction.

NUMERICAL RESULTS

The steel/epoxy 2D phononic crystals

We first consider the case of 2D phononic crystals made of two solid constituent materials. We choose steel for the cylindrical inclusions and epoxy for the matrix. Indeed these solids possess very different densities and elastic constants and the bulk phononic crystal exhibits very large absolute band gaps provided the filling factor of inclusion is sufficiently large. We used the elastic constants ${C_{11}}^A = 26.4$ and ${C_{44}}^A = 8.1$ (in units of 10^{10} $N.m^{-2}$) and mass density $\rho^A = 7780$ $kg.m^{-3}$ for steel, and ${C_{11}}^B = 0.754$ and ${C_{44}}^B = 0.148$ (in units of 10^{10} $N.m^{-2}$) and mass density $\rho^B = 1142$ $kg.m^{-3}$ for epoxy. Figure 2 represents the band structures of the bulk phononic crystal (hollow squares) and of the phononic crystal plates with different thicknesses h_2 (black filled circles) ranging from $0.1a$ to $4a$. The computations of the dispersion curves of the bulk phononic crystal were done with an usual two-dimensional PWE scheme by imposing that the propagation of the acoustic waves is limited to the plane perpendicular of the inclusions (see details in references [1,3]). In the course of the numerical calculations of the band structure of the phononic crystal plates, the thicknesses of slabs C and D were chosen equals to a and 1029 reciprocal lattice vectors were taken into account. This ensures satisfactory convergence of the PWE code. The array of cylindrical inclusions is square and the filling factor $f = \pi R^2/a^2$ is equal to 0.56. The results are rendered in terms of a reduced frequency $\Omega = \frac{\omega a}{2\pi \overline{C_t}}$, where $\overline{C_t} = \sqrt{\frac{\overline{C_{44}}}{\overline{\rho}}}$ with $\overline{C_{44}} = ({C_{44}}^A f h_2 + {C_{44}}^B (1-f) h_2 + {C_{44}}^C f h_1 + {C_{44}}^D f h_3)/\ell$ and $\overline{\rho} = (\rho^A f h_2 + \rho^B (1-f) h_2 + \rho^C f h_1 + \rho^D f h_3)/\ell$, is an average transverse speed of sound, versus a reduced wave vector $k = Ka/2\pi$. One first observes that the band structure of the phononic crystal plate strongly differs from the dispersion curves of the bulk phononic crystal. The vibrational modes in the plates are confined by the two free surfaces of the plates, and result in only plate modes namely Lamb modes. The spatial distribution of these different modes can be derived from the calcula-

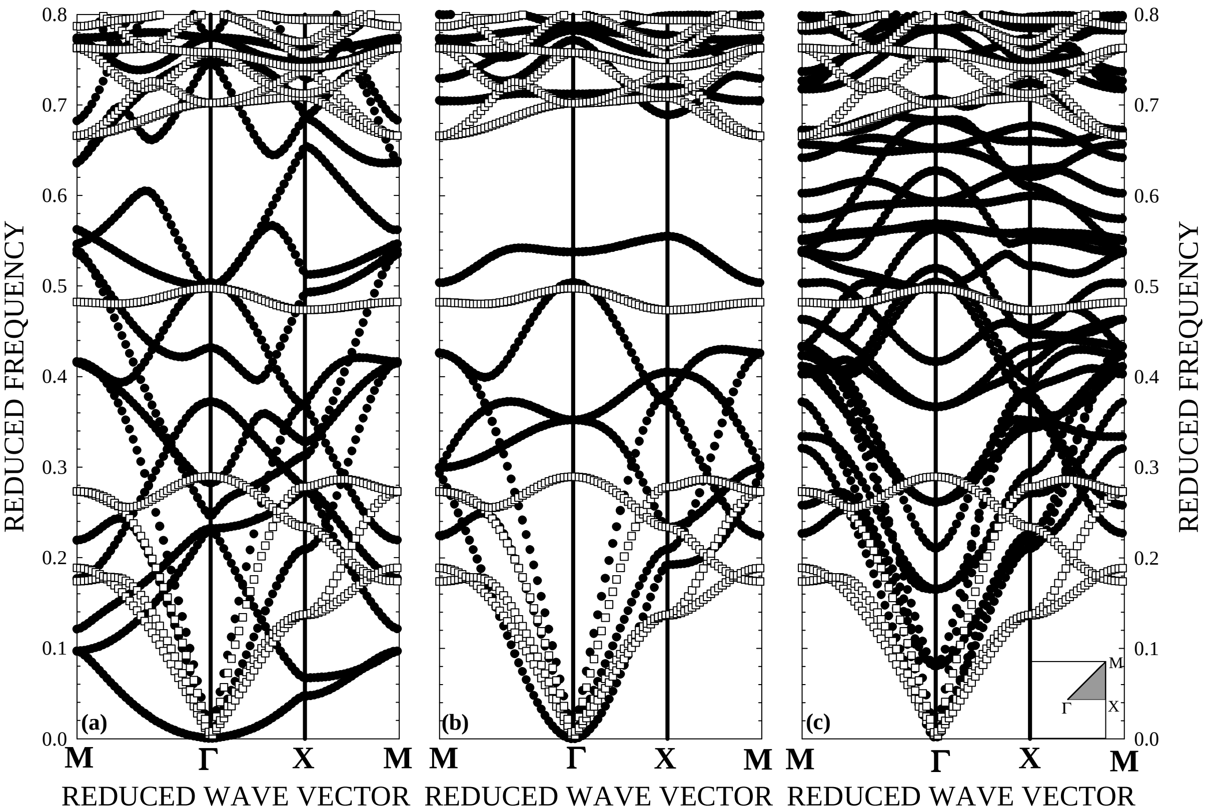

Figure 2. PWE ELASTIC BAND STRUCTURES FOR THE BULK 2D PHONONIC CRYSTAL (OPEN SQUARES) AND THE PHONONIC CRYSTAL PLATE OF THICKNESS h_2 (BLACK FILLED CIRCLES) MADE OF A SQUARE ARRAY OF STEEL CYLINDERS EMBEDDED IN AN EPOXY RESIN MATRIX WITH $f = 0.56$. (a) $h_2 = 0.1a$; (b) $h_2 = 0.7a$; (c) $h_2 = 4a$.

tion of the elastic displacement field associated with a specific mode. For example, Figure 3 shows the maps of the three components u_x, u_y and u_z of the displacement field in the plane xz (i.e. for $y = 0$) computed at the X point of Fig. 2(b). We restrict ourselves to the three dispersion curves that start from the point Γ. For the first mode, one deduces from Figs. 3(a,b,c) that u_x rapidly decreases from the surfaces $z/a = \pm 0.35$. In contrast, $u_y = 0$ and u_z remains nearly constant along the z direction (for a fixed value of x) and exhibits an oscillatory behavior along the x direction. This mode with a nearly parabolic dispersion curve corresponds to the A_0 mode i.e. the lowest order asymmetric Lamb mode. The displacement field associated with the second mode presents a non-vanishing value only along the y direction (see Figs. 3(c,d,e)) and is of transverse polarization. The third branch starting from the Γ point with a reduced frequency 0.38 at the X point presents a vanishing displacement along the y direction and u_z decreases from the surfaces. This is the S_0 mode i.e. the lowest order symmetric Lamb mode. These modes fold at the vicinity of the X point. Lamb modes of higher order occur at larger reduced frequencies. While in homogeneous plates, surface modes appear commonly below the bulk dispersion curves (as it can be seen in Fig. 2(a)), this is not observed in this particular case of phononic crystal plate. This was also observed in a semi-infinite phononic crystal made of a square array of holes in $LiNbO_3$, a piezoelectric material [9]. Of particular interest in Fig. 2(b) is the existence of an absolute band gap centered on $\Omega \cong 0.6$. This gap in which no plate mode can propagate offers the possibility of integrating at the scale of a thin slab of phononic crystals, structural defects such as cavities or waveguides. In that case, the vibrational modes associated with these structural defects should fall inside this absolute band gap. This may allow the design of functional devices for the filtering or the

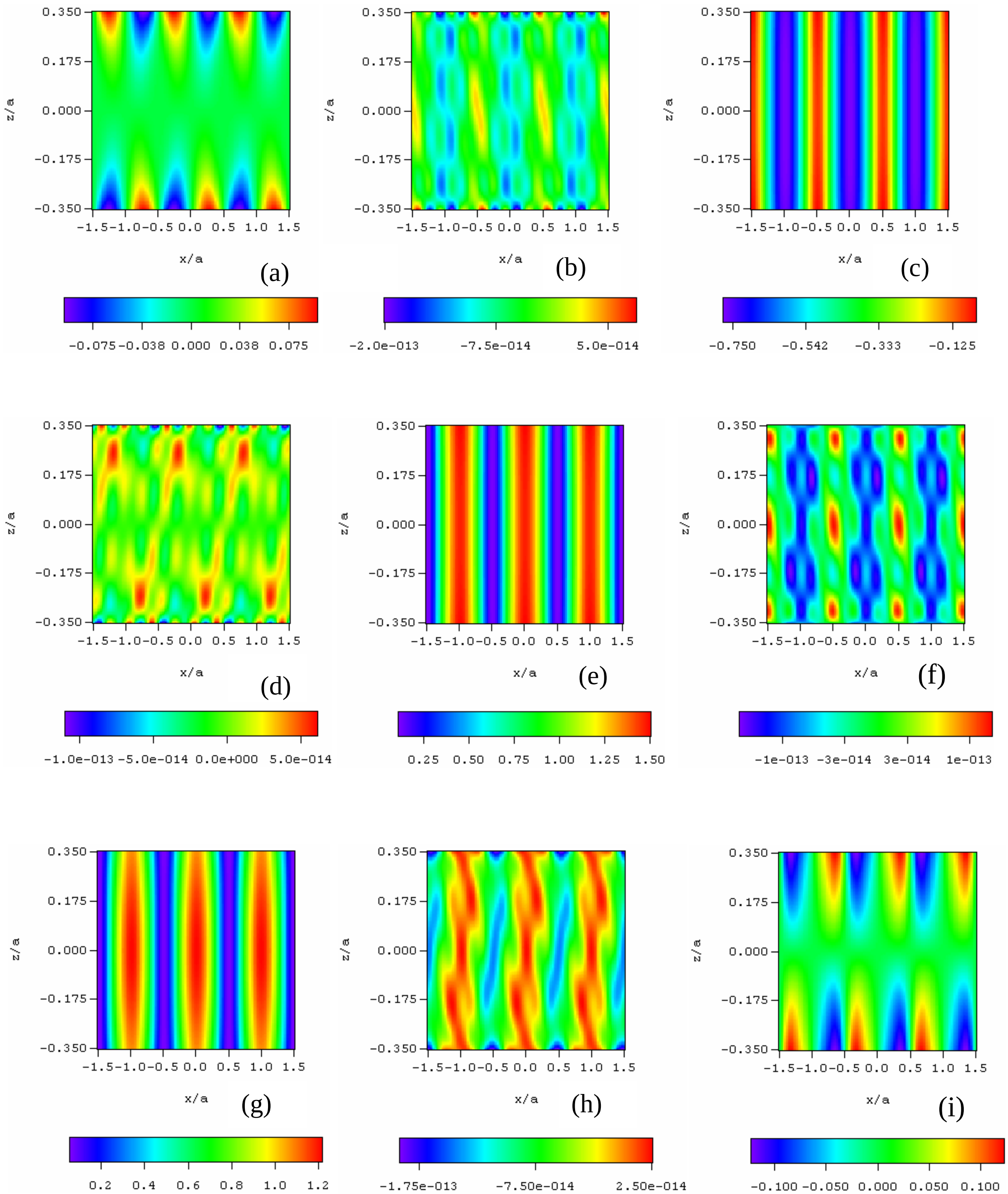

Figure 3. MAPS OF THE ELASTIC DISPLACEMENT FIELD IN THE xz PLANE ($y = 0$) FOR THE STEEL/EPOXY PHONONIC CRYSTAL PLATE OF FIG. 2(b). FIGS 3(a), (b) and (c) SHOW THE u_x, u_y AND u_z COMPONENTS OF THE DISPLACEMENT FIELD FOR THE A_0 LAMB MODE AT THE X POINT OF THE BRILLOUIN ZONE. (d), (e) AND (f) : THE SAME AS IN (a), (b) AND (c) BUT FOR THE FIRST TRANSVERSE MODE; (g), (h) AND (i) : THE SAME AS IN (a), (b) AND (c) BUT FOR THE S_0 MODE. THE COLOR SCALE INDICATES THE VALUE OF THE DISPLACEMENT FIELD IN ARBITRARY UNITS.

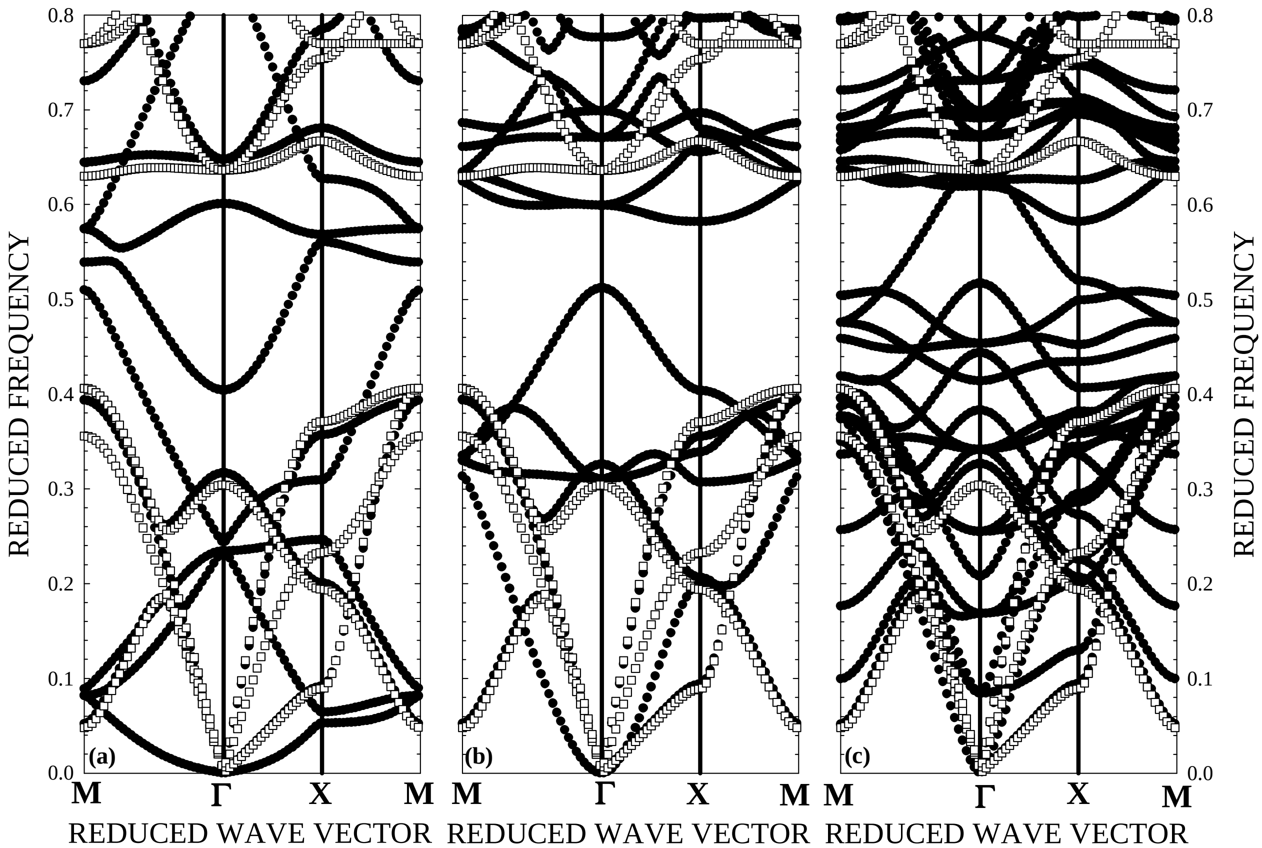

Figure 4. PWE ELASTIC BAND STRUCTURES FOR THE BULK 2D PHONONIC CRYSTAL (OPEN SQUARES) AND THE PHONONIC CRYSTAL PLATE OF THICKNESS h_2 (BLACK FILLED CIRCLES) MADE OF A SQUARE ARRAY OF CYLINDRICAL HOLES DRILLED IN STEEL WITH $f = 0.70$. (a) $h_2 = 0.1a$; (b) $h_2 = a$; (c) $h_2 = 4a$.

multiplexing of elastic waves. A detailed analysis of the band structures of steel/epoxy phononic crystal plates show that the width of the absolute band gaps depends on the filling factor of inclusion (larger gaps were observed for f larger than 0.5 as is the case for bulk waves [1]) and on the thickness of the plate. Indeed a comparison between Figs. 2(a), 2(b) and 2(c) shows clearly that for very thin ($h_2/a = 0.1$, for example) or very thick ($h_2/a = 4$) plates, full band gaps are not observed. With other constituent materials, our study shows that h_2/a ranging from 0.5 to 1.5 leads to the largest absolute band gaps.

The air/steel2D phononic crystals

From an experimental point of view, the realization at the micro- or at the nano-scale of 2D phononic crystals constituted of two different solid materials is a very challenging task while actual techniques based, for examples, on reactive ion etching (RIE) or focused ion beam (FIB) allows one to drill relatively easily regular network of holes in a solid [9]. Then with the aim of designing structures exhibiting absolute band gaps for very high frequencies ($\approx$ GHz), that can be fabricated experimentally, we focus our attention on arrays of holes drilled in a solid matrix. Figure 4 shows the elastic band structure of square arrays of cylindrical holes in steel for three different thicknesses of the phononic crystal plate. For the sake of comparison, we also report the bulk band structure. The band structures are rendered in the same way as those in Figs. 2. With these constituent materials, the choice of the filling factor is of particular importance. Indeed, most of the theoretical and experimental studies conducted on bulk 2D phononic crystals have shown that larger gaps are obtained when the inclusions (resp. the matrix) are made of the harder (resp. softer) material [1,3]. Nevertheless, this can be by-

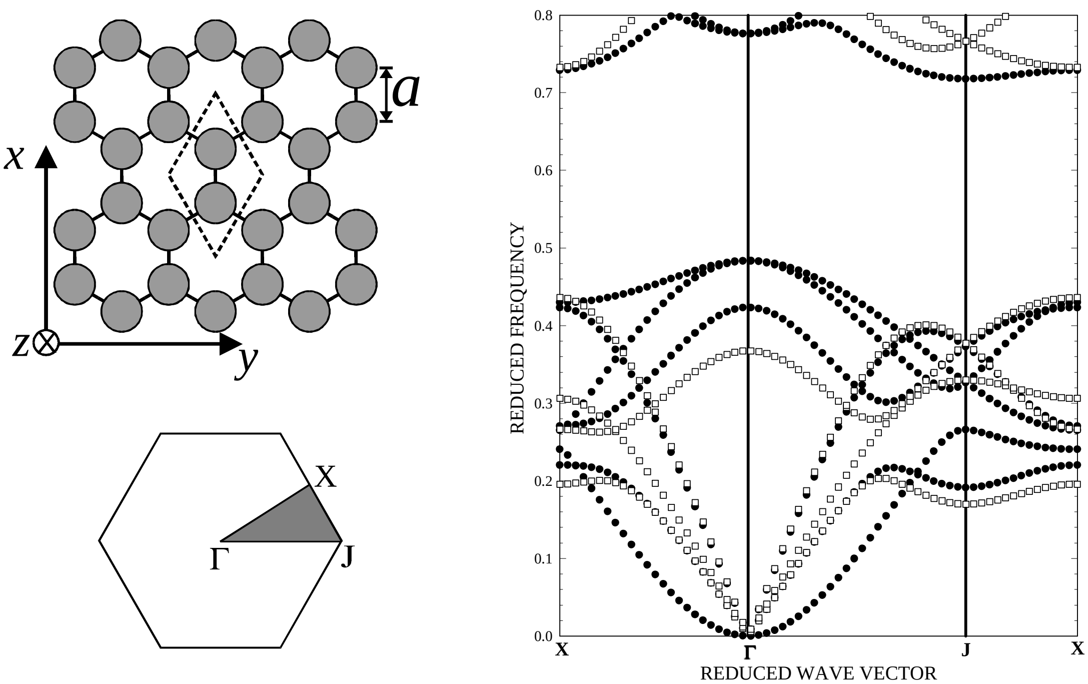

Figure 5. LEFT PANEL : SCHEMATIC REPRESENTATION IN THE xy PLANE (TOP) AND IRREDUCIBLE BRILLOUIN ZONE (BOTTOM) OF THE GRAPHITE ARRAY; RIGHT PANEL : PWE ELASTIC BAND STRUCTURES FOR THE BULK 2D PHONONIC CRYSTAL (OPEN SQUARES) AND THE PHONONIC CRYSTAL PLATE OF THICKNESS $h_2 = a$ (BLACK FILLED CIRCLES) MADE OF A GRAPHITE ARRAY OF CYLINDRICAL HOLES DRILLED IN STEEL WITH $f = 0.5$.

passed by considering a very compact array of holes. For example, a square array of holes drilled in a solid with a filling factor near the closed packed value (i.e. $f = \pi/4$) behaves like a square array of solid inclusions of singular shape embedded in air. Then one may expect large gaps for high filling factor of holes. This is illustrated in Figs. (4) where $f = 0.7$. One observes that the bulk band structure exhibits an absolute band gap centered on $\Omega \cong 0.5$. As in Fig. 2, an absolute band gap only appears for a thickness of the plate of the order of the lattice parameter namely $h_2/a = 1.0$ (see Fig. 4(b)). A vibrational mode associated with the plate falls inside the absolute band gap of the bulk phononic crystal but an absolute stop band still remains when the phononic crystal is of finite thickness. Furthermore one observes that the width of this absolute band gap is narrower than the one observed in Fig.2(b) for a phononic crystal made of two solid constituent materials. One may search for larger band gaps with the same constituent materials by changing the geometry of the array of inclusions. Indeed, it is well known that for bulk phononic crystals geometry plays a fundamental role in designing large elastic band gaps. Especially, it has been shown that for bulk phononic crystals, graphite arrays of soft inclusions in a hardest matrix leads to very large absolute gaps [3]. Subsequently we investigated the dispersion curves of 2D phononic crystal with the graphite structure. In the graphite network, the inclusions are located at the vertices of a regular hexagon and the distance between two nearest neighbors is a (see left panel of Fig.5). The super-cell considered in the PWE calculations contains two cylinders. In the schematic representation of the graphite array, the lozenge pattern drawn with dotted lines delimits the area of the super-cell in the xy plane. Along the z direction, the super-cell is similar to that depicted in Fig. 1(b). The filling factor of each inclusion is $f = 2\pi R^2/3\sqrt{3}a^2$ in the xy plane [3]. The irreducible Brillouin zone is the triangle ΓJX (see left panel of Fig. 5). Figure 5 shows the bulk band structure (hollow squares) and the dispersion curves of a phononic crystal plate (black filled circles) for a graphite array of holes in steel with $f = 0.25$ i.e. a total filling factor of inclusions equals 0.5, smaller than the close-packing value of 0.604. We consider a plate with a thickness equal to the lattice parameter a i.e. $h_2/a = 1$. As in the previous cases, the band structure of the plate differs from that of the infinite phononic crystal. One observes also the characteristic parabolic shape in the vicinity of the Γ point of the A_0 Lamb mode. In this particular structure, the S_0 Lamb mode and the first transverse mode overlap with the bulk dispersion curves. On the other hand, the width of the full band gap centered around 0.6 is markedly larger than the gaps reported in Figs. 2(b) and 4(b). As previously, the existence of this absolute stop band depends on the thickness h_2 of the plate and the optimum value of h_2 is of the order of magnitude of a. Thinner or thicker plates do not exhibit such absolute stop bands. Moreover, while for the square array of holes, absolute band gaps were obtained for filling factors approaching the close-packed value for which cylinders are in contact with one another, the graphite network shows wide gaps for non contacting cylinders. Consequently, the technical realization of phononic crystals made of holes in a solid matrix exhibiting absolute stop bands is probably much easier when the holes are arranged upon a graphite array than a square network especially at the scale of a thin plate.

CONCLUSION

The purpose of this paper was to investigate the existence of absolute stop bands in the elastic band structure of two-dimensional phononic crystal plates. A super-cell plane wave expansion method was applied for computing the dispersion curves of phononic crystals plates. Compared with previous works on waves propagating at the surface of 2D semi-infinite phononic crystals, our method does not require writing explicitly the boundary conditions on the free surfaces. This alleviates some numerical difficulties such as the computation of pseudo-modes without physical meaning [6]. PWE results show that the band structure of a phononic crystal plate strongly differs from that of a 2D composite material of infinite extent in the three spatial directions. Absolute stop bands in plates were observed for solid/solid systems such as steel inclusions in epoxy or for fluid/solid composites such as periodic arrays of holes in steel. We observed that the thickness of the plate plays an important role for designing artificial structures exhibiting absolute stop band. A thickness of the same order of magnitude as the lattice parameter of the array of inclusions seems to be the most favorable case for observing large absolute band gaps in phononic crystal plates. As far as arrays of holes drilled in a solid matrix are concerned, the graphite structure with the cylindrical inclusions placed at the vertices of a regular hexagon leads to the largest absolute band gaps. Structural defects such as point defects, cavities, channels inserted inside the phononic crystal plate could lead to the existence of vibrational modes inside such absolute stop bands. These defect modes could then be used to realize acoustic devices such as waveguides, specific frequency filters or wave length demultiplexers. In particular, these functionalities are of particular interest in radio-frequency devices for telecommunication applications. For example, surface acoustic waves (SAW) devices have been used extensively as radio-frequency (RF) band pass filters for the telecommunication industries [17]. Usual SAW devices are made of homogeneous piezoelectric films placed between two interdigital transducers. By replacing the piezoelectric film with a ”defective” phononic crystal plate, one will be able to introduce inside the device new functionalities such as wave guiding or wavelength demultiplexing. But in the range of radio-frequency (i.e. a few GHz), the thickness of absolute band gaps phononic crystal plates must be of the order of a few tens of nanometers (i.e. the same order of magnitude as the lattice parameter). Physical realization of such structures would then require that the thin plate of phononic crystal be deposited onto a thick substrate for support. It would then be interesting to investigate the influence of the substrate on the absolute band gap of the phononic crystal plate.

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