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Complete acoustic band gaps in periodic fibre reinforced composite materials: the carbon/epoxy composite and some metallic systems

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Abstract. We present results of elastic band structure for two-dimensional composite materials, composed of periodical square arrays of parallel cylinders in a background.

We reveal, for the first time, the existence of several very large complete band gaps in the band structure of a material of practical interest such as a C fibre reinforced epoxy composite. Within these gaps the propagation of acoustic waves is forbidden. The influence of the geometry of the cylinders and the effect of the composition of the composite material on the band structure are studied. We also compare these results with those obtained for metallic composites such as W (Al) cylinders in an Al (W) matrix.

The complete band gaps are observed in the cases of C cylinders in epoxy or W cylinders in Al, but not in the opposite situations. We discuss the existence of these gaps in relation to the physical parameters of the materials involved.

1. Introduction

During the last few decades, the propagation of waves in periodic or random composite systems has been studied extensively. Various structures and compositions of composite materials have been investigated using different approaches. The propagation of waves in periodic composite media such as a fluid containing immovable rigid spheres [1] or a solid containing spherical cavities [2] (inclusions being located periodically on a three-dimensional array) has been studied using the Floquet theory. The finite-element method has been extended to model the propagation of plane harmonic waves in one-, two- or three-dimensional periodic structures [3–5]. Wirgin and Ghariani [6] have studied the propagation of a shear horizontal wave in random composite fibrous media and have shown that the Urick–Ament formula gives a good description of the response of the system under some restrictions.

Moreover, there has been considerable interest, during the last few years, in the existence of band gaps in the optical [7–10] and acoustic [11–17] band structures and the presence of regions of very low density of states in periodic as well as in random composite systems. One motivation for these studies is a better understanding of wave localization in inhomogeneous media. In the case of the elastic composites with which we are dealing in this work, one can also consider engineering applications such as a vibrationless environment

for high-precision mechanical systems in a given frequency range or design of transducers and other devices. The elastic band structure of two-dimensional composite materials, formed from periodic arrays of parallel cylinders embedded in a background material, has been treated independently in a few recent works by Sigalas and Economou [11–14] and by Kushwaha *et al* [15–17]. Kushwaha *et al* [15] considered only the transverse polarization mode of vibration (with elastic displacement parallel to the cylinders and perpendicular to the wavevectors). The dispersion curves for Ni (Al) cylinders in an Al (Ni) background were presented. Phononic band gaps, extending throughout the first Brillouin zone, were found in both cases. On the other hand, the dependence of the band gap on the composition of the material and on the physical parameters of the constituents involved in the composite system was investigated [16]. In addition to the above polarization, Sigalas and Economou [13] also studied the coupled longitudinal–transverse polarization mode of vibration for which the elastic displacement as well as the Bloch wave vector are perpendicular to the cylinders' axis. They found that Au cylinders in a Be background exhibit a very narrow, albeit complete gap, shared by both polarizations. They proposed [14] that the cermet topology, in which the cylinders are made of a low-velocity material surrounded by a high-velocity host material, is the more favourable periodic binary composite structure for the appearance of acoustic gaps.

In this paper, we present results of elastic band structure for commercially available composite materials such as epoxy reinforced C or glass fibres. The dispersion curves for combinations of two isotropic metals such as W and Al are also calculated. One new result in this work is to emphasize the existence of several large complete band gaps in the epoxy reinforced C cylinder composite while one single narrow low-frequency gap was found in a previous work on elastic composites [13]. We also point out the possibility of very flat bands. The calculation of the band structure is performed for different shapes of the cylinder cross section, when the array of rods forms a square lattice. A general requirement for the existence of complete band gaps (which is fulfilled in our examples) is a large contrast between the parameters of the constituents. However, we obtain such gaps for C cylinders in an epoxy matrix or W inclusions in an Al matrix and not in the opposite situations. In the first case, the elastic constants are higher in the inclusions than in the background material; however C and epoxy have similar mass densities and very different elastic constants, whereas in W and Al both elastic constants and mass densities are rather different, the velocities of sound being almost the same. Therefore, our results show that a statement about the relative velocities of sound in the constituents cannot give a general rule for the existence of complete band gaps [14]; rather, the contrast between elastic constants as well as mass densities should be taken into account. The method of calculation is briefly presented in section 2 and followed by the numerical results in section 3. Section 4 contains the main conclusions of the paper.

2. Method of calculation

In this paper, we calculate elastic band structures of two-dimensional binary composite systems using a method developed by Kushwaha *et al* [15, 16].

These periodic systems are modelled as arrays of infinite cylinders of arbitrary cross section made of an isotropic material A embedded in an infinite isotropic elastic matrix B (see figure 1). The lattice constant is a and the filling fractions are f and $(1 - f)$ for the materials A and B respectively. The elastic parameters are periodic functions of the position. The mass density ρ and the elastic constants C_{ij} are ρ^A and C_{ij}^A inside the cylinders and

ρ^B and C_{ij}^B in the background. This means that ρ and C_{ij} are functions of the coordinates x and y where the z axis defines the direction of the cylinders. Considering the double periodicity in the xy plane, we can write ρ and C_{ij} as Fourier series:

$$\rho(\mathbf{r}) = \rho(x, y) = \sum_{\mathbf{G}} \rho(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}} \quad (1a)$$

$$C_{ij}(\mathbf{r}) = C_{ij}(x, y) = \sum_{\mathbf{G}} C_{ij}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}} \quad (1b)$$

where \mathbf{r} is the position vector of components x and y and \mathbf{G} are the reciprocal lattice vectors in the xy plane. The Fourier coefficients in equation (1a) take the form

$$\rho(\mathbf{G}) = \frac{1}{A} \int \int d^2\mathbf{r} \rho(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} \quad (2)$$

where the integration is performed over the unit cell of area $A = a^2$.

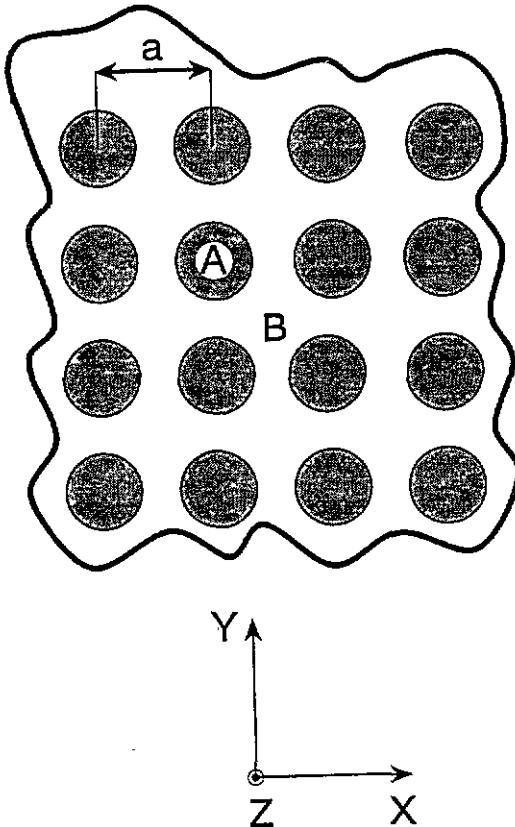


Figure 1. A transverse cross section of the binary composite system: a square array of infinite cylinders (A) periodically distributed in an infinite matrix (B).

For $\mathbf{G} = 0$, equation (2) gives the average density

$$\rho(\mathbf{G} = 0) = \bar{\rho} = \rho^A f + \rho^B (1 - f). \quad (3a)$$

For $\mathbf{G} \neq \mathbf{0}$, equation (2) may be written as

$$\rho(\mathbf{G} \neq \mathbf{0}) = (\rho^A - \rho^B)F(\mathbf{G}) = (\Delta\rho)F(\mathbf{G}) \quad (3b)$$

where $F(\mathbf{G})$ is the structure factor given by

$$F(\mathbf{G}) = \frac{1}{A} \int \int_A d^2\mathbf{r} \rho(\mathbf{r})e^{-i\mathbf{G}\cdot\mathbf{r}}. \quad (3c)$$

In (3c), the integration is only performed on material A. In an entirely similar way, equation (1b) gives

$$\begin{cases} C_{ii}(\mathbf{G} = \mathbf{0}) = \bar{C}_{ii} = C_{ii}^A f + C_{ii}^B(1 - f) \\ C_{ii}(\mathbf{G} \neq \mathbf{0}) = (C_{ii}^A - C_{ii}^B)F(\mathbf{G}) = (\Delta C_{ii})F(\mathbf{G}) \end{cases} \quad (4a)$$

$$(4b)$$

with $i = 1$ or 4 .

Let us now give the equations of motion in the composite material remembering that the elastic constants and the mass density are position dependent [18]:

$$\begin{aligned} \rho(\mathbf{r})(\partial^2 u_i / \partial t^2) &= \nabla \cdot [C_{44}(\mathbf{r})\nabla u_i] + \nabla \cdot [C_{44}(\mathbf{r})\partial u / \partial x_i] \\ &+ (\partial / \partial x_i)[(C_{11}(\mathbf{r}) - 2C_{44}(\mathbf{r}))\nabla \cdot \mathbf{u}] \end{aligned} \quad (5)$$

where \mathbf{u} represents the position and time dependent displacement vector $\mathbf{u}(\mathbf{r}, t)$.

For wave propagation in the xy plane, one can introduce a wave vector $\mathbf{K}(K_x, K_y)$ (which means $K_z = 0$) and use the Bloch theorem to write the displacement field

$$\mathbf{u}(\mathbf{r}, t) = e^{i(\mathbf{K}\cdot\mathbf{r} - \omega t)} \sum_{\mathbf{G}} \mathbf{u}_{\mathbf{K}}(\mathbf{G})e^{i\mathbf{G}\cdot\mathbf{r}} \quad (6)$$

where ω is the wave circular frequency. In this case the vibrations polarized parallel to the z axis become decoupled from those in the xy plane. The equations of motion for the former modes are written as

$$\begin{aligned} [(\bar{C}_{44}(\mathbf{K} + \mathbf{G})^2 - \rho\omega^2)u_{\mathbf{K}}^z(\mathbf{G}) + \sum_{\mathbf{G}' \neq \mathbf{G}} [(\Delta C_{44})(\mathbf{K} + \mathbf{G}) \cdot (\mathbf{K} + \mathbf{G}') - (\Delta\rho)\omega^2] \\ \times F(\mathbf{G} - \mathbf{G}')u_{\mathbf{K}}^z(\mathbf{G}')] = 0 \end{aligned} \quad (7)$$

whereas the latter modes are governed by the equation

$$\begin{aligned} [(\bar{C}_{44}(\mathbf{K} + \mathbf{G})^2 - \rho\omega^2) \cdot \mathbf{u}_{\mathbf{K}}^T(\mathbf{G}) + (\bar{C}_{11} - \bar{C}_{44})(\mathbf{K} + \mathbf{G})(\mathbf{K} + \mathbf{G}') \cdot \mathbf{u}_{\mathbf{K}}^T(\mathbf{G}) \\ + \sum_{\mathbf{G}' \neq \mathbf{G}} F(\mathbf{G} - \mathbf{G}')\{(\Delta C_{44})[(\mathbf{K} + \mathbf{G}) \cdot (\mathbf{K} + \mathbf{G}') \cdot \mathbf{u}_{\mathbf{K}}^T(\mathbf{G}')] \\ + (\mathbf{K} + \mathbf{G}')(\mathbf{K} + \mathbf{G}) \cdot \mathbf{u}_{\mathbf{K}}^T(\mathbf{G}') - 2(\mathbf{K} + \mathbf{G})(\mathbf{K} + \mathbf{G}') \cdot \mathbf{u}_{\mathbf{K}}^T(\mathbf{G}')\} \\ + (\Delta C_{11})(\mathbf{K} + \mathbf{G}) \cdot (\mathbf{K} + \mathbf{G}') \cdot \mathbf{u}_{\mathbf{K}}^T(\mathbf{G}') - (\Delta\rho)\omega^2 \mathbf{u}_{\mathbf{K}}^T(\mathbf{G}')\} = 0 \end{aligned} \quad (8)$$

where $\mathbf{u}^T = u_x \mathbf{x} + u_y \mathbf{y}$.

Equations (7) and (8) are two infinite sets of linear equations where the unknowns are the Fourier components of the displacement field. In practice, only a finite number of \mathbf{G} vectors are, of course, taken into account for the numerical calculation. The determinants of these systems of equations must vanish, which conditions yield the band structure $\omega_n(\mathbf{K})$. The eigenmodes of (7) correspond to transverse vibrations ($\mathbf{u} = u^z \mathbf{z} \perp \mathbf{K}$) and will be called Z modes or bands. On the other hand, the eigenvalues of (8) describe coupled longitudinal-transverse vibrations, to be denoted XY modes or bands.

3. Numerical results for the square lattice

We first consider composite systems of technological interest, namely C fibres reinforced epoxy composites, which are used, for example, in aeronautics and car manufacture [19]. We calculate the dispersion curves for different filling fractions and various cross sections of the cylinders. Epoxy and C are polycrystalline materials, and may be considered as isotropic on a macroscopic scale. Their physical parameters are listed in table 1.

Table 1. Physical parameters of Carbon [19], epoxy resin [19], W [21] and Al [21]. C_1 and C_t represent respectively the longitudinal and the transverse speed of sound.

	ρ (g cm ⁻³)	C_{11} (10 ¹¹ dyn cm ⁻²)	C_{44} (10 ¹¹ dyn cm ⁻²)	$C_l = \sqrt{C_{11}/\rho}$ (m s ⁻¹)	$C_t = \sqrt{C_{44}/\rho}$ (m s ⁻¹)
C	1.75	30.96	8.846	13310	7110
Epoxy	1.2	0.964	0.161	2830	1160
W	19.3	50.1	15.14	5090	2800
Al	2.692	11.2	2.79	6450	3220

It is assumed that the array of cylinders forms a square lattice of period a . Then the reciprocal lattice vectors \mathbf{G} are given by

$$\mathbf{G} = (2\pi/a)(n_x\mathbf{x} + n_y\mathbf{y}) \quad (9)$$

where n_x and n_y are two integers. In the course of the numerical calculations, these integers are limited to the interval $-N \leq n_x, n_y \leq +N$. For the sake of consistency, all the results sketched below are obtained with $N = 6$. However, some of the dispersion curves were also calculated with $N = 10$ and confirmed the good accuracy of the results for $N = 6$. The different shapes of the cylinders' cross sections are the following:

- (i) circular section of radius r_0 ;
- (ii) square section of width $2l$; and
- (iii) rotated square section of width $2l$ with a 45° angle of rotation with respect to the x, y axes.

The structure factors $F(\mathbf{G})$ associated with these shapes are respectively

$$(i) F(\mathbf{G}) = 2f J_1(Gr_0)/Gr_0 \quad \text{with } f = \pi r_0^2/a^2 \quad 0 \leq f \leq \pi/4$$

where J_1 is the Bessel function of the first kind,

$$(ii) F(\mathbf{G}) = f(\sin(G_x l)/G_x l)(\sin(G_y l)/G_y l) \quad \text{with } f = 4l^2/a^2 \quad 0 \leq f \leq 1$$

and

$$(iii) F(\mathbf{G}) = f \left(\frac{\sin[(l/\sqrt{2})(G_x + G_y)]}{[(l/\sqrt{2})(G_x + G_y)]} \right) \left(\frac{\sin[(l/\sqrt{2})(-G_x + G_y)]}{[(l/\sqrt{2})(-G_x + G_y)]} \right)$$

with $f = \frac{4l^2}{a^2}$ and $0 \leq f \leq \frac{1}{2}$.

In each case, the maximum value of the filling fraction f corresponds to the close packing of the cylinders.

The left part of figure 2(a) shows the first few Z and XY phononic bands for the square array of C cylinders of circular cross section in an epoxy matrix, the filling fraction f being equal to 0.55. We have plotted the band structure for the Z and XY modes in the three principal symmetry directions of the Brillouin zone (see the inset in figure 2(a)). The plots are given in terms of the reduced frequency $\Omega = \omega a/2\pi c_0$ (where c_0 is equal to $(\bar{C}_{44}/\bar{\rho})^{1/2}$) versus the reduced Bloch wave vector $k = Ka/2\pi$.

In the range of frequency of figure 2(a), three complete band gaps were found between the XY and the Z mode bands. These gaps are defined by the high-symmetry points Γ, X, M of the first Brillouin zone except for the bottom of the first gap. One can also notice that the higher dispersion curves in figure 2(a) are rather narrow and we especially mention the presence of a nearly flat Z band between the second and third forbidden bands. These behaviours may indicate the existence of localized states in this structure, even though we did not search for the eigenvectors in our computation.

The right panel of figure 2(a) presents the variations of the densities of states of XY and Z modes, scanning the interior of the irreducible triangle ΓXM of the Brillouin zone at 1275 points. The phononic gaps in the band structure coincide exactly with regions of null density of states. This leads us to confirm that the existing band gaps extend throughout the Brillouin zone and are not only on its periphery. One can also notice that for the nearly flat Z band, the density of states resembles a Dirac δ function.

The band structure in figure 2(a), is computed for a filling fraction of 0.55 because this is the value of f that leads to the largest complete gaps. Indeed, in figure 2(b), the widths of these three gaps are presented as a function of the filling fraction f . We note the opening of complete band gaps over a large range of the filling fraction, namely, $0.2 < f < 0.65$. One can also notice that the most usual commercially available C fibre reinforced epoxy composite corresponds to a filling fraction equal to 0.6 [19].

In figure 3(a), the Z and XY band structures for the square array of C cylinders of square cross section in an epoxy matrix are drawn for $f = 0.65$. Two complete gaps appear in the range of energy considered, as well as a few rather narrow bands. The value of the largest gap width is now $\Delta\Omega = 0.14$ as compared to a value of $\Delta\Omega = 0.09$ in figure 2(a). It is noteworthy, for this cylinder geometry, that there exists a very large gap between the second and the third XY bands, which explains the presence of a very large complete gap.

As a function of the filling fraction, complete band gaps open up for $0.25 < f < 0.8$ with a maximum of their width around $f = 0.65$ (figure 3(b)). The gap widths are greater than those calculated for the cylinders of circular cross section.

We have also investigated the case of square cylinders rotated through 45° with respect to the x, y axes. In figure 4(a), the band structure for $f = 0.35$ displays two complete band gaps. The third, the fifth and the sixth Z bands are quite flat. The largest gap width is $\Delta\Omega = 0.033$ in this case.

Figure 4(b) shows that the domain of existence of complete band gaps in this structure corresponds to filling fractions in the range $0.225 < f < 0.4$. In this composite system, the gap widths are much lower than those obtained in the two preceding geometries.

Let us notice that for the three geometries, the maximum gap width is obtained for $f/f_{\max} \simeq 0.6$ where f_{\max} corresponds to the close-packing value of f .

The acoustic band structures of the C fibres reinforced epoxy composites are very sensitive to the cylinders' cross section as well as to the filling fraction. The existence of rather large gaps is here associated with the very large contrast between the elastic constants of the cylinders and the background, while the mass densities of these materials are of the same order of magnitude (see table 1). Notice that for these usual composite systems

DENSITY OF STATES

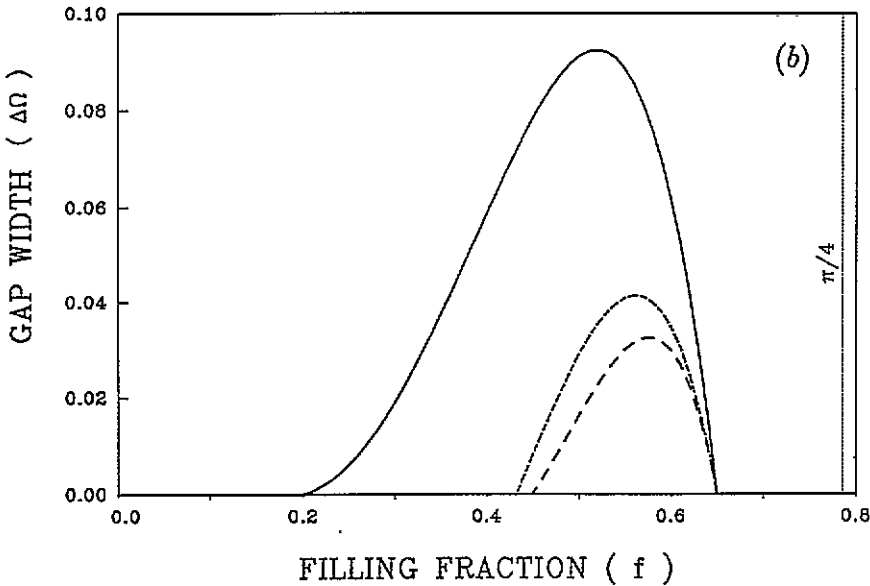
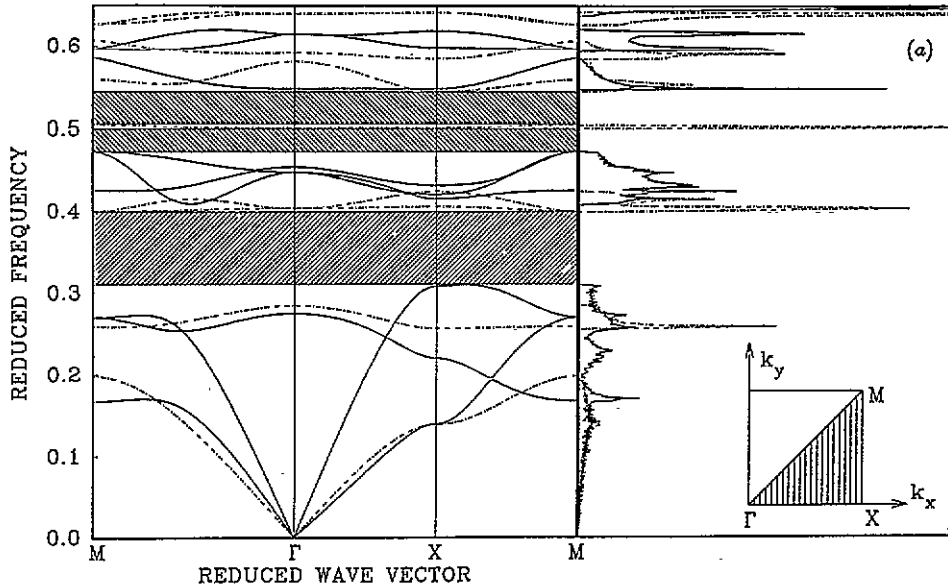


Figure 2. (a) The elastic band structure and density of states for C cylinders of circular cross section in an epoxy resin matrix, for $f = 0.55$. In the left panel of the figure, the band structure is plotted for Z (dashed lines) and for XY (solid lines) modes of vibration, in the three high-symmetry directions ΓXM of the first Brillouin zone (see inset). One can notice three complete band gaps (a fourth one of lower width exists between the ninth XY band and the eighth Z band) as well as the existence of nearly flat bands such as the fifth Z band. The right panel of the figure shows the density of states for Z (dashed lines) and XY (solid lines) modes of vibration. The phononic complete band gaps in the elastic band structure appear in this figure as regions of null densities of states. (b) The width of the first three complete band gaps as a function of the filling fraction: solid line, first gap; dash-dotted line, second gap; dashed line, third gap.

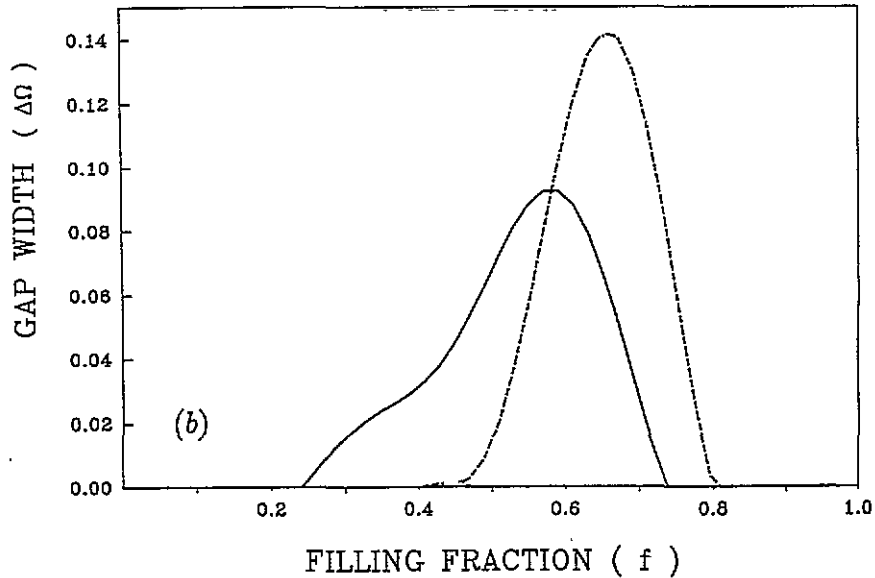
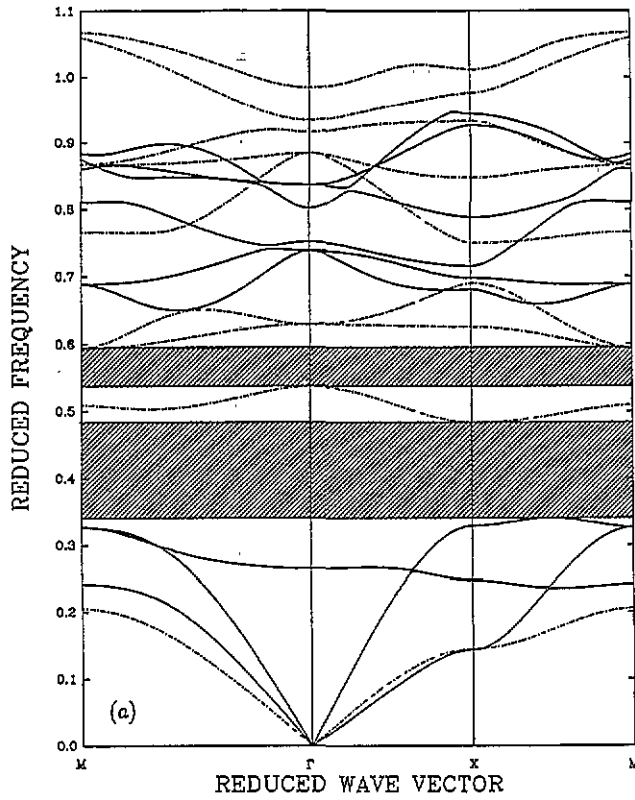


Figure 3. (a) Elastic band structures for C cylinders of square section in an epoxy matrix, for $f = 0.65$; (b) the width of the first two complete band gaps as a function of the filling fraction: solid line, first gap; dash-dotted line, second gap. It is noteworthy that the second complete band gap, which appears for higher filling fraction, is larger than the first one.

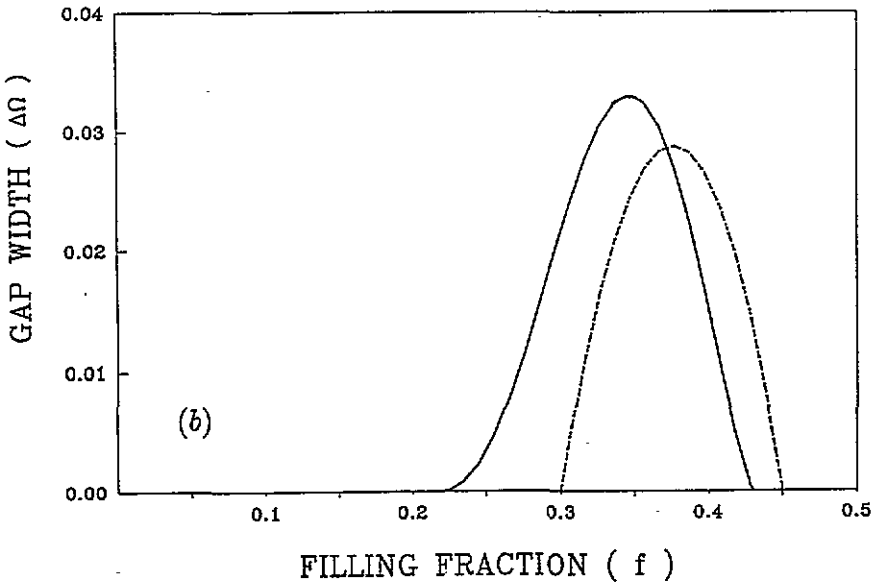
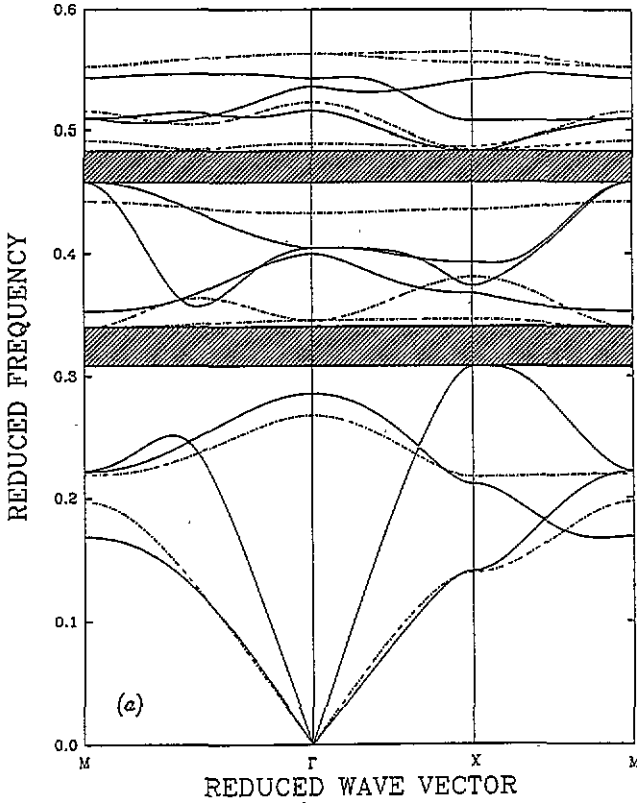


Figure 4. (a) Elastic band structures for C cylinders of square cross section rotated through 45° around the Z axis, in an epoxy matrix for $f = 0.35$. (b) The width of the first two complete band gaps as a function of the filling fraction: solid line, first gap; dash-dotted line, second gap.

presenting very large complete acoustic gaps, the cylinders are made of the high-velocity material.

We also studied another composite of technological interest, namely glass fibre reinforced epoxy matrix, using a filling fraction of 0.6. Only one complete gap was found in this case, having a width smaller than that of the first gap in the C-epoxy composite. The glass fibres' elastic constants being approximately three times lower than those of the C fibres [19], the contrast between the elastic constants of the matrix and the background is in this case less important than in the C-epoxy system.

Finally, as a matter of comparison, we also considered the case of metallic composites where there is a contrast between both elastic constants and mass densities of the constituents whereas their velocities of sound have the same order of magnitude. W and Al are two quasi-isotropic metals presenting a large ratio between the parameters although the contrast is far from being comparable to the C-epoxy case (see table 1). With a filling fraction of $f = 0.30$, figures 5 and 6 give the dispersion curves of W (Al) cylinders in an Al (W) background. Only one complete gap, of width $\Delta\Omega = 0.05$, is found in the first case while there is no such gap in the second case. Qualitatively similar results are also obtained for $f = 0.15$, with a smaller width of the gap than at $f = 0.30$. These behaviours are similar to those found in [13] for the Au-Be system. We can notice that the velocities of sound in W are slightly lower than those in Al.

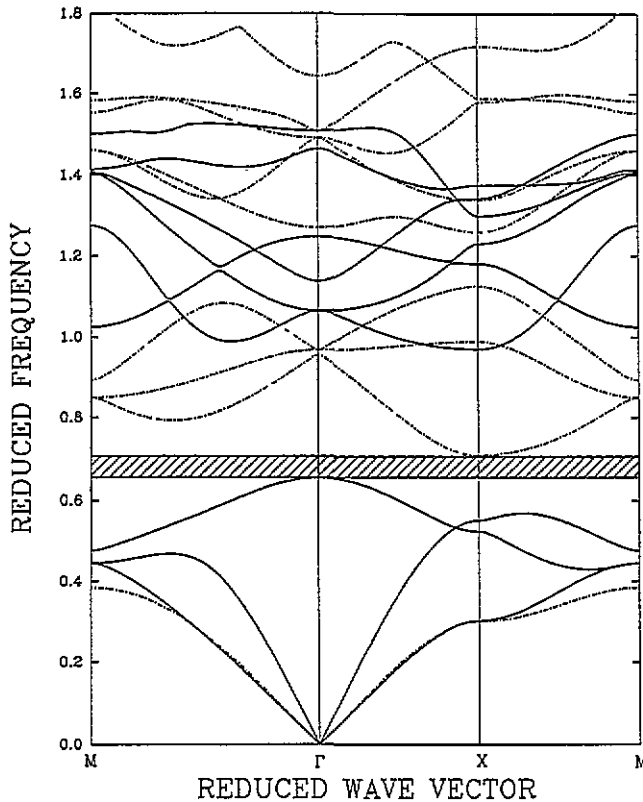


Figure 5. Elastic band structures for W cylinders in an Al matrix for $f = 0.30$. One phononic band gap appears between the third XY band and the second Z band.

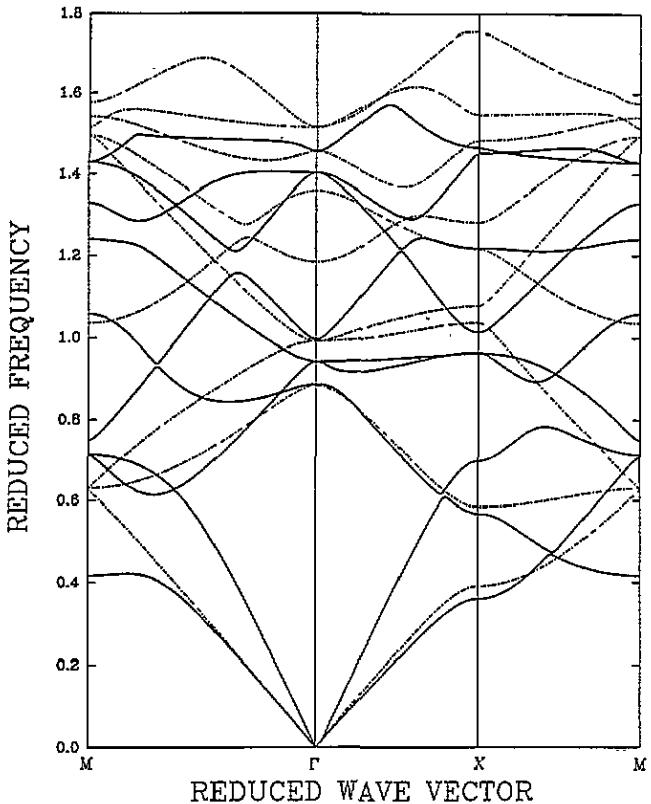


Figure 6. The same as in figure 5 for Al cylinders in a W matrix for $f = 0.30$. There is no band gap in this case.

4. Conclusion

The purpose of this paper was to investigate theoretically the existence of complete band gaps in the acoustic band structure of periodic elastic fibres reinforced composite materials such as the C-epoxy system. We obtained relatively large complete gaps where the propagation, perpendicular to the cylinders, of acoustic waves is forbidden. The influence of the geometry of the inclusions, and the effect of the composition of the composite material, on the band structure were studied. In the case of a square array of C cylinders embedded in an infinite epoxy background, larger complete band gaps appear for a square section parallel to the lattice than for the other two configurations studied. The existence of a strong contrast between the physical parameters of the inclusions and the matrix seems to be a general rule to obtain complete band gaps in the band structure of elastic composite systems. Of the materials considered in this work, C and epoxy have rather similar mass densities and very different elastic constants, whereas in W and Al the velocities of sound are in the same range, the elastic constants and mass densities being much higher in W than in Al. With these constituents, we have obtained complete band gaps for C fibres in epoxy and W fibres in an Al matrix, but not in the opposite situations. We conclude that the contrast between both elastic constants and mass densities is important for the existence of complete band gaps, which cannot be solely predicted by a requirement concerning the relative velocities of sound [14].

In this paper, we have considered square arrays of cylinders perfectly embedded in an infinite elastic background. This means that we neglected the effects due to decohesion of the fibres from the matrix and to roughness at the interface between the cylinders and the matrix. Such defects could alter the acoustic wave propagation in composite materials and consequently modify the band structure of such composites or introduce wave attenuation.

In a forthcoming publication [20], we present theoretical and experimental investigations of a binary composite consisting of a square array of Duralumin cylinders in a PVC matrix, exhibiting a good correlation between the predicted local gaps and the dips in the transmission spectrum of the *XY* acoustic waves.

It could be interesting to extend our calculation to other geometries of practical interest and to non-periodic systems, and especially to weakly disordered composites, in order to improve our understanding of acoustic wave localization.

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