Computational Problems and Numerical Techniques for the Analysis of Phononic Crystals

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Abstract The propagation of elastic or acoustic waves in phononic crystals can be described *via* wave equations with periodically varying coefficients. In this chapter, we give an overview of different methods that have been used to compute phononic band structures and transmission through phononic crystals, and investigate the properties of phononic crystal waveguides and cavities. We first present general considerations on the equations and the types of problems that have been considered. We then introduce four different methods: (layer) multiple scattering theory, plane wave expansion, finite-difference time-domain, and finite element methods. Rather than giving a full account of each method, we stress their generic properties, capacities, and limitations. We hope this discussion will be useful for the reader to decide which method to select for a specific problem.

1 Basic equations for wave propagation

As a general rule, computational problems for phononic crystals are the combination of equations in a domain of a given geometry, supplemented with some given boundary conditions. This introductory section focuses on the basic equations that govern wave propagation inside a domain composed of either, or both, fluids and solids. It also briefly introduces how material loss can be represented, and exposes the Bloch-Floquet theorem and its consequences.

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1.1 Equations for solids

In the absence of internal sources, the basic equations for elastic waves propagating in solid media are written as

$$T_{ij}(\mathbf{r},t) = c_{ijkl}(\mathbf{r})\, u_{k,l}(\mathbf{r},t), \tag{1}$$

$$T_{ij,j}(\mathbf{r},t) = \rho(\mathbf{r}) \frac{\partial^2 u_i(\mathbf{r},t)}{\partial t^2}, \tag{2}$$

with u_i the three displacements in space and T_{ij} the stress tensor. In these equations, we have explicitly written the dependence on spatial coordinates and time. Note that we assume that the solid material with density ρ (in kg.m^{-3} units) and elastic constants c_{ijkl} (in Pa units) is static but has a spatially varying composition. As a general rule, indices like i, j, k, or l run between 1 and 3 for the three directions of space, a coma before an index indicates derivation (e.g., $u_{k,l} = \partial u_k / \partial x_l$), and summation over repeated indices is implied (e.g., we have $T_{ij,j} = \sum_{j=1}^{3} \partial T_{ij}/\partial x_j$). Such tensorial notations are useful to keep expressions in tractable length and are easily transposed as loops in computer programs.

The rank-4 elastic tensor c_{ijkl} has symmetries that are directly dictated by the lattice symmetry of the solid material. It is not the purpose of this chapter to discuss these symmetries and the corresponding number of independent elastic constants, as such a discussion and practical values for usual materials can be found in classical textbooks [1, 2]. In many papers on wave propagation in solid phononic crystals, the equations are specified for specific cases such as isotropic or cubic media; we note however that as long as the tensor formulation is understood and correctly applied, such simplifications do not generate any practical computational gains.

Stresses can be eliminated from Equations (1-2) to obtain a wave equation for the displacements only

$$\left(c_{ijkl}(\mathbf{r})\, u_{k,l}(\mathbf{r},t)\right)_{,j} = \rho(\mathbf{r}) \frac{\partial^2 u_i(\mathbf{r},t)}{\partial t^2}. \tag{3}$$

This last equation is often taken as the basis for formulating models for phononic crystals, because it only involves one unknown field, but we stress that it is not directly suited to surface and evanescent wave problems, for which mixed displacement / stress formulations are both elegant and efficient.

In case the propagation medium (i.e., the phononic crystal) is perfectly periodic and the fields are monochromatic, we can further make use of the Bloch-Floquet theorem to obtain equations limited to the unit-cell (please see Chapter 2 for a definition of the unit-cell). Specifically, if $\mathbf{a}$ is any vector giving the repetition of the structure in space, we have $\rho(\mathbf{r}) = \rho(\mathbf{r}+\mathbf{a})$ and $c_{ijkl}(\mathbf{r}) = c_{ijkl}(\mathbf{r}+\mathbf{a})$ and all elastic quantities describing an eigenmode can be written in the form

$$u_i(\mathbf{r},t) = \bar{u}_i(\mathbf{r}) \exp(\imath(\omega t - \mathbf{k}\cdot\mathbf{r})), \tag{4}$$

with ω the angular frequency, $\mathbf{k}$ the Bloch-Floquet wave vector, and $\bar{u}_i(\mathbf{r})$ a periodic function defined in the unit-cell ($\bar{u}_i(\mathbf{r}) = \bar{u}_i(\mathbf{r}+\mathbf{a})$). A similar expression holds for the stresses. We can write for the periodic part of the solution

$$\bar{T}_{ij}(\mathbf{r}) = c_{ijkl}(\mathbf{r})(\bar{u}_{k,l}(\mathbf{r}) - \imath k_l \bar{u}_k(\mathbf{r})), \tag{5}$$

$$\bar{T}_{ij,j}(\mathbf{r}) - \imath k_j \bar{T}_{ij}(\mathbf{r}) = -\rho(\mathbf{r})\omega^2 \bar{u}_i(\mathbf{r}). \tag{6}$$

The case of piezoelectric solids is a bit more involved but actually follows exactly the same line. In piezoelectric materials, an electromagnetic wave travels along with the elastic wave and provides a very efficient way to generate and detect elastic waves with electrical signals. In the quasi-static approximation of Maxwell equations, it suffices to consider the electric field vector to derive from a scalar potential ϕ, and the constitutive laws are taken in the linear limit as [3]

$$T_{ij}(\mathbf{r},t) = c_{ijkl}(\mathbf{r})\, u_{k,l}(\mathbf{r},t) + e_{kij}\phi_{,k}(\mathbf{r},t), \tag{7}$$

$$D_i(\mathbf{r},t) = e_{ikl} u_{k,l}(\mathbf{r},t) - \varepsilon_{ij}\phi_{,j}(\mathbf{r},t). \tag{8}$$

Here $\mathbf{D}$ is the electric induction vector, e_{ikl} is the piezoelectric tensor, and ε_{ij} is the dielectric tensor considered at low frequency (i.e., as opposed to optical frequencies). In addition to the above two equations, Eq. (2) still holds, and the auxiliary Maxwell equation $D_{i,i} = 0$ must be added. As explained for instance in Ref. [4], the equations for piezoelectric solids can be cast in a form similar to those of elastic solids by defining a general displacement vector with $u_4 = \phi$ and a generalized stress tensor with $T_{4i} = D_i$.

To summarize this sub-section, elastic wave propagation in solids can be described by either a constitutive relation relating stresses and displacements and the fundamental relation of dynamics, such as the set of equations (1-2), or by a wave equation for the displacement only, such as Eq. (3). As long as only linear phenomena are considered, this model can be enriched in a straightforward manner to include effects such as piezoelectricity, piezomagneticity, chemical potentials, and so on.

1.2 Equations for fluids

It is well known that wave propagation in fluids (gazes, liquids) only involves longitudinal displacements as long as viscoelasticity can be neglected. As a consequence, it might be thought that propagation in fluids can be treated as a limiting case of elastic wave propagation in isotropic solids with only the longitudinal displacements considered; but it turns out that this simplification is not correct. In the absence of applied external forces, the basic equations for propagation of acoustic waves in a still fluid can instead be taken as

$$-\nabla p(\mathbf{r},t) = \rho(\mathbf{r})\frac{\partial \mathbf{v}(\mathbf{r},t)}{\partial t}, \tag{9}$$

$$\frac{\partial p(\mathbf{r},t)}{\partial t} = -B(\mathbf{r})\nabla\cdot\mathbf{v}(\mathbf{r},t), \tag{10}$$

where variable dependence has been stressed and will not be repeated in the following. ρ is again the mass density and B is a bulk modulus expressed with the same units as the elastic constants. We have purposely employed vector notations instead of tensorial notations because it is the customary way to present these equations, but of course both are equivalent. The velocity can be eliminated from Eq. (10) to get a scalar wave equation for the pressure

$$\frac{1}{B}\frac{\partial^2 p}{\partial t^2} = \nabla\cdot\left(\frac{1}{\rho}\nabla p\right). \tag{11}$$

If we had eliminated the pressure instead, we would have obtained a vector wave equation for the velocity (or the displacement) similar (but not equivalent) to Eq. (3). Obviously, solving the pressure wave equation is the best choice in practice, in particular for band structure computations.

Nevertheless, when surface and evanescent wave problems are considered, the set of first-order differential equations (9-10) relating pressure and velocity is the logical choice. Further assuming monochromaticity and making use of the Bloch-Floquet theorem as in the previous sub-section, we have for the periodic part of the solution

$$-\frac{1}{\rho}(\bar{p}_{,i} - \imath k_i \bar{p}) = \imath\omega\bar{v}_i, \tag{12}$$

$$\imath\omega\frac{1}{B}\bar{p} = -(\bar{v}_{i,i} - \imath k_i \bar{v}_i). \tag{13}$$

The case of phononic crystals containing both solid and fluid materials has been considered quite often in the literature, especially in relation with experiments, for instance for the steel rods in water or air cases. The reason is that macroscopic realizations of phononic crystals are rather easy with these material systems. As is apparent from the equations given above for the solid and the fluid cases, it is not possible to use just one set of equations with coefficients assuming different values in different regions of space. The rigorous way to consider the problem is to solve the problem known as fluid-structure interaction. For instance, if the displacement field has been computed inside the solid, Eq. (10) and use of the divergence theorem from vector calculus leads to a boundary condition relating the pressure created in the fluid with the normal acceleration of the solid boundary. Such boundary conditions can be employed naturally with FDTD and FEM methods described later in this chapter. The reverse reasoning shows that the pressure exerted by the fluid on the solid boundary leads to a boundary condition for the acceleration inside the solid. Simpler but only approximate methods can be followed if the solid is considered very rigid: either the solid boundary can be considered to have no motion

(hence it is assumed there are no elastic waves in the solid), or the solid material can be regarded as an equivalent fluid supporting only longitudinal waves (and thus having an equivalent bulk modulus). The latter approximate solution gives results less distant from the exact solution than the former. Such approximate solutions have been employed mostly with PWE methods, but are not restricted to them.

1.3 Consideration of material loss

We end this section on basic equations with a short discussion of the representation of material losses. There are several physical origins for loss occurring during the propagation of elastic waves and thus not one unique solution to represent them. Losses occurring because of microscopic defects in the materials or because of scattering at random rough surfaces can be described in statistical terms and are thus in some limit amenable to macroscopic *ad hoc* loss terms. Elastic waves in solids naturally interact with thermal acoustic phonons and this loss mechanism can be viewed as dominating in perfectly ordered crystalline solids such as silicon, quartz, or lithium niobate, to cite a few materials that are used for the realization of hypersonic phononic crystals by microfabrication techniques. In general, it is found that losses in the best elastic materials increase with the square of the frequency. A simple approach to viscous losses that results in this behavior is to consider that at a fixed temperature we can add a restoring term depending on a viscosity tensor η_{ijkl} and the time derivative of the strain tensor so that the constitutive relation is modified to [2]

$$T_{ij} = c_{ijkl}\, u_{k,l} + \eta_{ijkl} \frac{\partial u_{k,l}}{\partial t}. \tag{14}$$

The viscosity tensor has the same symmetries as the elastic tensor. Such an expression is well suited to time-domain methods such as FDTD. For monochromatic waves, the elastic constants are then seen to be modified from real to complex valued as

$$c'_{ijkl} = c_{ijkl} + \imath\omega\eta_{ijkl}. \tag{15}$$

This modification offers a simple means to include the effect of losses at a fixed frequency, e.g. with the extended PWE method [5].

2 Computational problems of phononic crystals

Before turning to the different type of methods that are used to describe wave propagation in phononic crystals, we outline in this section the different kinds of problems that one encounters and their characteristics in terms of numerical computation. There is a first obvious separation of problems depending on whether they are considered in the spectral or the time domain. However, it is in principle always pos-

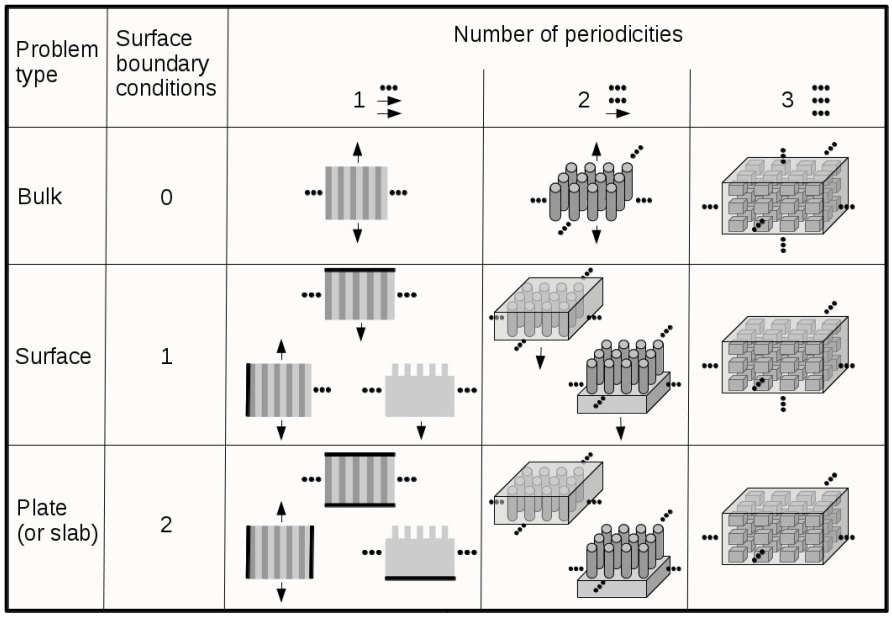


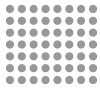
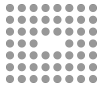
Fig. 1 Classification of phononic crystals according to their geometry. Three consecutive dots indicate a direction of periodic repetition of the unit-cell, while an arrow means the structure extends homogeneously to infinity.

sible to go from one type to the other with the help of Fourier transforms. A deeper separation of problems, in our opinion, stems from the boundary conditions that are considered, as these lead to different types of waves (i.e. bulk, surface, and plate waves). This is exposed in subsection 2.1. Less fundamental in character, but very important for the understanding of the physics behind phononic crystals are the different problem types that can be considered: band structures, waveguides, cavities, scattering problems. These are considered in subsection 2.2.

2.1 Classification by geometry

In case the phononic crystal is unbounded, there are no boundary conditions required to terminate the infinite domain of definition. We speak of the propagation of bulk elastic or acoustic waves. In a physical three-dimensional space, we can consider from 1 to 3 periodicities and it is customary to refer to 1D, 2D, and 3D phononic crystals. When the phononic crystal fills a semi-infinite domain terminated by a given surface, there are additional waves that can be guided along the surface that we term surface waves. In case there can be radiation to the remaining half space, we speak of interface waves. Plate (or slab) phononic crystals are limited by 2 parallel planes and thus 2 surface or interface boundary conditions. Rather than

Table 1 Basic computational problems for perfectly periodic and defect-based phononic crystals.

Structure		Dispersion (infinite structure)	Scattering (finite structure)
Phononic crystal		Band structure $\omega(k)$ Complex BS $k(\omega)$	Transmission, reflection, and diffraction of an incident plane wave
Waveguide		Guided modes	Waveguide transmission
Cavity		Confined modes	Cavity transmission

attempting a lengthy description, we depict in Fig. 1 the different possibilities that arise from this discussion. Note that there are even more complicated cases that can be considered (e.g., finite phononic crystals with arbitrary enclosing surfaces), so that our tentative classification is clearly not exhaustive.

2.2 Classification by problem type

The previous classification by geometry insists upon the physical properties of phononic crystals, and especially upon the types of waves that they can support. A second classification can be performed based on the phononic crystal structure, as attempted in Table 1. Perfectly periodic phononic crystal can be thought ideally as extending to infinity, in which case any solution of the wave equation can be written as a superposition of Bloch waves. The dispersion relation of all Bloch waves forms the band structure which can in general be obtained by solving a generalized eigenvalue problem, possibly supplemented with surface or interface boundary conditions. Note that Bloch waves constitute a complete basis (in the monochromatic sense) only if all complex $k(\omega)$ solutions are considered [6]. If a perfectly periodic phononic crystal of finite size is considered, for instance for comparison with experiments, then the scattering of an incident plane wave to all orders of diffraction is an important basic problem. Phononic crystal cavities and waveguides can be formed by breaking locally the periodicity of the phononic crystal structure. Defect-based phononic structures are generally mostly interesting for frequencies that fall inside a complete phononic band gap, in which case perfect guidance or confinement can be achieved. Otherwise, phononic crystal waveguides and cavities are leaky. By defining a supercell that artificially restores periodicity[1], waveguide and cavity modes

[1] A supercell extends a few periods away from the defect it encloses. Modal computations then give physically meaningful results when only evanescent Bloch waves of the elementary phononic crystal exist, i.e., inside a complete band gap. Furthermore, the number of phononic crystal rows

can be estimated, and their band structures can be obtained. Finite-size defect-based phononic crystal structures are in general considered for comparison with experiments, with the accent on obtaining the transmission of the waveguide or the resonance properties of the cavity.

3 Multiple scattering theory (MST) and layer multiple scattering (LMS) methods

Multiple scattering type computation methods (MST) have a long history in condensed matter and particle physics. The methods used for phononic crystals have a close relation with those used for the treatment of electron scattering in solids and computing the band structure of photonic crystals and transmission through them. The basic idea is to make use of the superposition principle for non overlapping scatterers. Considering a single scatterer with a given shape, one first obtains the field scattered from an incident plane wave with given angular frequency and wave vector. Then the scattered field from an assembly of scatterers is constructed by summing properly all individual contributions. The method thus works very efficiently if the single scatterer problem can be solved analytically, as is the case of isotropic spherical scatterers in a homogeneous isotropic medium (for which spheroidal expansions are known) or of infinite isotropic cylinders in a homogeneous isotropic medium. Multiple scattering methods have been employed with great success for the computation of band structures, density of states, and transmission trough finite phononic crystals, though almost always for isotropic spheres or cylinders embedded in a isotropic background, as is the case for sonic crystals. Generalization of multiple scattering methods to arbitrary anisotropic periodic materials still stands as a highly difficult problem.

Arguably the most developed and versatile MST method is the layer-multiple-scattering (LMS) method [7, 8, 9]. We refer the reader to these papers for a full description of the method and only outline here the method. The basic principle of the method is that the wave incident on a given scatterer is the sum of the waves outgoing from all the other scatterers and the externally incident wave. A scattering matrix relating the amplitudes (which are expansion coefficients in a given basis, e.g., spheroidal harmonics) of the scattered wave with those of the incident wave is obtained for the composite system from the corresponding matrices of the individual scatterers and proper propagator functions in the host medium. The LMS method considers a phononic crystal to be constituted by a stack of phononic crystal layers. It proceeds layer by layer by evaluating the scattering properties of the phononic crystal from those of the constituent phononic crystal layers, for given frequency and wave vector. The layers can be either planes of 3D scatterers with the same 2D periodicity, or homogeneous layers. For each plane of scatterers, the method cal-

must be sufficient so that the Bloch wave with the least imaginary part of the wave vector can be considered negligible on the boundary of the supercell.

culates the full multipole expansion of the total multiply scattered wave field and deduces the corresponding transmission and reflection matrices in the plane-wave basis for the surrounding media. For homogeneous layers, the transmission and reflection matrices are directly obtained in the plane-wave basis of the homogenous material.

In any multiple scattering calculation, the angular frequency is a fixed quantity. The wave vector only appears as a eigenvalue in band structure computations or as a particular component of the wave vector of the wave incident on a finite phononic crystal. As such, MST and LMS methods give access to complex band structures and to the consideration of propagation loss in the form of frequency-dependent viscous elastic constants [10].

4 Plane wave expansion method

The discussion in this section relies on the presentation of the plane wave expansion (PWE) method proposed in Refs. [4, 11]. However, whereas these papers contained the full piezoelectric formulation, we restrict it here to the (anisotropic) elastic case for simplicity of the presentation. The PWE method relies on a literate application of the Bloch-Floquet theorem. As discussed in Section 1.1, any eigenmode of a perfectly periodic medium (termed a Bloch wave) is the product of a plane-wave like term and a function periodic in the unit cell. In the PWE method, the periodic function is considered explicitly through its Fourier series expansion. Specifically, we write for any displacement component

$$u(\mathbf{r},t) = \sum_{\mathbf{G}} u_{\mathbf{G}}(\omega,\mathbf{k}) \exp(\imath(\omega t - \mathbf{k}\cdot\mathbf{r} - \mathbf{G}\cdot\mathbf{r})), \tag{16}$$

where the vectors of the reciprocal lattice are (for the square lattice case) $\mathbf{G} = (2\pi m_1/a, 2\pi m_2/a, 2\pi m_3/a)^T$. One should note that the Fourier coefficients $u_{\mathbf{G}}(\omega,\mathbf{k})$ are those of the periodic part of the Bloch wave solution, $\bar{u}$.

The periodicity of the structure is also used to expand the material constants as Fourier series

$$\alpha(\mathbf{r}) = \sum_{\mathbf{G}} \alpha_{\mathbf{G}} \exp(-\imath\mathbf{G}\cdot\mathbf{r}), \tag{17}$$

where α is either ρ or c_{ijkl}. The Fourier harmonics $\alpha_{\mathbf{G}}$ are easily calculated for various scatterers and lattice geometries [12, 13].

4.1 Band structures with PWE

Assuming a truncation to a total of N harmonics in the Fourier expansions, the following vector notations are considered for the harmonics of the generalized stress and displacement fields ($3N$ components each)

$$\mathbf{T}_i = \left(\mathbf{t}_{i\mathbf{G}_1} \dots \mathbf{t}_{i\mathbf{G}_N}\right)^T, \tag{18}$$

$$\mathbf{U} = \left(\mathbf{u}_{\mathbf{G}_1} \dots \mathbf{u}_{\mathbf{G}_N}\right)^T, \tag{19}$$

where the vectors of the reciprocal lattice, $\mathbf{G}_m$, are labeled using a single index m. Bulk waves are then obtained as the eigensolutions of the secular equation

$$\omega^2 R\mathbf{U} = \sum_{i,l=1,3} \Gamma_i A_{il} \Gamma_l \mathbf{U}, \tag{20}$$

with the $3N \times 3N$ matrices Γ_i, A_{il} and R defined by the $N \times N$ blocks with 3×3 elements

$$(\Gamma_i)_{mn} = \delta_{mn}(k_i + G_{im}) I_3, \tag{21}$$

$$(A_{il})_{mn} = A_{il\mathbf{G}_m - \mathbf{G}_n}, \tag{22}$$

$$(R)_{mn} = \rho_{\mathbf{G}_m - \mathbf{G}_n} I_3, \tag{23}$$

with I_3 the 3×3 identity matrix and

$$A_{il\mathbf{G}}(j,k) = c_{ijkl\mathbf{G}}, \tag{24}$$

with $i,j,k,l = 1,2,3$ and $m,n = 1 \dots N$. Eq. (20) defines a generalized eigenvalue problem which can be solved for ω^2 as a function of $\mathbf{k}$ to obtain the band structure of bulk waves. This formulation encompasses 1D, 2D, and 3D bulk wave problems, plus the out-of-plane 2D bulk wave propagation problem [14].

It is also instructive to consider the problem of surface waves propagating on the surface of a 2D phononic crystal. The phononic crystal is assumed to be periodic in the directions x_1 and x_2 and invariant along direction x_3, except for the presence of a surface at $x_3 = 0$. Surface waves are defined by the angular frequency ω and a wave vector $\mathbf{k} = (k_1, k_2, 0)^T$ defined in the plane of the surface. The two-dimensional phononic crystal is not periodic along the x_3 axis and k_3 can be obtained as a function of the other parameters of the model – i.e. k_1, k_2 and ω. We group the displacements and the stresses normal to the surface in the $6N$-components state vector $\mathbf{H} = (\mathbf{U}, \mathbf{T}_3)^T$ and obtain k_3 as the eigenvalue of the equation

$$\begin{bmatrix} \omega^2 \widetilde{R} - B & 0 \\ -C_2 & I_d \end{bmatrix} \mathbf{H} = k_3 \begin{bmatrix} C_1 & I_d \\ D & 0 \end{bmatrix} \mathbf{H} \quad , \tag{25}$$

where

$$B = \sum_{i,j=1,2} \Gamma_i \widetilde{A}_{ij} \Gamma_j, \; C_1 = \sum_{i=1,2} \Gamma_i \widetilde{A}_{i3},$$
$$C_2 = \sum_{j=1,2} \widetilde{A}_{3j} \Gamma_j, \qquad D = \widetilde{A}_{33}. \tag{26}$$

Solving this system yields $6N$ complex-valued eigenvalues k_{3q} and eigenvectors $\mathbf{H}_q$. By grouping in the eigenvectors the 6 components corresponding to the m-th

harmonic, we introduce the notation

$$\mathbf{h}_{mq} = \begin{pmatrix} (u_i)_{\mathbf{G}_m q} \\ (T_{3j})_{\mathbf{G}_m q} \end{pmatrix}, \tag{27}$$

with $i, j = 1,2,3$, $m = 1,\ldots,N$, and $q = 1,\ldots,6N$. The generalized displacement and normal stress fields are obtained from the superposition with relative amplitudes A_q

$$\mathbf{h}(\mathbf{r},t) = \sum_{m=1}^{N} \sum_{q=1}^{6N} A_q \tilde{\mathbf{h}}_{mq} \exp((\omega t - (\mathbf{G}_m + \mathbf{k}_q)\cdot\mathbf{r})). \tag{28}$$

This superposition is a finite approximation to the infinite series (16). From this partial wave expansion, boundary conditions can be constructed to solve surface and plate problems [4, 11].

The PWE method has one drawback that is apparent in Eq. (16). The Fourier series expansion of the displacement and the stress fields implicitly makes the solution continuous everywhere inside the unit-cell. Whereas the displacements and the normal stresses can be considered continuous at an interface between different solid materials, such is not the case for shear stresses applying along the interface. Also, the boundary condition at the interface of a solid and a fluid cannot in general be satisfied, which makes the PWE method rather unsuitable for solid-fluid problems (its application can result in the appearance of spurious modes in the fluid part).

4.2 Evanescent waves in phononic crystals

A limitation of the PWE method for band structure computations is that the eigenvalue problem of Eq. (20) gives eigenfrequencies at fixed values of the Bloch wave vector. Thus, it is not easy to consider materials with frequency-dependent elastic constants describing viscous losses, contrary to the LMS case. The extended PWE method relieves this particular limitation and enables the computation of the full complex band structure [6, 5], as we outline here.

It is well-known in the theory of diffraction gratings and near-field optics or acoustics that evanescent waves play a essential role in all wave propagation problems. The set of all propagative and evanescent Bloch waves constitutes a complete basis for phononic crystal problems [6]. Evanescent Bloch waves can be characterized as eigensolutions of the periodic Helmholtz equation describing monochromatic wave propagation, for which the wave vector can be complex-valued. Usual band structures are obtained assuming the wave vector to be a real-valued quantity (through the $\omega(\mathbf{k})$ eigenvalue problem); complex band structures are obtained by assuming real-valued frequencies and solving for the (generally complex-valued) wave vector (the $\mathbf{k}(\omega)$ problem).

As an example, let us outline how the complex band structure for solid phononic crystals can be obtained from the equations we have written in Section 1. Multiply-

ing Equation (3) with α_j we get

$$\bar{T'}_i = \alpha_j \bar{T}_{ij} = c_{ijkl}\alpha_j \bar{u}_{k,l} - \imath k c_{ijkl}\alpha_j\alpha_l \bar{u}_k. \tag{29}$$

Inserting Equation (3) into Equation (4) we also get

$$\rho\omega^2 \bar{u}_i = -c_{ijkl}\bar{u}_{k,jl} + \imath k c_{ijkl}\alpha_l \bar{u}_{k,j} + \imath k \bar{T'}_i. \tag{30}$$

$\bar{T'}_i$ is the component along x_i of the stress tensor projected along the propagation direction. In the two last equations, the modulus of the wave vector, k, appears in factor of terms that are linear in the unknown periodic fields $\bar{u}$ and $\bar{\phi}$. Thus these equations can be used to formulate a generalized eigenvalue problem for the eigenvalue k. Written in terms of the PWE notations given in Section 3, the eigenvalue problem is as follows [6]

$$\begin{pmatrix} -C_2 & I_d \\ \omega^2 R - B & 0 \end{pmatrix} \begin{pmatrix} U \\ \imath T' \end{pmatrix} = k \begin{pmatrix} D & 0 \\ C_1 & I_d \end{pmatrix} \begin{pmatrix} U \\ \imath T' \end{pmatrix}, \tag{31}$$

with $B = \Gamma_i A_{ij} \Gamma_j$, $C_1 = \Gamma_i A_{ij} \alpha_j$, $C_2 = \alpha_i A_{ij} \Gamma_j$, $D = \alpha_i A_{ij} \alpha_j$, and $(\Gamma_i)_{mn} = (k_{0i} + G_i^m)\delta_{mn}$. It can be checked easily that Eq. (25) appears as a special case of the above generalized eigenvalue problem. Eqs. (29-30) can also be used to formulate the finite element version of the generalized eigenvalue problem, by using a mixed displacement-stress formulation.

5 Finite element method

The finite element method (FEM) is a numerical technique to solve partial differential equations (PDE) and integral equations in the time domain as well as in the spectral domain. The primary challenge is to create an equation that approximates the equation to be studied and that is numerically convergent. FEM is a powerful method suitable for solving PDE over complicated domains, when the domain changes – e.g., for moving boundaries – and when the desired precision varies over the entire domain. Several authors of the phononic community have recently proposed FEM to study different geometries and compositions, through the calculation of band structures [15, 16] or the design of cavities and waveguides – defect modes – in perfect structures [17]. The commercial software COMSOL, for instance, is now widely used to compute band structures of phononic crystals. In the following, we describe an example of such a calculation in the case of the phononic crystal slab.

The geometry of a square lattice phononic crystal slab is depicted in Fig. 2. The phononic crystal is assumed to be infinite and arranged periodically in the x and y directions. a_1 and a_2 are the pitches of the array, with $a_1 = a_2 = a$ in the square lattice case. The slab has a finite thickness d in the z direction. Each unit cell is indexed by (m, p). The whole domain is split into successive unit cells, consisting

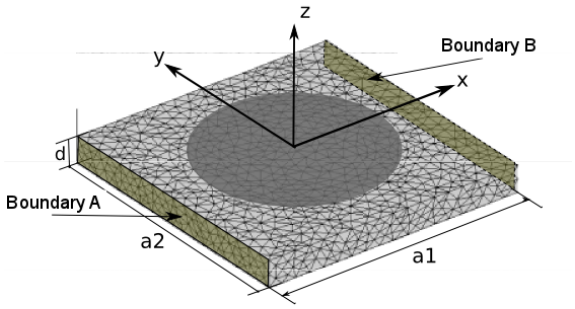


Fig. 2 Unit cell of phononic crystal slab.

of a single cylinder surrounded by a matrix. The inclusions are assumed to have a circular cross section so that the filling fraction is $F = \pi r^2/a^2 = 0.5$, where r is the radius of the inclusion. The unit cell is meshed and divided into finite elements connected by nodes as shown in Fig. 2. According to the Bloch-Floquet theorem, all fields obey a periodicity law, yielding for instance the following relation between the mechanical displacements u_i for nodes lying on the boundary of the unit cell

$$u_i(x+ma_1, y+pa_2, z) = u_i(x,y,z)\exp\left(-\imath(k_x ma_1 + k_y pa_2)\right), \tag{32}$$

where k_x and k_y are the components of the Bloch wave vectors in the x and y directions, respectively. Considering the periodic boundary conditions above allows us to reduce the model to a single unit cell which can be meshed using finite elements. A mechanical displacement (for elastic solids) and electrical potential (for piezoelectric solids) FE scheme is used. Considering a monochromatic variation of mechanical and electrical fields with a time dependence $\exp(\imath\omega t)$, where ω is the angular frequency, the general piezoelectric problem with no applied external force can be written

$$\begin{pmatrix} K_{uu} - \omega^2 M_{uu} & K_{u\phi} \\ K_{\phi u} & K_{\phi\phi} \end{pmatrix} \begin{pmatrix} u \\ \phi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{33}$$

where K_{uu} and M_{uu} are the stiffness and mass matrices of the purely elastic part of the problem, $K_{u\phi}$ and $K_{\phi u}$ are piezoelectric-coupling matrices, and $K_{\phi\phi}$ accounts for the purely dielectric problem. u and ϕ represent, respectively, all displacements and electrical potential at the nodes of the mesh, gathered together in vector form. As the angular frequency ω is a periodical function of the wave vector, the problem can be reduced to the first Brillouin zone. Practically, we relate all the degrees of freedom on boundary A to those on boundary B along the x direction, according to

$$\begin{pmatrix} u_{i(B)} \\ \phi_{(B)} \end{pmatrix} = \begin{pmatrix} u_{i(A)} \\ \phi_{(A)} \end{pmatrix} \exp\left(-\imath(k_x a)\right), \tag{34}$$

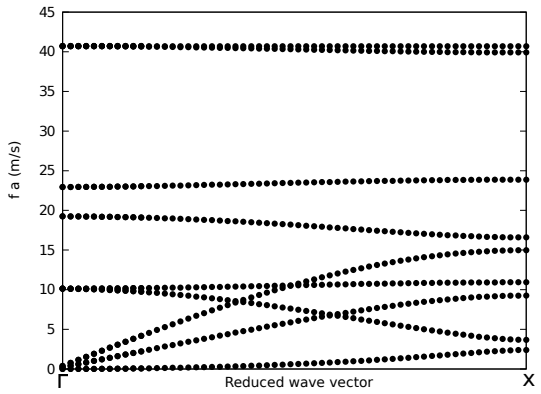


Fig. 3 Band structure of a periodic array of tungsten rods in epoxy. The lattice is based on square symmetry. The filling fraction is about 0.35. A large band gap extending from $fa = 23$ to 42 m/s is obtained.

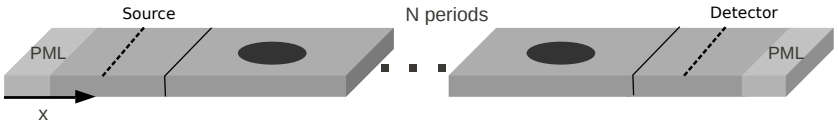


Fig. 4 Phononic crystal slab geometry for transmission calculation.

in which k_x varies in the interval $(0, \pi/a)$ along the x direction. Similar periodic boundary conditions are applied to the boundaries orthogonal to the y axis. The dispersion curves are then obtained by varying the wave vector in the first Brillouin zone for a given propagation direction and by solving the eigenvalue problem to obtain the eigenfrequency solutions, or angular pulsations, ω. The full band structure is then deduced using symmetries. An example of a dispersion calculation is presented in Fig. 3.

In transmission calculations involving a phononic crystal of finite size, an acoustic wave with specific polarization (u_x, u_z, u_y) can be generated by applying a line source vibration on the upper surface. We apply in addition in the y direction periodic boundary conditions to account for the lateral size of the structure. The line source generates monochromatic waves propagating along the x direction. To prevent reflections of the scattering wave from the edge, a perfectly matched layer (PML) [18] is applied. The PMLs have the property that the mechanical disturbances are gradually absorbed in the layers before they reach the outer boundaries. In this way, there will be no reflections that can disturb the propagation of the source wave. Indeed, we can write the dynamical equation as

$$\frac{1}{\gamma_j}\frac{\partial T_{ij}}{\partial x_j} = -\rho\omega^2 u_i, \tag{35}$$

where ρ is the density of the material. The parameter γ_j is an artificial damping factor at position x_j in the PML. As the PML is added to attenuate the acoustic wave propagating in the plane of the structure, for propagation in direction x only γ_x is different from 1 and is given by

$$\gamma_x(x) = 1 - \imath\sigma_x(x - x_l)^2, \tag{36}$$

where x_l is the coordinate at the interface between the regular domain and the PML, and σ_x is a suitable constant. There is no damping outside the PMLs and $\gamma_x = 1$ there. A suitable thickness of the PML as well as the value of σ_x must be found by calculations such that the mechanical disturbances are absorbed before reaching the outer boundaries. Absorption, however, must also be sufficiently low as reflections will occur at the interface between the regular domain and the PML if their material properties are not comparable. Mechanical stresses depend on the strains as usual

$$T_{jk} = c_{jklm} S_{lm}, \tag{37}$$

Where c_{jklm} are the elastic stiffness constants, but strains are now defined from the displacements as

$$S_{ij} = \frac{1}{2}\left(\frac{1}{\gamma_j}\frac{\partial u_i}{\partial x_j} + \frac{1}{\gamma_i}\frac{\partial u_j}{\partial x_i}\right). \tag{38}$$

6 Finite-difference time-domain method

Finite-difference time-domain (FDTD) is a well-known computational electro- and elastodynamics modeling technique. It is usually considered easy to understand and easy to implement. Since it is a time-domain method, with the advantage that the solutions can cover a wide frequency range with a single simulation run. The FDTD method belongs in the general class of grid-based differential time-domain numerical modeling methods. Generally, the time-dependent wave equations -in partial differential form- are discretized using central-difference approximations to the space and time partial derivatives. The resulting finite-difference equations are solved in a leapfrog manner: in the case of elastic wave, the displacement field vector components in a volume of space are solved at a given instant in time; then the stress field tensor components in the same spatial volume are solved at the next instant in time; and the process is repeated until the desired transient or steady-state acoustic or elastic displacement field behavior has fully evolved. Since the rise of phononic crystal field, FDTD has emerged as an alternative technique to PWE when dealing with finite size structure – to evaluate the transmission through a finite number of period – and more important with acoustic / elastic wave interactions in solid / fluid mixed phononic structures. In the later case, PWE fails in getting stable solutions due to the non consideration of shear waves in the equations describing the fluid. In the following, we describe how FDTD can obtain the band structure of infinite periodic 2D phononic crystals composed and the spectral transmission through a finite size structure.

We first consider a perfect 2D elastic or acoustic system composed of a periodic array of cylinders of a material A embedded in a background material B according to a square lattice array (see Fig. 5). Both materials are assumed to be elastically isotropic. We choose the z ($= x_3$) direction parallel to the cylinder axis of the

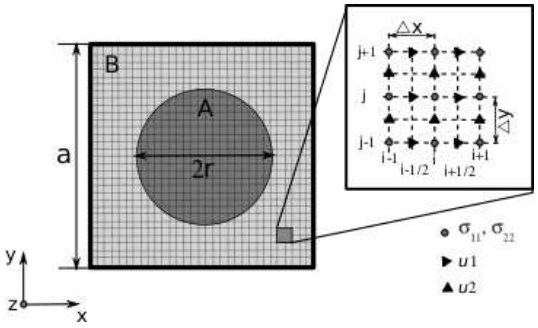


Fig. 5 Gridded unit cell of a phononic crystal composed of a cylinder (A) embedded in a background (B) and arranged according to a square lattice. A closer view of spacial discretization of elastic fields is shown.

2D phononic crystal. The mass density ρ and the elastic tensor c_{ijmn} of the system depend only upon coordinates $(x,y) = (x_1,x_2)$ in the plane perpendicular to the cylinder axis. The equations of motion for the lattice displacement are those of Eqs. (1-2). In the phononic crystals composed of isotropic materials and for acoustic waves propagating in the (x,y) plane, the equations of motion can be decomposed into two independent sets of equations. One is in explicit form

$$\rho(x,y)\frac{\partial^2 u_1(x,y,t)}{\partial t^2} = \frac{\partial T_{11}(x,y,t)}{\partial x} + \frac{\partial T_{12}(x,y,t)}{\partial y}, \tag{39}$$

$$\rho(x,y)\frac{\partial^2 u_2(x,y,t)}{\partial t^2} = \frac{\partial T_{21}(x,y,t)}{\partial x} + \frac{\partial T_{22}(x,y,t)}{\partial y}, \tag{40}$$

$$T_{11}(x,y,t) = c_{11}(x)\frac{\partial u_1(x,y,t)}{\partial x} + c_{12}(x,y)\frac{\partial u_2(x,y,t)}{\partial y}, \tag{41}$$

$$T_{12}(x,y,t) = T_{21}(x,y,t) = c_{44}(x,y)\left(\frac{\partial u_2(x,y,t)}{\partial x} + \frac{\partial u_1(x,y,t)}{\partial y}\right), \tag{42}$$

$$T_{22}(x,y,t) = c_{12}(x,y)\frac{\partial u_1(x,y,t)}{\partial x} + c_{11}(x,y)\frac{\partial u_2(x,y,t)}{\partial y}. \tag{43}$$

In these equations, the c_{IJ} are the contracted elastic constants with two indices and the relations $c_{21} = c_{21}$, $c_{22} = c_{11}$ and $c_{66} = c_{44}$ have been used. The equations are restricted to mixed modes consisting of both longitudinal and transverse vibrations, which means that shear modes with a pure transverse vibration along z is not included in these equations.

The basic FDTD space grid and time-stepping algorithm traces back to a paper written by K. Yee, which was originally applied to electromagnetic wave propagation in dielectric media [19]. To solve Eqs. (39-43), we extend Yee's discretization scheme in the framework of the FDTD method. The variables involved in those equations are now defined on rectangular grids with side lengths Δx and Δy. Displacement fields are separated in time by a unit time step Δt and the displacement and stress fields are spatially interleaved by half a grid cell. Based on this scheme, center differences in both space and time are used to approximate the equations of motion for mixed modes. The explicit expressions for this discretization version are

given as

$$u_1^{i+\frac{1}{2},j;n+1} = 2u_1^{i+\frac{1}{2},j;n} - u_1^{i+\frac{1}{2},j;n-1} + \frac{(\Delta t)^2}{\rho^{i+\frac{1}{2},j}}\left[\frac{\sigma_{11}^{i+1,j;n} - \sigma_{11}^{i,j;n}}{\Delta x} + \frac{\sigma_{12}^{i+\frac{1}{2},j+\frac{1}{2};n} - \sigma_{12}^{i+\frac{1}{2},j-\frac{1}{2};n}}{\Delta y}\right], \tag{44}$$

$$u_2^{i,j+\frac{1}{2};n+1} = 2u_2^{i,j+\frac{1}{2};n} - u_2^{i,j+\frac{1}{2};n-1} + \frac{(\Delta t)^2}{\rho^{i,j+\frac{1}{2}}}\left[\frac{\sigma_{21}^{i+\frac{1}{2},j+\frac{1}{2};n} - \sigma_{21}^{i-\frac{1}{2},j+\frac{1}{2};n}}{\Delta x} + \frac{\sigma_{22}^{i,j+1;n} - \sigma_{12}^{i,j;n}}{\Delta y}\right], \tag{45}$$

$$\sigma_{11}^{i,j;n} = c_{11}^{i,j}\frac{u_1^{i+\frac{1}{2},j;n} - u_1^{i-\frac{1}{2},j;n}}{\Delta x} + c_{12}^{i,j}\frac{u_2^{i,j+\frac{1}{2};n} - u_2^{i,j-\frac{1}{2};n}}{\Delta y}, \tag{46}$$

$$\sigma_{22}^{i,j;n} = c_{12}^{i,j}\frac{u_1^{i+\frac{1}{2},j;n} - u_1^{i-\frac{1}{2},j;n}}{\Delta x} + c_{11}^{i,j}\frac{u_2^{i,j+\frac{1}{2};n} - u_2^{i,j-\frac{1}{2};n}}{\Delta y}, \tag{47}$$

$$\sigma_{12}^{i+\frac{1}{2},j+\frac{1}{2};n} = \sigma_{21}^{i+\frac{1}{2},j+\frac{1}{2};n} = C_{44}^{i+\frac{1}{2},j+\frac{1}{2}}\left[\frac{u_1^{i+\frac{1}{2},j+1;n} - u_1^{i-\frac{1}{2},j;n}}{\Delta y} + \frac{u_2^{i+1,j+\frac{1}{2};n} - u_2^{i,j+\frac{1}{2};n}}{\Delta x}\right], \tag{48}$$

where (i, j) defines a 2D grid point (grid spacings are Δx and Δy), n specifies the time step with an interval Δt. In the fluid region, $c_{44} = 0$ and $c_{11} = c_{12}$, which simplifies the equations without disturbing the stability of the solution process as no matrix inversion is required.

6.1 Boundary conditions

Two major boundary conditions can be distinguished depending on the purpose of calculations: (1) the periodic boundary condition simulating an infinite structure and (2) the absorbing boundary condition or absorbing region applied when a truncation of an open region is needed.

1. When we calculate the dispersion relation of bulk waves with a 2D wave vector in the (x,y) plane, we may consider a 2D unit cell of a square shape involving just one cylinder and may impose periodic boundary conditions in both x and y directions. Here we note that the periodic boundary conditions in the (x,y) plane are expressed as

$$u_i(x+L_x, y+L_y, t) = \exp(-\imath(k_x L_x + k_y L_y))u_i(x,y,t)), i = 1,2 \tag{49}$$

where (L_x, L_y) are the periods in the x and y directions, respectively, and in the present case $L_x = L_y = a$. These equations define the two-dimensional wave vector $k = (k_x, k_y)$ in the first Brillouin zone $-\pi/L_x < k_x < \pi/L_x$ and $-\pi/L_y < k_y < \pi/L_y$.

2. When we compute the transmission of acoustic or elastic waves through a finite phononic crystal structure with, say, 5 periods, homogeneous regions consisting of the background material are added to the lattice in the regions $x < 0$ and $x > 5a$. At the far ends of these regions in the longitudinal (x) direction, absorbing boundary conditions are imposed and periodic boundary conditions are applied at boundaries orthogonal to the lateral y direction. Basicaly, the most commonly used grid truncation techniques for open-region FDTD modeling problems are the Mur absorbing boundary condition (ABC), the Liao ABC and various perfectly matched layer (PML) formulations. The Mur and Liao techniques are simpler than the PML. However, PML (which is technically an absorbing region rather than a boundary condition) can provide orders-of-magnitude lower reflections. In this work, we use Mur absorbing boundary conditions (ABC) where we impose that the elastic or acoustic wave is propagating – at the ends of the medium in the x direction for instance – in the forward direction and is leaving the medium without reflexion. The condition is, therefore,

$$V_L \frac{\partial u_i(x,y,t)}{\partial x} + \frac{\partial u_i(x,y,t)}{\partial t} = 0, \tag{50}$$

where the longitudinal speed of sound in the radiation medium V_L is used for both the x and y components of the displacement field. A finite-difference approximation of that condition may be used.

6.2 Calculation of dispersion relations

In the example of Fig. 6, we consider a perfect 2D periodic crystal where elastic circular steel cylinders of radius r are embedded periodically in a water medium, forming a square lattice with lattice spacing a. For the calculation of dispersion relations, a small disturbance at a randomly chosen position of the structure is set as the initial condition. Thus all possible wave modes are excited inside the considered 2D unit cell, and the displacement can be recorded and subsequently expanded into Fourier series. Then the eigenfrequencies for a given wave vector k_x, k_y (imposed via the periodic boundary conditions) are obtained by selecting the resonance peaks of the spectrum. This procedure allows us to find all possible types of bulk waves. In the numerical calculations, the spacings of the grid points are chosen as $\Delta x = \Delta y = a/60$ and the unit time step Δt is selected as $\Delta t = 0.95\Delta t_{\max}$, where the stability criterion for the FDTD method requires

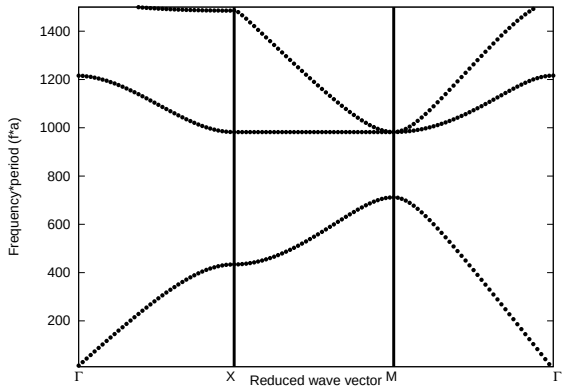


Fig. 6 Band structure of a square lattice array of steel rods in water computed with FDTD. The filling fraction is 0.41 approximately. A full band gap extending from 700 to 1000 m/s is obtained.

$$\Delta t < \Delta t_{\max} = \frac{1}{v_{\max}\sqrt{(\frac{1}{\Delta x})^2 + (\frac{1}{\Delta y})^2}}, \tag{51}$$

with $v_{\max} = v_{\text{steel}}$. In practical cases, after $t = 2^{17}\Delta t = 131,100\Delta t$ time steps, the vibration of the system become stationary and is composed of a superposition of eigenmodes.

Fig. 6 shows the low frequency part of the dispersion curves of bulk waves along the boundary of the irreducible Brillouin zone. The filling fraction is f = 0.41. We can notice the existence of a large complete gap that prohibits bulk wave propagation in the (x,y) plane.

6.3 Calculation of transmission spectra

To gain a better insight into the effects of band gaps, and also to investigate the qualitative behavior of transmission inside pass bands, the FDTD method is a powerful tool to calculate the transmission through finite size samples. To do so, the samples are composed of three adjacent regions (see the inset in Fig. 7). The probing signal, a longitudinal wave that propagates along the x direction, is launched from the first region and detected in the third one. The signal is the superposition of a few sinusoidal waves with frequencies centered around the central frequency of interest and is usually weighed by a Gaussian profile. Transmission of this signal through a homogeneous water medium produces a broad band spectrum that covers the frequency range of interest. The central region contains the phononic crystal. To probe the transmission, severals output displacements (longitudinal vibrations) are detected at different locations in the third region. Transmission spectra are calculated as an average of their Fourier transforms. As an example, Fig. 7a show the

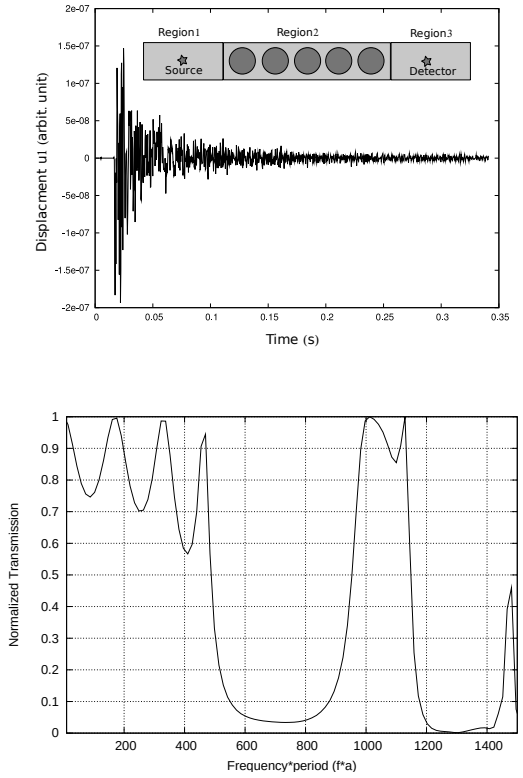


Fig. 7 (a) Time response of displacement detected at some position after the phononic crystal. (b) Calculated transmission power spectrum along the ΓX direction of the irreducible Brillouin zone of the square lattice of steel cylinders in water. A strong attenuation in transmission extending from 700 to 1000 m/s in reduced frequency is obtained.

time evolution of bulk waves received at a spatial position located in the third region. The Fast Fourier transform of the time signal gives the transmission spectrum of wave propagation through the finite size phononic crystal structure.

In addition, the FDTD method allows to visualize the spatial profiles of the displacement amplitudes in the structure at a precise frequency. Indeed, displacement amplitudes averaged over one period of oscillation give the displacement fields of the mode. Fig. 8, shows a bended waveguide in steel/water structure for a frequency inside the complete band gap. We can notice the high confinement of the acoustic field inside the defect waveguide.

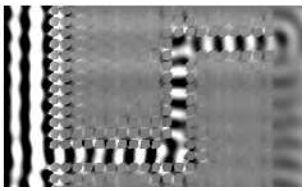


Fig. 8 Calculated longitudinal displacement amplitude averaged over one period of oscillation in bended waveguide.

7 Conclusion

In this chapter, we have presented an overview of the different computational problems that are encountered wen studying wave propagation in phononic crystals. We have outlined the characteristics, and pros and cons of four dominant methods: the MST method (and its improvement, LMS), the PWE method (and the extended PWE method for complex band structures), the FDTD method, and the FEM. As a final useful comment for the reader, we may summarize the usage of these methods as follows.

- The layer multiple scattering (LMS) method is the method of choice for both infinite periodic and finite phononic crystals composed of non-overlapping spheres or cylinders in a uniform background, provided all materials are isotropic. Its usage for surface or plate problems is possible but much more involved, and its usage for arbitrary anisotropic scatterers is presently out of reach. Sainidou *et al.* propose a free LMS code [9].
- The plane wave expansion (PWE) method is very popular for band structure computations because it is general purpose (arbitrary scatterers and background, anisotropy, piezoelectricity). However, it has slow convergence properties (the number of Fourier harmonics that have to be included can make the computation rather slow). To the authors' opinion, the finite element method (FEM) is to be preferred over classical PWE in most cases. The extended PWE was introduced recently and enables the computation of complex band structures and the consideration of losses without sacrificing the general purpose character of the original PWE method. No free or commercial phononic PWE codes are available to the authors' knowledge.
- The finite-difference time-domain (FDTD) method is very popular because it allows to solve the wave equation directly in space and time, thus mimicking real experiments. It is a general purpose method, though the consideration of anisotropy and piezoelectricity is not trivial in the general case. Convergence can be very slow, especially for resonant structures with high quality factors (Q-values). No free or commercial phononic FDTD codes are available to the authors' knowledge.
- The finite element method (FEM) is a general purpose method that solves all drawbacks of the PWE method. It allows the consideration of various boundary

conditions (e.g., solid-fluid phononic crystals), the computation of band structures (it is especially efficient for thin plate problems because of the reduced size of the 3D mesh in this case), and the study of finite phononic crystals. FEM is more often used for time-harmonic or band structure problems. However, it can also be employed in the time-domain, much as the FDTD method, though this property has not been really exploited so far in the litterature. Comsol Multiphysics®, a commercial FEM software, has recently become increasingly popular because of its ease of use (the obvious drawback being its "black-box" character). Many free or even open-source softwares can be employed as well, and one of the authors (VL) has for instance been using FreeFem++ (http://www.freefem.org/ff++/) with success.

References

1. B. A. Auld. *Acoustic Fields and Waves in Solids*. Wiley, New-York, 1973.
2. D. Royer and E. Dieulesaint. *Elastic waves in solids*. Wiley, New York, 1999.
3. IEEE standard on piezoelectricity 176-1987. IEEE Trans. Ultrason., Ferroelec., Freq. Control, vol. 43, no. 5, p. 717, 1996.
4. M. Wilm, S. Ballandras, V. Laude, and Th. Pastureaud. A full 3-D plane-wave-expansion model for piezocomposite structures. *J. Acoust. Soc. Am.*, 112:943–952, 2002.
5. R. P. Moiseyenko and V. Laude. Material loss influence on the complex band structure and group velocity in phononic crystals. *Phys. Rev. B*, 83(6):064301, 2011.
6. Vincent Laude, Younes Achaoui, Sarah Benchabane, and Abdelkrim Khelif. Evanescent Bloch waves and the complex band structure of phononic crystals. *Phys. Rev. B*, 80(9):092301, 2009.
7. I. E. Psarobas, N. Stefanou, and A. Modinos. Phononic crystals with planar defects. *Phys. Rev. B*, 62(9):5536–5540, 2000.
8. R. Sainidou, N. Stefanou, and A. Modinos. Formation of absolute frequency gaps in three-dimensional solid phononic crystals. *Phys. Rev. B*, 66(21):212301, 2002.
9. R. Sainidou, N. Stefanou, I. E. Psarobas, and A. Modinos. A layer-multiple-scattering method for phononic crystals and heterostructures of such. *Computer Physics Communications*, 166:197–240, 2005.
10. I. E. Psarobas. Viscoelastic response of sonic band-gap materials. *Phys. Rev. B*, 64(1):012303, 2001.
11. V. Laude, M. Wilm, S. Benchabane, and A. Khelif. Full band gap for surface acoustic waves in a piezoelectric phononic crystal. *Phys. Rev. E*, 71:036607, 2005.
12. J. O. Vasseur, B. Djafari-Rouhani, L. Dobrzynski, M. S. Kushwaha, and P. Halevi. Complete acoustic band gaps in periodic fibre reinforced composite materials: the carbon/epoxy composite and some metallic systems. *J. Phys.: Condens. Matter*, 6(42):8759–8770, 1994.
13. T.-T. Wu, Z.-G. Huang, and S. Lin. Surface and bulk acoustic waves in two-dimensional phononic crystal consisting of materials with general anisotropy. *Phys. Rev. B*, 69(9):094301, 2004.
14. M. Wilm, A. Khelif, S. Ballandras, V. Laude, and B. Djafari-Rouhani. Out-of-plane propagation of elastic waves in two-dimensional phononic band-gap materials. *Phys. Rev. E*, 67:065602, 2003.
15. A. Khelif, B. Aoubiza, S. Mohammadi, A. Adibi, and V. Laude. Complete band gaps in two-dimensional phononic crystal slabs. *Phys. Rev. E*, 74:046610, 2006.
16. Mahmoud I. Hussein. Reduced bloch mode expansion for periodic media band structure calculations. *Proceedings of the Royal Society A-Mathematical Physical and Engineering Sciences*, 465(2109):2825–2848, 2009.

17. Vincent Laude, Jean-Charles Beugnot, Sarah Benchabane, Yan Pennec, Bahram Djafari-Rouhani, Nikos Papanikolaou, Jose M. Escalante, and Alejandro Martinez. Simultaneous guidance of slow photons and slow acoustic phonons in silicon phoxonic crystal slabs. *Opt. Express*, 19(10):9690–9698, May 2011.
18. J.-P. Berenger. A perfectly matched layer for the absorption of electromagnetic waves. 114:185, 1994.
19. Kane Yee. Numerical solution of initial boundary value problems involving maxwell's equations in isotropic media. *IEEE Transactions on Antennas and Propagation*, 14(3):302–330, 1966.