

Material loss influence on the complex band structure and group velocity in phononic crystalsRayisa P. Moiseyenko^{1,2} and Vincent Laude¹¹*Institut FEMTO-ST, Université de Franche-Comté and CNRS, 32 avenue de l'Observatoire, F-25044 Besançon Cedex, France*²*Unité Mixte Internationale GT-CNRS, Georgia Tech Lorraine, 2 rue Marconi, Metz 57070, France*

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The influence of material loss on the complex band structure of two-dimensional phononic crystals is investigated. A viscoelasticity model is added to the extended plane-wave expansion (EPWE) method, with viscosity proportional to the frequency. It is found that losses have a stronger influence on the real than on the imaginary part of Bloch waves, in contrast with propagation in homogeneous media. Flat bands, i.e., bands initially showing low group velocity without losses, acquire an enhanced damping as compared to bands with larger group velocities. Losses are also found to limit the appearance of large group slownesses, or conversely small group velocities.

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I. INTRODUCTION

Phononic crystals (PC) are two- or three-dimensional periodic structures that are made of at least two materials with different mechanical properties. They can exhibit complete band gaps, i.e., finite continuous frequency regions where energy propagation is forbidden for all possible wave directions,¹ or conversely where only evanescent waves are allowed.² For band gaps to appear as a result of Bragg interference, such factors as the lattice type, the shape, and the size of inclusions, the material velocities contrast, or the density contrast are important. A composite material comparison was held by Ao *et al.*³ for metamaterials, and photonic or phononic crystals. The key distinction among these systems is that metamaterials can be homogenized in the sense that effective constitutive parameters can be meaningfully extracted and used whereas the latter cannot. In any case, the full complex dispersion relation for all waves is needed for a complete description of both types of composite materials.

The most common way to obtain the dispersion relation of phononic crystals is to solve an eigenvalue problem where the Bloch wave vector k is considered a fixed quantity within the first Brillouin zone and the appropriate frequency of allowed modes are sought for as $\omega(k)$.¹ Such an approach treats the wave vector and the frequency as implicitly real-valued. However, when considering evanescent Bloch waves, the wave vector becomes complex-valued.^{4,5} Several methods have been proposed to obtain the complex band structure of phononic crystals. The layer-multiple scattering (LMS) method is an on-shell method that operates at a fixed frequency and can yield all complex k vectors.^{3,6} A plane-wave expansion (PWE) method was proposed by Suzuki and Yu⁷ for solving three-dimensional problems based on complex eigenfrequencies. They focused their attention on tunneling modes appearing when the eigensystem becomes complex nonsymmetric, thus resulting in eigenvalues that are not necessarily real-valued. Recently, an extended plane-wave expansion (EPWE) method was introduced to obtain the full complex band structure of solid phononic crystals.² In all these works, however, loss is not considered, and complex wave vectors are found as a result of either the opening of a band gap or the frustrated character of higher-order diffracted Bloch waves below their cut-off frequency.²

In actual experiments, one or more of the constituent materials can be lossy in the frequency range of interest. Viscoelastic materials such as epoxy are for instance often used to form the matrix phase of phononic crystal composites. For crystalline solids such as silicon, quartz, or lithium niobate, losses are non-negligible starting from the GHz frequency range and can be adequately described by a viscosity tensor.^{8,9} Taking losses into account may obviously lead to changes in the appearance of band structures. Material loss has not been extensively considered in the various theories of phononic crystals, though several viscosity models exist that have been considered to describe propagation losses. Psarobas has investigated the Kelvin-Voigt model and its influence on the transmission on a phononic crystal.¹⁰ Based on the LMS method, he observed enhanced absorption at the frequencies of flat bands of a three-dimensional phononic crystal of close-pack rubber spheres in air. Another popular model closely related to the Kelvin-Voigt model is to consider the elasticity tensor (or more generally the material constants) as complex-valued. In the case of viscoelastic materials, the elastic moduli are complex numbers that are dependent on the frequency. Based on the finite-difference time-domain (FDTD) method, it has been argued that viscoelasticity impacts the transmission properties of phononic crystals not only by attenuating the transmitted acoustic waves but also by shifting the passing bands frequencies toward lower values.^{11,12} Damped Bloch waves were investigated by Hussein¹³ assuming the Rayleigh model. He introduces, in a finite element method, a damping operator proportional to both the mass and the stiffness operators in the governing equation of motion, of form $C = \alpha M + \beta K$. This formulation results in a generalized eigenvalue problem for the complex eigenfrequencies, the imaginary part of which can be used to estimate the damping of each mode. However, the problem of finding proportionality coefficients α and β for a given material is not obvious.

Artificial crystals offer design control over the dispersion of waves. Much attention has indeed been paid during the last decade to the group velocity of light passing through dispersive material.^{14,15} Low group velocity, also known as slow light or slow sound, finds a fundamental application to the enhancement of nonlinear wave interactions.^{16–18} Generally, zero group velocities can be found in a lossless periodic

structure when the Bloch wave vector sits on the boundary of the Brillouin zone. It is however well known in slow light optics that loss can play nasty tricks. Based on a simple model where the dielectric constant has a small imaginary part, Pedersen *et al.* have shown that the group velocity is limited to finite values larger than zero.¹⁹ The interplay of slow group velocities with losses arising for scattering or imperfections in photonic crystal slabs has also been widely discussed.^{20,21}

In this paper, we consider obtaining the full complex band structure of phononic crystals containing viscoelastic media. Through the EPWE method, we can thus monitor the effect of losses on both the real and the imaginary part of the frequency-dependent wave vector. We give a simple formula for the precise evaluation of the group velocity at any point of the band structure. We show that the minimal group velocity that can be achieved is limited by loss, but also that enhanced losses are observed for flat bands.

II. LOSSY PHONONIC CRYSTALS

We consider monochromatic wave propagation in a perfectly periodic phononic crystal composed of homogeneous viscous materials. Figure 1 shows the definition of the geometrical parameters in the case of a square-lattice two-dimensional phononic crystal. The relevant EPWE method is summarized in this section. From the Bloch-Floquet theorem, all fields are expressed as the product of a periodic function times an exponential term. The three displacements u_i ($i = 1, 2, 3$) are, for instance,

$$u_i(\mathbf{r}) = \sum_n u_{in} \exp(-i\mathbf{G}^n \cdot \mathbf{r}) \exp[i(\omega t - \mathbf{k} \cdot \mathbf{r})], \quad (1)$$

where the \mathbf{G}^n are the reciprocal lattice vectors and \mathbf{k} is the Bloch wave vector. A similar expression holds for the stresses.

In order to include material damping, the rank-4 viscosity tensor η_{ijkl} is introduced. This tensor has the same symmetry as the elastic tensor c_{ijkl} .⁸ Attenuation is assumed to increase linearly with frequency as it proper to polymers⁸ but also to crystalline solids such as silicon, quartz or lithium niobate.⁹ For monochromatic waves, a complex-valued elastic tensor can then be written as

$$c'_{ijkl} = c_{ijkl} + i\omega\eta_{ijkl}. \quad (2)$$

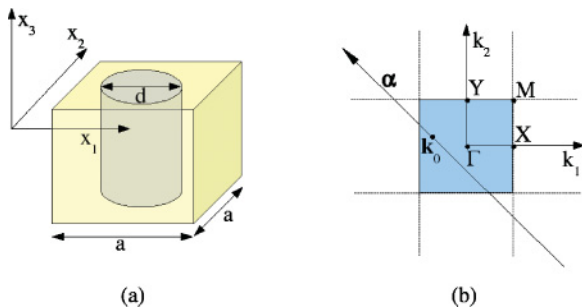


FIG. 1. (Color online) (a) Unit-cell of a square-lattice two-dimensional phononic crystal. The rod diameter and the pitch of the array are d and a , respectively. (b) Sketch of the corresponding first Brillouin zone.

More generally, any frequency dependent complex elastic tensor could be considered to model loss, without any further modification of the method.

We focus our attention on the evaluation of complex wave vectors as a function of frequency. We can formulate the same generalized eigenvalue problem as in lossless elastic media,² but for the generalization of the elastic tensor to the form in Eq. (2),

$$\begin{pmatrix} -C_2 & I_d \\ \omega^2 R - B & 0 \end{pmatrix} \begin{pmatrix} U \\ {}_i T' \end{pmatrix} = k \begin{pmatrix} D & 0 \\ C_1 & I_d \end{pmatrix} \begin{pmatrix} U \\ {}_i T' \end{pmatrix}. \quad (3)$$

In this equation, the propagation direction is given by a unit vector α and the modulus of the wave vector is the eigenvalue k . The eigenvector contains both the displacements and the stresses measured along the propagation direction, $T' = \alpha_i T_i$. The expressions for the submatrices are equally valid for 1D, 2D, and 3D phononic crystals and are given by

$$B = G_i A_{ij} G_j, \quad (4)$$

$$C_1 = G_i A_{ij} \alpha_j, \quad (5)$$

$$C_2 = \alpha_i A_{ij} G_j, \quad (6)$$

$$D = \alpha_i A_{ij} \alpha_j, \quad (7)$$

with the definition $(G_i)_{mn} = (k_{0i} + G_i^m) \delta_{mn}$, with \mathbf{k}_0 some fixed wave vector. \mathbf{k}_0 is introduced so that band structures can be generated along directions in the Brillouin zone that do not cross the Γ point. In all the previous equations, summation is implicit over any repeated index. Material constants (elastic constants, and piezoelectric and dielectric constants in the case of piezoelectric solids) enter the A_{ij} matrices; the mass density enters the R matrix. Note that the generalized eigenvalue problem for the case of plate and surface waves in 2D phononic crystals,²² but also out-of-plane propagation in 2D phononic crystals,^{23,24} appear as special cases of the above formulation.

As compared to the lossless case, the difference is that the matrices C_1, C_2, B, D are now complex-valued and frequency dependent. As a consequence, the propagative or evanescent character of eigenvalues cannot be predicted anymore: there are no purely real solutions nor complex-conjugate pairs of solutions, only complex solutions. A complex wave vector describes a wave attenuated or amplified along its propagation, depending on the sign of the imaginary part. Furthermore, band gaps are not truly apparent anymore, except by comparing to the related lossless problem obtained by setting viscosity values to zero.

As the wave vector is complex-valued, care should be taken in the definition of the group velocity. We introduce the group slowness as

$$s_g(\omega) = \text{Re} \left(\frac{\partial k(\omega)}{\partial \omega} \right) \quad (8)$$

and consider the group velocity as the inverse of this quantity. There are several possibilities in practice to calculate group quantities. The crudest approach consists in approximating the derivative by finite differences between two consecutive points of the band structure; this approach is both inefficient and imprecise. Another possibility could be to use the equality of the group velocity with the energy velocity. We rather make use of the properties of right and left eigenvectors, following an idea by Thurston.²⁵ Using the shorthand notations

$\mathbf{h} = (U, T')^T$ and $A_1 \mathbf{h} = k A_2 \mathbf{h}$ for the generalized eigenvalue problem in Eq. (3), the Appendix shows that

$$s_g(\omega) = \text{Re} \left(\frac{\mathbf{h}_l^T \left(\frac{\partial A_1}{\partial \omega} - k \frac{\partial A_2}{\partial \omega} \right) \mathbf{h}_r}{\mathbf{h}_l^T A_2 \mathbf{h}_r} \right), \quad (9)$$

where $\mathbf{h}_l(\omega)$ and $\mathbf{h}_r(\omega)$ are, respectively, a left and a right eigenvector of the same eigenvalue $k(\omega)$. This formula offers a practical and accurate means of evaluating the group slowness and group velocity at any point of the band structure. Note that we do not attempt in this paper to attribute a physical meaning to the imaginary part of the group slowness.

III. RESULTS

We consider for definiteness a two-dimensional square lattice phononic crystal made of steel rods in epoxy. The rod diameter and the pitch of the array are denoted d and a , respectively. Because the viscosity model is frequency dependent, we cannot simply reduce frequencies as is usual when displaying the band structure of lossless phononic crystals. We specify $d = 2.5$ mm and $a = 3$ mm in all the computations of this paper. With the rod axis aligned along the x_3 axis, there is a complete decoupling of waves polarized in-plane (with displacements u_1 and u_2 only) from pure shear waves (with displacement u_3 only). For simplicity, we consider only pure shear wave propagation, but the conclusions of this paper apply to in-plane wave propagation as well. Material constants used for representing isotropic steel and epoxy are given in Table I. With the dimensions chosen for the phononic crystal, the shear band gap would appear around 300 kHz, approximately. Losses in steel are neglected compared to those in epoxy, and three different levels for the shear viscosity of epoxy are considered in Table I. It should be pointed out that precise values of the viscosity are not available and that many different epoxy compositions can be obtained experimentally. The values for the shear viscosity in this paper are arbitrary and are intended for qualitative comparison only.

The complex band structures presented in Figs. 2, 4, 5, and 6 were computed along the ΓX direction of the first Brillouin zone with 11 Fourier harmonics in each direction of space. Complex band structures were obtained by solving the eigenvalue problem for a discrete number of frequencies followed by sorting using the continuity of $k(\omega)$, of the polarization and of the group slowness. One third of the eigenvalues in Eq. (3) correspond to pure shear (out-of-plane) waves and the rest to in-plane waves; only pure shear waves are shown in the band structures. In order to ease the reading

TABLE I. Material constants for steel and epoxy, restricted to pure shear wave propagation. Four different arbitrary viscosity values are considered for epoxy.

Material	c_{44} (GPa)	ρ (kg/m ³)	η_{44} (Pa.s)
Steel	82	7630	0
Epoxy 0	1.331	1100	0
Epoxy 1	1.331	1100	8
Epoxy 2	1.331	1100	80
Epoxy 3	1.331	1100	160

of complex band structures, they are presented using three panels, showing the frequency as a function of the real and the imaginary part of the wave vector, and the group slowness as a function of frequency. Real parts of the wave vector are displayed within a range slightly exceeding the first Brillouin zone in order to highlight periodicity. In contrast, imaginary parts of the wave vector are not subjected to periodicity.² They are displayed within a limited range, but there are other complex bands outside this range. Each band was assigned a color and a line type, so that modifications caused by viscosity can be monitored from one band structure to another.

Figure 2 displays the complex band structure in the lossless case. There are two shear band gaps indicated by the gray regions. Two Bloch waves are propagative at low frequencies and are labeled $B0+$ and $B0-$. The plus (+) and minus (-) signs are used to indicate propagation to the right and to the left, respectively. According to the analysis in Ref. 2 making an analogy between phononic crystals and diffraction gratings, they have a (0,0) order of diffraction. Starting from the reduced frequency $\omega a / (2\pi) \approx 1.7$ they interact with bands $B1b+$ and $B1b-$, respectively. The latter bands, like $B1a+$ and $B1a-$, have a (1,0) order of diffraction. Also apparent are bands $B2a+$, $B2a-$, $B2b+$, and $B2b-$, all having a (2,0) order of diffraction. Note that all bands with an order of diffraction larger than zero start with a rather large value of the imaginary part of the wave vector at low frequencies. Such phonons are then strongly damped even in the lossless phononic crystal.

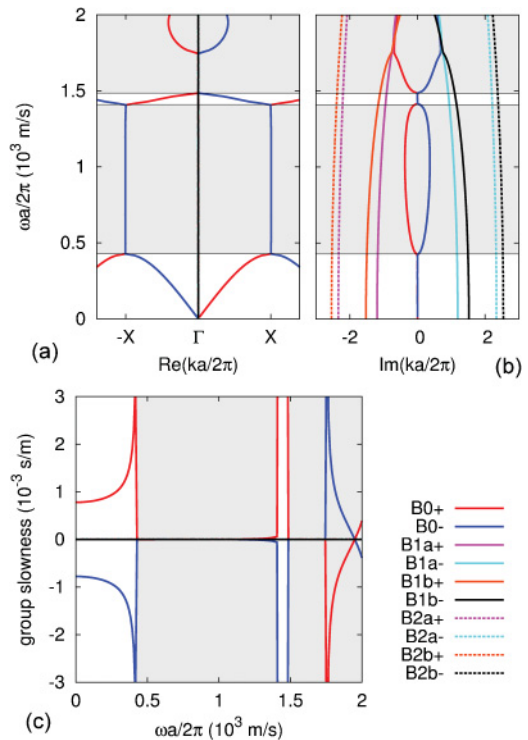


FIG. 2. (Color online) Complex dispersion relation computed with the EPWE method for a lossless square-lattice phononic crystal of steel rods in epoxy, with parameters $a = 3$ mm and $d = 2.5$ mm. In the complex band structure, the reduced frequency is presented as a function of (a) the real part and (b) the imaginary part of the wave vector. (c) The group slowness is shown as a function of the reduced frequency. Frequency band gaps are underlined in gray.

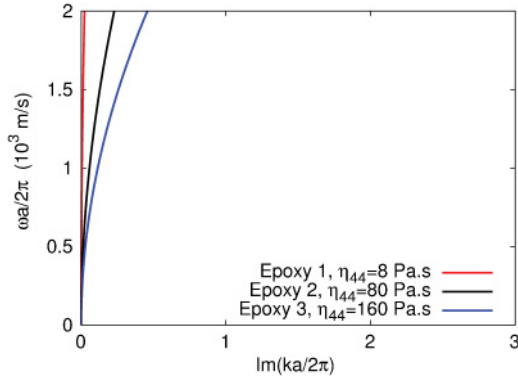


FIG. 3. (Color online) Imaginary part of the wave vector for propagation of shear waves in epoxy with various values of the shear viscosity.

The group slowness of bands $B0+$ and $B0-$ is infinite at the entrance and at the exit of the band gaps, or equivalently the group velocity vanishes at these points. In contrast, the group slowness for these two bands vanishes throughout the first band gap, since the real part of the wave vector is a constant in this frequency range. However, this apparent infinite group velocity is found in conjunction with exponential decay on propagation. The physical picture is that of classical wave tunneling in periodic structures and no violation of causality can be found in this case.^{26–28} Within the second band gap, the

group slowness of bands $B0+$ and $B0-$ then goes to infinity at $\omega a/(2\pi) \approx 1.75$. Again, these phonons are simultaneously attenuated within this frequency range.

Before turning to the effect of viscosity on phononic crystals, we recall its influence on homogeneous materials. It is well known that viscosity has a larger influence on the imaginary part than on the real part of the wave vector of initially propagative modes in homogeneous media.^{29,30} Indeed, in the limit of small viscosity the real part is almost unaffected while the damping of a pure shear plane wave is given by⁹

$$\text{Im}(k) = \frac{\eta_{44}\omega^2}{2\rho V_T^3}, \quad (10)$$

with the shear velocity $V_T = \sqrt{c_{44}/\rho}$. This equation stresses the dependence of damping with the square of the frequency in the frame of the viscoelastic model of Eq. (2). This homogeneous damping is plotted in Fig. 3 in the same units as the band structures and for the values of shear viscosity considered in Table I.

The shear viscosity is given the value $\eta_{44} = 8 \text{ Pa}\cdot\text{s}$ in Fig. 4. For this small value, propagation of waves in homogeneous epoxy is only made slightly lossy at higher frequencies, as Fig. 3 illustrates. However, the complex band structure of the phononic crystal is in contrast much more affected, though the steel inclusions remain non viscous in the EPWE computation.

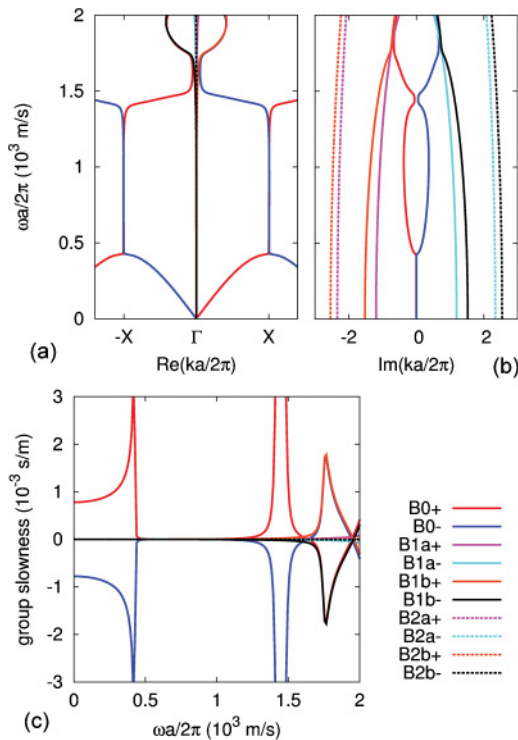


FIG. 4. (Color online) Complex dispersion relation computed with the EPWE method for a lossy square-lattice phononic crystal of steel rods in epoxy, with parameters $a = 3 \text{ mm}$, $d = 2.5 \text{ mm}$, and $\eta_{44} = 8 \text{ Pa}\cdot\text{s}$. In the complex band structure, the reduced frequency is presented as a function of (a) the real part and (b) the imaginary part of the wave vector. (c) The group slowness is shown as a function of the reduced frequency.

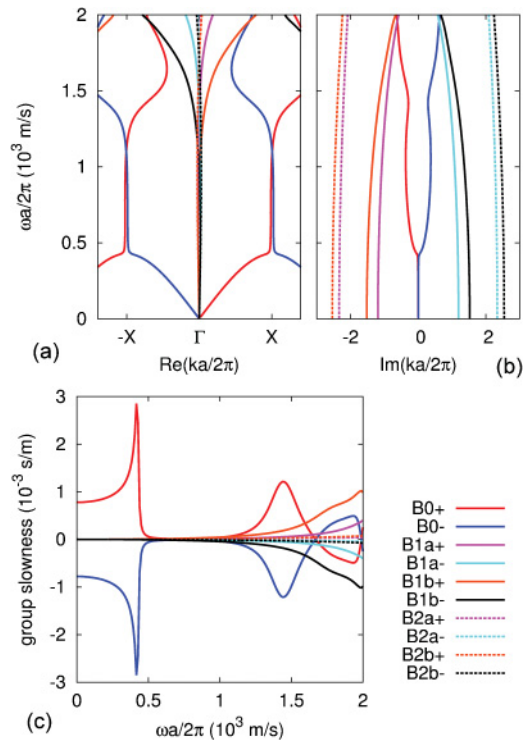


FIG. 5. (Color online) Complex dispersion relation computed with the EPWE method for a lossy square-lattice phononic crystal of steel rods in epoxy, with parameters $a = 3 \text{ mm}$, $d = 2.5 \text{ mm}$, and $\eta_{44} = 80 \text{ Pa}\cdot\text{s}$. In the complex band structure, the reduced frequency is presented as a function of (a) the real part and (b) the imaginary part of the wave vector. (c) The group slowness is shown as a function of the reduced frequency.

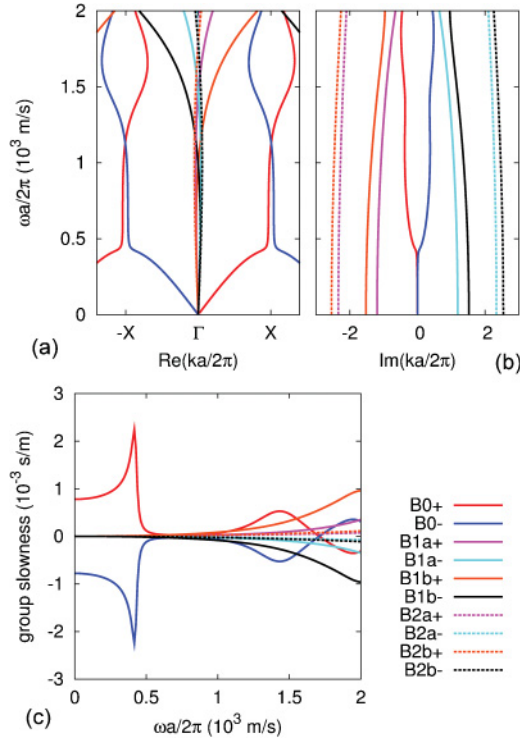


FIG. 6. (Color online) Complex dispersion relation computed with the EPWE method for a lossy square-lattice phononic crystal of steel rods in epoxy, with parameters $a = 3$ mm, $d = 2.5$ mm, and $\eta_{44} = 160$ Pa·s. In the complex band structure, the reduced frequency is presented as a function of (a) the real part and (b) the imaginary part of the wave vector. (c) The group slowness is shown as a function of the reduced frequency.

The most striking modification of the band structure occurs around the zero group velocity points, including the edges of the stop bands at the Γ and the X points of the Brillouin zone. Indeed, every sharp corner of the band structure becomes rounded. This rounding effect is more pronounced at higher frequencies, as the effect of viscosity on the elastic constants increases linearly with frequency. It can also be seen that viscosity is affecting more the real part than the imaginary part of the wave vector, in striking contrast with the homogeneous case.

The shear viscosity is further increased to $\eta_{44} = 80$ Pa·s and 160 Pa·s in Figs. 5 and 6, respectively. The trends observed with the smaller value of η_{44} are naturally amplified, and it can be further observed that the influence of viscosity is greater on the bands with the smallest imaginary part of the wave vector and the smallest group velocity in the lossless case. Frustrated evanescent Bloch waves, i.e., bands with a diffraction order larger than one, are almost not affected as long as the frequency remains well below their cutoff. The rather flat real bands that were connecting the first and the second band gap in the lossless case (part of $B0+$ and $B0-$) are washed out with increasing viscosity. It can also be observed that band gaps cannot anymore be defined when viscosity is important, because all k values are complex and the band gap edges have no precise value. Again, because the effects of viscosity increase with frequency, this is even more pronounced at the exit than at the entrance of a band gap. On the technical side,

one good point is that there are no more degenerated points in the band structures, so that it becomes easier to distinguish between the different Bloch waves.

The group slowness was going to infinity at four different frequencies in the lossless case of Fig. 2. As the viscosity is increased in Figs. 4, 5, and 6, the corresponding peaks become more and more attenuated. Similarly to the photonic crystal case discussed by Pedersen *et al.*,¹⁹ the group velocity is then limited to finite values larger than zero, the value of the limit increasing with viscosity. We finally note that the group slowness (or the group velocity) can change from positive to negative as a result of a combination of damping and dispersion for some bands.

IV. CONCLUSION

We have constructed a model for lossy phononic crystals containing viscoelastic media. We have shown how complex band structures can be computed in this case via the extended plane-wave expansion method (EPWE). As any material is intrinsically lossy, especially at high frequencies, such a model is important when analyzing the results of actual experiments. Significantly, we have found that contrary to homogeneous materials, the real part of the wave vector is more affected by losses than is its imaginary part. This effect is especially pronounced whenever the group velocity is small, for instance at the edges of a band gap. It also causes flat bands to acquire enhanced losses. Furthermore, the group velocity is limited by losses to finite values larger than zero, the value of the limit increasing with the level of viscosity. The combination of damping and dispersion could give rise to an increase in the absorption of waves by phononic crystals, with potential applications to sound shields or backing materials for ultrasound.

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APPENDIX

Let us rewrite Eq. (3) as

$$A_1(\omega)h_r(\omega) = k(\omega)A_2(\omega)h_r(\omega), \quad (\text{A1})$$

with

$$A_1(\omega) = \begin{pmatrix} -C_2 & I_d \\ \omega^2 R - B & 0 \end{pmatrix}, \quad (\text{A2})$$

$$A_2(\omega) = \begin{pmatrix} D & 0 \\ C_1 & I_d \end{pmatrix}, \quad (\text{A3})$$

$$h_r(\omega) = \begin{pmatrix} U \\ jT' \end{pmatrix}. \quad (\text{A4})$$

Note that the dependence on frequency of matrix A_2 is only active with loss, because of the viscosity term in the elastic constants. However, matrix A_1 is frequency dependent even for lossless materials, because of the ω^2 term in factor of the R sub-matrix in Eq. (A2). In Eq. (A1), $h_r(\omega)$ is a right

eigenvector associated with the eigenvalue $k(\omega)$. Conversely, a left-eigenvector of the same eigenvalue satisfies

$$h_l(\omega)^T A_1(\omega) = k(\omega) h_l(\omega)^T A_2(\omega), \quad (\text{A5})$$

where $()^T$ stands for the transposition of a vector. Left and right eigenvectors of the same eigenvalue are generally not equal.

We differentiate Eq. (A1) with respect to ω to get

$$\frac{\partial A_1}{\partial \omega} h_r + A_1 \frac{\partial h_r}{\partial \omega} = \frac{\partial k}{\partial \omega} A_2 h_r + k A_2 \frac{\partial h_r}{\partial \omega} + k \frac{\partial A_2}{\partial \omega} h_r. \quad (\text{A6})$$

We then left-multiply the result by h_l and make use of Eq. (A5) to get

$$h_l^T \frac{\partial A_1}{\partial \omega} h_r = \frac{\partial k}{\partial \omega} h_l^T A_2 h_r + h_l^T \frac{\partial A_2}{\partial \omega} h_r, \quad (\text{A7})$$

and finally the following expression for the group slowness:

$$s_g(\omega) = \text{Re} \left(\frac{\mathbf{h}_l^T \left(\frac{\partial A_1}{\partial \omega} - k \frac{\partial A_2}{\partial \omega} \right) \mathbf{h}_r}{\mathbf{h}_l^T A_2 \mathbf{h}_r} \right). \quad (\text{A8})$$

The group velocity is simply the inverse of this expression. It can be noted that the group velocity goes to zero if $\mathbf{h}_l^T A_2 \mathbf{h}_r = 0$. According to Eq. (A1) or (A5), then in this case we also have $\mathbf{h}_l^T A_1 \mathbf{h}_r = 0$, though the ratio of the two quantities has a finite value, $k(\omega)$. This explains why the value of $k(\omega)$ is very sensitive to any perturbation around a zero group velocity point, as for instance incurred when losses are turned on in the computation.

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