Theoretical study of a tunable phononic band gap system

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The control of acoustic-frequency gaps by altering the geometry of the system is analyzed in the particular case of a set of parallel solid square-section columns distributed in air on a square lattice. This system is shown to be sensitive enough to the rotation of the columns to be considered for practical sonic band-gap-width engineering. For different geometric configurations, specific interpretation models are used, taking into account the important mismatch of the impedance between the compounds. The accuracy of the plane-wave calculation is discussed in the different cases.

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I. INTRODUCTION

The propagation of elastic or acoustic waves in periodic heterogeneous materials has received much renewed attention in the last years. Periodic realizations of elastic heterostructures, called *phononic crystals*, make possible the achievement of complete frequency band gaps, useful to prohibit the specific vibrations in accurate technologies such as transducers or sonars.[1–4]

Different ways for enlarging a gap were already described in the literature for both photonic and phononic crystals. For example, the reduction of the total symmetry of the crystal can remove some band degeneracies, allowing for the appearance of complete gaps.[5–7] A common example consists of a comparison between diamond and zinc-blende crystals.[4] A widening of photonic band gap was also previously achieved by inserting a material at well-chosen places in the unit cell.[8]

A different approach to obtain a tunable phononic band-gap width is proposed here. It consists of a rotation of a two-dimensional periodic system of hard inclusions hosted in air. By choosing square-section rods distributed according to a square lattice, and by increasing the rotation angle of these rods with respect to the lattice orientation, we can obtain a progressive widening of the gap.

Figure 1 represents a geometric assembly of the columns in air in two different configurations. In the left part, the columns are aligned with the square lattice. In the right part of the same figure, an angle (θ) of 30° is formed between the alignment of the rods and that of the lattice. The representation is shown for a filling fraction, expressed as the ratio between the rod section and the surface of the two-dimensional unit cell, of 0.50.

This tuning technique differs from those described in the literature, where no additional insertions are made. We will see that a reduction of the symmetry cannot be used to explain the gap widening when the angle is increased. Even if the symmetry is reduced for angles differing from 0° or 45°, 45° seems to be the best angle for generating the largest gap, as the following discussion will point out.

Geometric tuning was already suggested in photonic crystals, but no emphasis was given to a detailed origin of the wave stopping.[9] Here we will reach for a plausible explanation of the wave transmission by regarding the geometric effects induced on the gap by the rotation of the rods.

II. NUMERICAL FORMULATION

It is well established that homogeneous elastic media present no gap in their dispersion relations. The linear branches issuing from the Γ point have slopes equal to the different sound velocities. Periodic inhomogeneities play a crucial role in the opening of gaps. The periodic insertion of components, characterized by different elastic constants, reshapes the spectral response. The adjustment of parameters such as the mass densities or the sound velocities allows for an opening of partial or complete gaps. We have built a *phononic crystal*.[1–4]

The study of elastic mode propagation through inhomogeneous solid structures is not straightforward, since a coupling between the transverse and longitudinal modes is expected in comparison with homogeneous systems. Nevertheless, for two-dimensional periodic systems, a partial decoupling is achieved by assuming a normal incidence of the waves with respect to the direction normal to the plane of the periodicity. Pure transverse modes are found along this axis (denoted by the z index). These modes are independent of the related coupled modes propagating in the plane of the periodicity (denoted by index i, $i=1,2$).[10] Equations

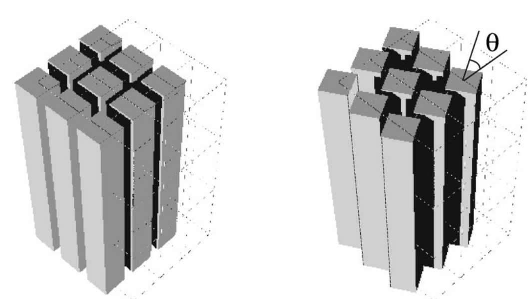

FIG. 1. Geometric representation of the two-dimensional periodic systems of hard rods in air arranged in a square lattice. The rods have a square section, and the filling fraction is 0.50. The left part of the figure represents a column array having the same orientation as the empty lattice. The right part deals with the same array rotated by 30° (rotation angle θ).

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describing these distinct modes can be expressed in the harmonic approximation by

$$-\rho(\mathbf{r_t})\omega^2 u_z = \nabla \cdot [\mu(\mathbf{r_t})\nabla u_z], \tag{1}$$

$$-\rho(\mathbf{r_t})\omega^2 u_i = \frac{\partial}{\partial x_i}[\lambda(\mathbf{r_t})\nabla\cdot\mathbf{u}] + \nabla\cdot[\mu(\mathbf{r_t})\nabla u_i] + \nabla\cdot\left(\mu(\mathbf{r_t})\frac{\partial}{\partial x_i}\mathbf{u}\right) \quad (i=1,2), \tag{2}$$

where $\mathbf{r_t}$ represents a direct-space vector in the plane of the periodicity, ∇ is the two-dimensional Laplace operator, $\rho(\mathbf{r_t})$ is the mass density distribution, and $\mu(\mathbf{r_t})$ and $\lambda(\mathbf{r_t})$ are the so-called Lamé coefficients. u_z and u_i $(i=1,2)$ are the three components of the elastic displacement vector $\mathbf{u}$.

In the case of heterostructures composed of fluids, shearing can be neglected $(\mu=0)$, and we can remove the coupling difficulty by using another variable, the pressure p, defined as a pure scalar dilatation motion:

$$p = -\lambda(\mathbf{r_t})\nabla\cdot\mathbf{u}. \tag{3}$$

The basic equations which describe the wave propagation then reduce to a simple scalar equation[4]

$$-\frac{\omega^2}{\lambda(\mathbf{r_t})}p = \nabla\cdot\left(\frac{1}{\rho(\mathbf{r_t})}\nabla p\right). \tag{4}$$

This describes the so-called *acoustic* case, to be contrasted with the *elastic* case. It is interesting to note the similarity between this equation and Eq. (1) introduced above for describing the pure transverse motion in the *elastic* case.

In both cases, we decided to make use of a plane-wave formulation. We set up Fourier developments of the periodic parameters and the Bloch theorem to express the elastic displacement vector or the pressure field. For a two-dimensional periodic system, we can obtain a two-dimensional generalized eigenvalue problem by canceling the component of the wave vector in the direction normal to the plane of the periodicity $(k_z=0)$.[10] For practical applications, a good convergence is obtained by using a basis set of 600 plane waves.

III. TUNABLE PHONONIC BAND-GAP SYSTEM

The modeling of systems mixing a solid and a fluid using a plane-wave representation is not known to be an easy task. Unrealistic results or problems of convergence are commonly encountered difficulties.[11,12] In many cases, these systems offer a huge density contrast between various parts of the unit cell, and this property is of real interest for the generation of a wide complete gap.[13–15] With an adequate modeling, these systems allow one to use a plane-wave method. In this section, we will introduce these models, in relation with the tuning effect.

A. Air modes for low solid filling fractions

First, we examine the case of isolated solid rods in air. It was shown that these inclusions can be considered as perfectly hard,[16,17] which implies that the sound does not propagate inside the columns. The rods are thus strong reflectors, and the propagation is predominant in the background of air. It is thus a good approximation to consider the solid rods as fluid inclusions with very high stiffness and specific mass.

Indeed, it is well known that the huge contrast of acoustic impedances in fluid systems induces a total reflection of the waves with a confinement of the waves inside the lowest impedance region, that is to say, in the region of low density or low longitudinal velocity. In the calculations, this justifies the use of the acoustic wave equation described above [Eq. (4)]. This approximation is coherent with existing experimental results,[1] and we call it the *acoustical model* in this paper. Two particular band structures are presented in Fig. 2 for different symmetry directions of the two-dimensional first Brillouin zone. The first one (in the left part of the figure) was calculated for a filling fraction of 0.40 and a rotation angle of 35°. A sketch of the two-dimensional periodicity is presented below the band structure. Except in the near neighborhood of the zone center Γ, a restructuring of the bands with regard to the homogeneous case is shown.[18,19] A large complete phononic band gap is clearly established between the first and second bands.

The next band structure (in the right part of the same figure) was calculated for a filling fraction of 0.50, and for an angle of 45°. The gap has increased in comparison with the first result, due to the higher angle of rotation and the higher filling fraction. In the last example, the picture of the periodic distribution of columns shows that the close-packing limit is reached: the columns are in contact at their corners.

A summary of the calculated results is presented in Fig. 3. For different filling fraction values (with a maximum of 0.50), we can see curves of the normalized width of a complete gap, lying between the first and second bands, as functions of the rotation angle of the columns (θ). The normalized band-gap width is taken as the gap width divided by the midgap frequency. For each filling fraction, we clearly see that the gap width increases progressively with the increasing angle and, at a fixed angle, increases with the filling fraction.

We explain the widening of the gap by some effects induced by the change of the geometry. At 0°, the space left between the columns is large enough to allow for propagation of the waves in the whole structure with little wave interferences. This leads to dispersion relations without gap. On the other hand, as the angle increases, this space is reduced, and more reflection on the columns can be expected, involving more destructive interferences. The increasingly destructive interferences are at the origin of the progressive widening of the gap. This explanation cannot be transferred directly in the photonic case,[9] because a huge contrast of the dielectric functions is not possible.

We already showed that waves propagate mainly inside low-density or low-velocity regions of fluid systems. Isolated cavities of low density can even lead to a confinement of waves in these regions, responsible for the appearance of flatbands in the band structure.[20,21] We could show that a high contrast of densities is the main condition in order to confine the waves. In this case, the contrast of velocities does not affect the shape of the band structures, and only the

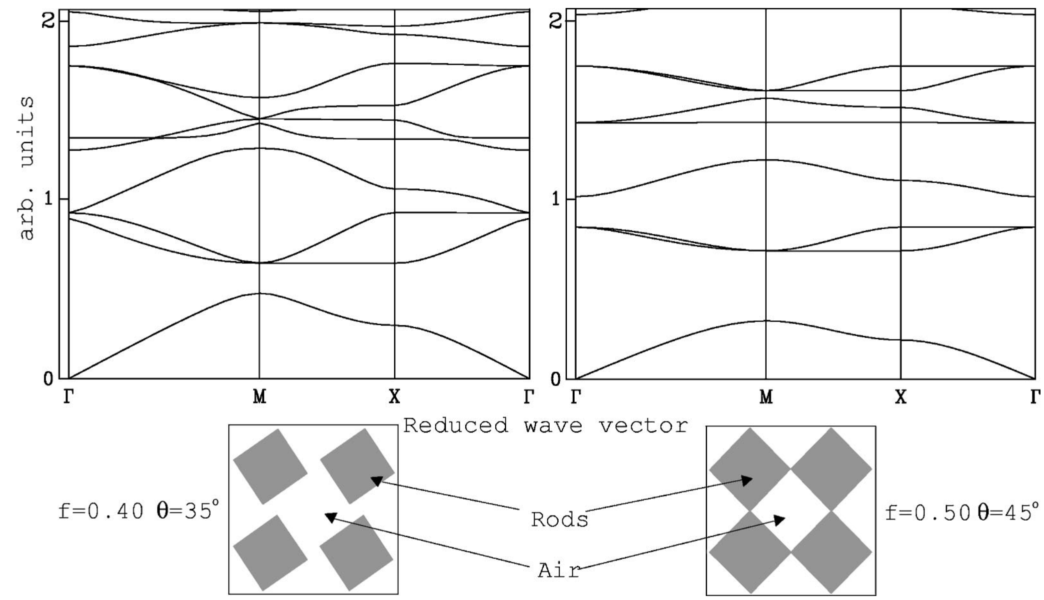

FIG. 2. Dispersion relations calculated for the structure described in Fig. 1 in different directions of the two-dimensional Brillouin zone (the vertical scale is the frequency expressed in arbitrary units, $\nu a/c$, where a is the cell parameter and c is the sound speed in air). In the left part, the filling fraction was set at 0.40, and the rotation angle as 35°. A gap is clearly visible between the first and second bands. The second part, in the right, was calculated for a filling fraction of 0.50 and for an optimum rotation angle of 45°. The gap is then larger due to the higher values of the angle and the filling fraction. In both cases, a plane of the two-dimensional periodicity is given below the dispersion relations. We note that the close-packing arrangement is reached in the second case.

frequency scale can be modified. On the other hand, a system offering high contrasts of velocities without high contrasts of densities will not allow for the confinement of the modes.

Note that the mechanisms responsible for the confinement are explained by the settling of interferences in the wave propagation process, as described in this work. These are far different from those used to explain the localization in a disorder system;[22] however, in the two cases, localized modes are characterized by an exponential decay as the distance from the localization center increases.

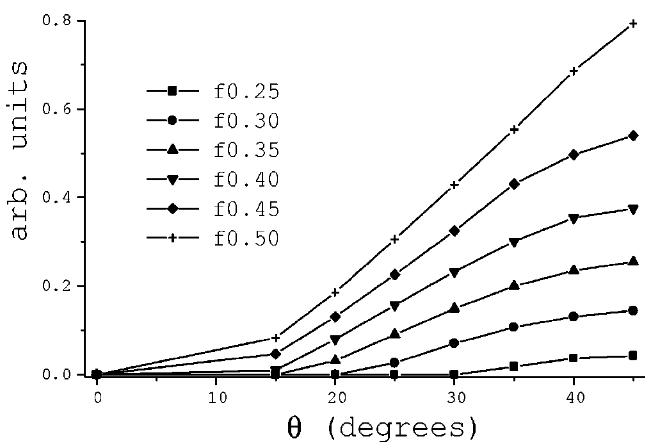

FIG. 3. Representation of the normalized first gap width (lying between the first and second bands) vs the rotation angle (θ) calculated for hard rods in air with different filling fractions (f). The normalized gap width (expressed in arbitrary units) is obtained by dividing the gap width by the midgap frequency. A widening of the gap value with increasing rotation angle is observed in all the cases. The elastic parameters chosen for the calculations are $\rho_{air} = 1\ \mathrm{kgm}^{-3}$, $\rho_{rod} = 1500\ \mathrm{kgm}^{-3}$, $c_{air} = 340\ \mathrm{ms}^{-1}$, and $c_{rod} = 2000\ \mathrm{ms}^{-1}$.

B. Elastic modes for high solid filling fractions

Such kinds of flatband structures could appear if the inclusions are in contact, so that the air host forms isolated cavities. This means that we exceed the close-packed arrangement of the hard prisms. This situation can be found for filling fractions higher than 0.50, and above a critical value of the rotation angle (θ_c). This value is related with the filling fraction (f) by the following simple law:

$$\cos \theta_c = \sqrt{f}. \tag{5}$$

Nevertheless, for an infinite crystal, this pattern is equivalent to that obtained with air columns inserted in an homogeneous solid matrix. Thus the acoustical model cannot be properly employed, and the shearing inside the host must be accounted for by using the full elastic equations [see Eqs. (1) and (2)].

As already suggested, systems composed of both fluids and solids are not easily described with the plane-wave method.[11,12] The existing inaccuracies[11] were attributed to problems encountered during the diagonalization step, when huge contrasts are found in the system. Other methods, such as the finite-difference time-domain method[12] (FDTD) or the so-called Kornage-Kohn-Rostoker approach,[11] shed some light on this particular plane-wave limitation.

As an example, consider the system described above for a filling fraction of 0.60 and a rotation angle of 45°, which is

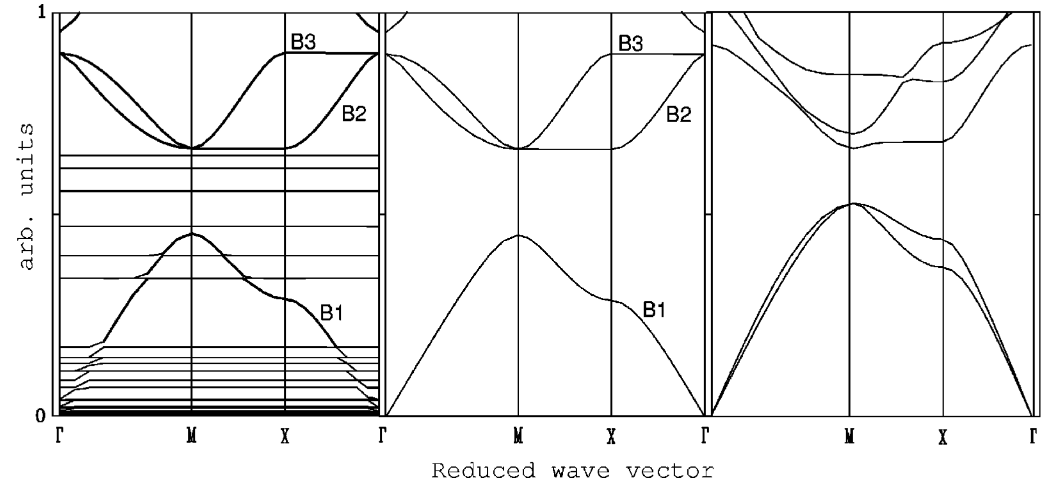

FIG. 4. Dispersion relations calculated for the inverted structure of air cavities in a solid host. The filling fraction of the hard component is 0.60, and the rotation angle is 45°. The vertical scale is the frequency expressed in arbitrary units $\nu a/c_t$, where a is the cell parameter and c_t is the transverse velocity in the host. In the left part, the band structure was calulcated for the pure transverse motion with a null transverse velocity in the fluid. Many flatbands are found. Three bands, denoted by $B1$, $B2$, and $B3$, present a normal character. In the middle part, the same band structure is calculated with a high artificial transverse velocity in the fluid. The flat bands are removed, and the $B1$, $B2$, and $B3$ bands stay in the same position. A strong similarity with the band structure presented in Fig. 2 is found. In the right part, the band structure associated with the mixed motions is calculated with the same approach. In the last two cases a phononic band gap is found. The elastic parameters chosen for the calculations are $\rho_{air}=1$ kgm^{-3}, $\rho_{host}=1500$ kgm^{-3}, $c_{l,air}=340$ ms^{-1}, $c_{l,host}=3500$ ms^{-1}, and $c_{t,host}=2000$ ms^{-1}. The value of the artificial transverse velocity inside the fluid is discussed in the text.

higher than the critical angle of the close-packed arrangement of the solid rods ($\theta_c=39.2°$). A more realistic approach consists of considering the equivalent infinite elastic crystal of air columns occupying 40% in a heavy solid matrix.

We calculated the band structure associated with the pure transverse motion u_z. The result is shown in the left part of Fig. 4. Three bands denoted by $B1$, $B2$, and $B3$ converge. In the other hand, some unphysical flatbands appear. We can show that these bands do not converge, and appear randomly according to the number of plane waves. Moreover, for an equivalent number of plane waves, their position can differ according to the routines employed in the calculation, suggesting a bad numerical problem condition.

In the case of a huge contrast of densities, the FDTD (Ref. 12) method showed that only the $B1$, $B2$, and $B3$ bands constitute the *physical* band structure. Using a plane-wave method, the flatbands can be removed by taking an artificial transverse velocity inside the fluid. For the calculations, a value of 1500 ms^{-1} was chosen. This can be only done for very low-density fluid, in order to keep the ratio between the density and the artificial velocity small compared with the one in the solid.[12] As already suggested, this value depends on the routines and on the convergence.

Our band structure is presented in the middle part of Fig. 4. The three remaining bands in the pure transverse case are the $B1$, $B2$, and $B3$ bands. The flatbands have disappeared, and a gap has settled between the $B1$ and $B2$ bands. In the right part of Fig. 4, the band structure associated with the in-plane motions is calculated with a similar approach. In this case, an artificial transverse velocity of 10^5 ms^{-1} is introduced in order to remove the unrealistic flatbands. By overlaying the two band structures, a full phononic band gap is still obtained.

We claim that this model is justified by the same geometric arguments as before. Instead of postulating a purely longitudinal behavior of the solid, we now give an artificial transverse character to the fluid.

As for the shape of the equations, we find a strong similarity between the acoustic case and the pure transverse case. The band structures presented in Fig. 2 and in the middle of Fig. 4 are roughly similar. These analogies suggest that the shearing coefficient μ plays the same important role as the mass density in the fluid case. Thus the waves will propagate mainly in the region of high μ. The air cavities are reflectors, because the waves now propagate mainly in the solid. This justifies the use of an artificial transverse character of the fluid. This simple model, deduced from the simplest case, gives a good account of the insertion of a low-density fluid in a solid. This is not valid for massive fluids such as mercury.[12] The higher density in the fluid does not allow one to consider the fluid as a perfect reflector, as a strong mode conversion between the transverse modes and the longitudinal ones is expected.

In the case of the in-plane motions, this simple model is still valid. Nevertheless, the nontrivial shape of the equations does not allow for the same kind of analogy, so that the explanation for the use of a high artificial transverse velocity in air is not straightforward.

A gap tuning is then also expected for large filling fractions, due to geometric effects similar to those found for small filling fractions. The orientation of the air cavities will induce exactly the same opening of the gap as the rotation angle is increased. The frequency scale is larger, since the material host is now a solid. This theoretical example is illustrated in Fig. 5. The normalized gap width is drawn for a host filling fraction of 0.70. Above the close-packing arrangement of the solid compound ($\theta_c=33.2°$), the elastic

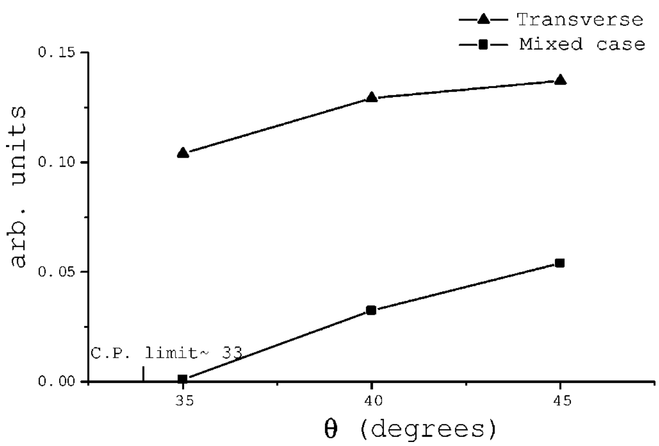

FIG. 5. Representation of the normalized first gap width vs the rotation angle (θ) calculated for air cavities inserted in a solid host. The normalized gap width (expressed in arbitrary units) is obtained by dividing the gap width by the midgap frequency. The filling fraction of the host is 0.70. The normalized width is calculated for both the transverse and mixed cases beyond the close packing angle, $\theta_c = 33.2°$, denoted by the C.P. limit. A widening of the gap value with higher rotation angles is observed in both cases, as in the acoustic system.

model of reflective air columns suggests a widening of the gap for both pure transverse and coupled motions. Nevertheless, the normalized gap width of the resulting full gap is smaller than in the former case.

IV. CONCLUSION

In this work, we used a plane-wave method for analyzing the band structure of a periodic assembly of hard rods of square section distributed in air. This system is of practical interest in order to achieve a phononic crystal with a tunable gap width, adjustable by rotating the columns.

Such a system, mixing fluid and solid compounds, is not easy to study with a plane-wave method. Nevertheless, two models were developed in order to avoid the difficulties for low and high filling fractions of the solid component in the air host. In a complementary way, these models explained the effects induced by the progressive change of the geometry on the gap size. They take into account the important contrast of impedances responsible for a strong reflective action in the interfaces of the compounds.

The real interest of the introduction of this device can be stressed by underlining that the tuning mechanisms provides a nondestructive method of influencing the phononic structure, as we can obtain the desired value of the gap without acting on the shape or the constitution of the rods. Several direct applications can be envisaged in the field of a selective filtering of the acoustic power.

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