DESIGN OF FUNCTIONALLY GRADED PHONONIC BAND GAPS USING TOPOLOGY OPTIMIZATION

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Abstract. *Phononic band-gap materials prevent elastic waves from propagating at certain frequency ranges. These materials are called Phononic Crystals (PCs). PCs have been applied to manufacture frequency filters, vibration protection devices, waveguide and to improve ultrasound imaging transducers. Periodic band-gap materials are designed by choosing the location and the size of the band gaps. Many works have been performed on the systematic design of band-gap materials by using topology optimization method (TOM) which is applied to design and optimize periodic materials containing different types of inclusions. Topology optimization is a method which defines the best distribution of material in a design domain in according to an objective function and some constraints. In usual formulation a design domain is discretized into finite elements and a pseudo density is assigned at each element as a design variable. However, the optimal solution presents some elements with intermediate density values. To obtain the manufactured solution the gray scale is often removed which implies changes in the dynamic behavior of the material. To minimize this problem, in this work, the concept of FGM is applied. Functionally graded materials (FGMs) are two component composites characterized by a continuous gradient from one material phase to the other. By combining TOM with FGM an optimal solution closer to the manufactured solution can be found. The modelling of phononic band-gap materials is obtained by using the linear finite element method based on four nodes isoparametric elements combined with Bloch-Floquet relations. This model provides dispersion curves from which results of physical interest can be extracted, such as: identification of propagation modes, cutoff frequencies, passbands and stopbands. In the topology optimization formulation a material model based on the Solid Isoparametric Microstructures with Penalization (SIMP) is used. Sequential Linear Programming (SLP) is used for solving the non-linear optimization problem. To validate the proposed approach bi-dimensional phononic structures are designed and their performance are evaluated.*

Keywords: *phononic band gaps, topology optimization, functionally graded materials, finite element method, Bloch-Floquet*

1. INTRODUCTION

Periodic material, such as porous or fibrous materials and composites, have arisen a great deal of interest and are now widely used in underwater acoustics, signal processing, as well as for medical imaging applications. Particularly, elastic composite materials (phononic materials) exhibit frequency band gaps within which sound and vibrations at certain frequencies are forbidden to propagate. Wave propagation in heterogeneous media is dispersive, it means that a wave decomposes into multiple waves with different frequencies. In this kind of media there are ranges of frequencies, known as stopbands or band gaps, over which all incident waves are effectively attenuated.

Because of the potential application of the band gap property of phononic materials there has been growing interest in the systematic design of structure that possesses a desired band gap (Tanaka *et al.*, 2000). Although it is very challenging issue, a plenty of works has been done to enlarge the width of band gaps (Sigmund and Jensen, 2003; Wu *et al.*, 2009; Vatanabe and Silva, 2010). Many authors (Langlet *et al.*, Nov. 1995; Sigmund and Jensen, 2003) have built accurate mathematical models for the propagation of harmonic elastic waves through periodic materials based on the Bloch-Floquet theory. Thanks for Bloch-Floquet only one unit cell needs to be analysed.

Functionally graded materials (FGMs) are composites characterized by a continuous gradient from one material phase to the other (Suresh and A., 1988; Miyamoto *et al.*, 1999). They are characterized by spatially varying microstructures which intend to take advantage of certain desirable features of each of the constituent phase.

In the literature, the design of phononic materials are usually found by parameters studies based on fixed inclusions shapes, however a powerful method for systematic design of band gap structures is the topology optimization method (TOM) (Sigmund, 2003). In topolology optimization the design domain is discretized by finite elements and a pseudo-density is analysed at each element node as a design variable, i.e., it is determined which elements should be solid and which ones should be void inside a given domain (Sigmund, 2000). Although, the binary $(0-1)$ design is an ill-posed problem and a typical way to seek a solution consists of relaxing the problem by defining a material model that allows for intermediate (composite) property values (Sigmund, 2003), it means that the discrete material function is substituted by

a continuous function. The material model applied is called Simple Isotropic Material with Penalization (SIMP) which tries to recover the binary design of the optimal solution by applying a penalization coefficient. Despite of applying the penalization coefficient to recover the binary model design $(0 - 1)$, some gray scale remains. It can be treated by post-processing the optimal solution. However, those small corrections imply changes in the material dynamic behaviour which means changing of bandgaps. On the other hand, if the FGM concept is applied the gray scale is intrinsic to the model and it does admit solutions with intermediate values of the material field. This approach has been recently explored by Silva and Vatanabe (2010) who used the chain matrix method together to TOM to design one-dimensional functionally graded piezocomposite materials with prescribed band gaps.

In the present work, the objective is to systematically study the design of two-dimensional functionally graded materials that maximize the first band gap for different unit cell symmetry conditions. It is considered a two-dimensional model based on finite element method (FEM) combined with Bloch-Floquet relations (Langlet *et al.*, Nov. 1995). During the development of the work it is intended to explore two-dimensional models considering a non bi-symmetric unit cell. This paper is organized as follows: in Section 2, the theoretical formulation regarding mathematical model, unit cell modelling and the boundary conditions applied are presented. In Section 3, the topology optimization problem is described by defining material model and the gradient control applied. Finally, in Section 4, preliminary results are presented and in the Section 5, some conclusions are given.

2. Theoretical formulation

2.1 Mathematical model

The presented model is based on a doubly periodic material. It is a infinite elastic medium with periodic array of a inclusion in a matrix. It is considered that inclusions are infinite and set parallel to the z axis. Consequently, the problem is bidimensional and only depends on the x and y coordinates, using plane strain conditions.

The whole domain is split into successive unit cells. Due to the material symmetry conditions and thanks for the Bloch-Floquet relations it is only necessary to analyse one unit cell. Therefore, A_1 and A_2 lines are parallel to the y axis and B_1 and B_2 lines are parallel to the x axis. Those lines limit the unit cell which is $2d_a$ wide in the x direction and $2d_b$ wide in the y direction. Corners are marked by the letter C.

The material is excited by a plane and monochromatic wave, the direction of incidence of which is marked by an angle θ with respect to the positive y axis. The incident wave is characterized by a real wave vector $\mathbf{k}$. The modulus of which is called the wave number and it is denoted by k. The time dependence is written as $e^{-j\omega t}$. The schematic description of the unit cell is presented in Fig.(1).

Considering the Bloch-Floquet relation, any spacial function F has to verify the following equation Eq.(1).

$$F(x + 2d_a, y + 2d_b) = e^{j2d_a k \sin\theta} e^{j2d_b k \cos\theta} F(x,y) = e^{j\varphi_a} e^{j\varphi_b} F(x,y) \tag{1}$$
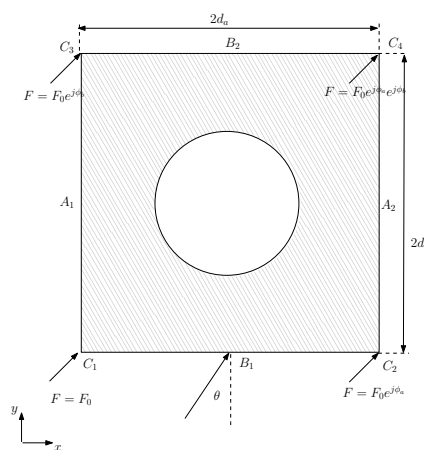

Figure 1. Unit cell schematic description.

2.2 Unit cell finite element modelling

By using Eq.(1) only one unit cell needs to be analysed by finite element. Using Eq.(1) for node displacement values separated by one period, the boundary conditions between adjacent cells are obtained. Considering a modal analysis the whole system of equations is represented by Eq. (2).

$$([\mathbf{K}] - \omega^2[\mathbf{M}])\mathbf{U} = 0 \tag{2}$$

where $[\mathbf{K}]$ and $[\mathbf{M}]$ are respectively, the structure stiffness and mass matrices, ω is the angular frequency, $\mathbf{U}$ is the nodal displacement unknown vector.

This problem is characterized as a complex eigenvalue problem with $\mathbf{k}$ varying on the first Brillouin zone. Eq.(2) should be solved for any wave vector $\mathbf{k}$, however due to the periodicity it is possible to restrict the wave vector to the first Brillouin zone $\mathbf{k} \in [-\pi, \pi]^2$ (Brillouin, 1953), as presented in Fig. (2).

Firstly, due to the square symmetry of the unit cell, it is adopted that the area can be restricted further to the triangle defined by the lines. In principle the whole triangle should be searched, but, although unproved, many researches claim that the information required can be obtained by searching points only on the boundary lines. Later, it will be explored another formulation, based on the non-symmetry of the unit cell. Besides, it will be considered the whole area and not just the points in the boundary lines in the First Brillouin zone.
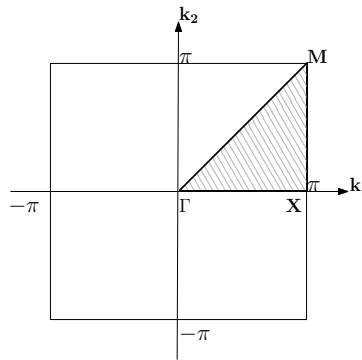

Figure 2. The first Brillouin zone.

2.3 Periodic boundary conditions

The application of the periodic boundary conditions implies that the phase relation Eq. (1) between nodal values belonging to the A_1 and A_2 lines, on one hand, to the B_1 and B_2 lines, on the other hand, has to be incorporated in the matrix equation Eq. (2). The unit cell is divided into nine parts: the four lines A_1, A_2, B_1, and B_2, the four corners C_1, C_2, C_3 and C_4, and the inner domain I. Displacement vector $\mathbf{U}$ and force vector $\mathbf{F}$ are then split into the corresponding nine parts. Due to Eq. (1), their components have to verify:

$$\mathbf{U}_{A2} = \mathbf{U}_{A1}e^{j\varphi_a}, \mathbf{U}_{B2} = \mathbf{U}_{B1}e^{j\varphi_b}, \mathbf{U}_{C2} = \mathbf{U}_{C1}e^{j\varphi_a}, \mathbf{U}_{C3} = \mathbf{U}_{C1}e^{j\varphi_b}, \mathbf{U}_{C4} = \mathbf{U}_{C1}e^{(j\varphi_a + \varphi_b)} \tag{3}$$

Defining the reduced vector $\mathbf{U}_R$ as a vector containing the nodal values of the displacement on the A_1 and B_1 lines, on the C_1 corner and in the inner domain I, Eq. (3) implies a simple matrix relation between $\mathbf{U}$ and $\mathbf{U}_R$. In the same way, a matrix relation can be defined between the vector $\mathbf{F}$, which contains the nodal values of applied forces, and the reduced vector $\mathbf{F}_R$. Also, the same is done for the mass matrix. Consequently, the equation to be solved can be reduced to:

$$([\mathbf{K_R}] - \omega^2[\mathbf{M_R}])\mathbf{U_R} = \mathbf{F_R} \tag{4}$$

where $\mathbf{K_R}$ and $\mathbf{M_R}$ are, respectively, the stiffness and mass reduced matrix.

The dispersion curves are built by varying $\mathbf{k}$ (wave vector) on the first Brillouin zone, for a given propagation direction.

3. Topology optimization method

3.1 Material model

The topology optimization formulation implemented in this work considers a material model based on the SIMP (Solid Isotropic Material with Penalization) (Sigmund, 2003). After all the considerations in the above section, the design domain is defined by the unit cell domain. The objective is to maximize the first band gap. The SIMP model defines that the effective property Ψ_H at each point of the domain is a mixture defined by the linear interpolation between the two constitutive materials. That relation can be applied to calculate the density and elastic property. A generic equation is given by Eq. (5).

$$\Psi_H = \rho_i\Psi_B + (1 - \rho_i)\Psi_A \quad i = 1 \ldots N \tag{5}$$

where Ψ_A and Ψ_B are the constituent material properties. The variable ρ is a design variable describing the amount of material at each point of the domain, which can assume values between 0 and 1, also N is the number of nodes in the finite element mesh.

In this work the design variables are defined for each finite element node and the distribution of the design variables inside the finite elements is calculated by interpolation, considering a continuous distribution. Besides, the optimization problem is solved by using the MMA (Method of Moving Asymptotes) algorithm (Svanberg, 1987), which requires the calculation of gradients of the objective with respect to the design variables. It is also applied a gradient control constraint in the unit cell based on projection technique aiming to control the influence of FGM gradation in the unit cell. By this way, it is possible to impose a smoother gradation, making manufacturing easier.(Carbonari *et al.*, 2007).

3.2 Optimization process

The objective of the optimization process is to maximize the PC first band gap. Thus, the optimization problem is described as follows:

$$
\begin{aligned}
Maximize: & \quad F(\rho_i) = \omega_{n+1} - \omega_n \\
\rho_i(\mathbf{x}) & \\
subject\ to: & \quad ([K] - \omega^2[M])U = F \\
& \quad 0 < \rho_i \leq 1, i = 1\dots N
\end{aligned}
\tag{6}
$$

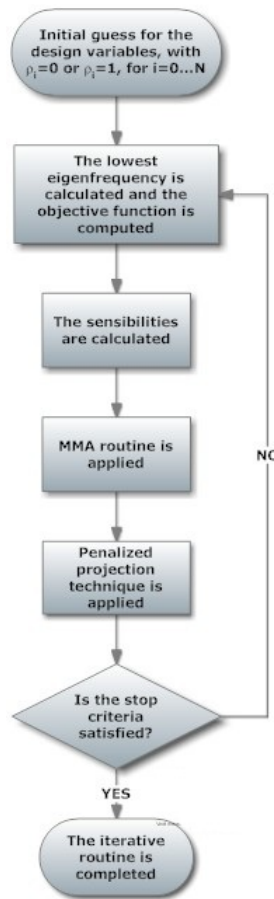The optimization problem is solved following the steps described by the flowchart above.

Figure 3. Iterative routine flowchart

4. Results

Here the results of the optimization are presented considering the maximization of the first band gap width. For the preliminary tests it is observed the influence of material choices in PC's design. It is important to emphasize that the more is the difference between the constituent material properties values, better are the chances to obtain a large band gap. The results are presented for two pairs of material:

1. Cooper and resin

2. Alumina and aluminium

The constituent material properties values are described in Tab. 1.

Table 1. Constituent materials properties.

Property	Cooper	Resin	Alumina	Aluminium
Density (Kg/m^3)	8940	1180	4000	2700
Young's Modulus (GPa)	129.8	3.6	400	70
Poisson's coefficient	0.343	0.376	0.24	0.325

4.1 Material analysis

Considering the two pairs of materials, the following results are obtained.

After 7 iterations the unit cell design and the corresponded dispersion diagram are obtained. Normalized frequencies of the first band gap are 0.422 and 1.167.
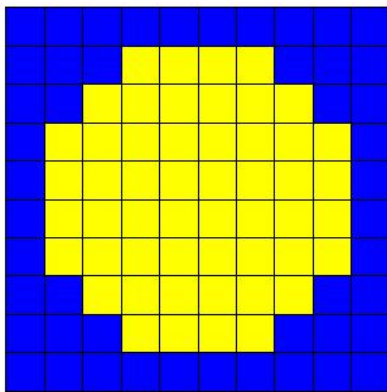
Figure 4. Unit cell designed (cooper and resin).
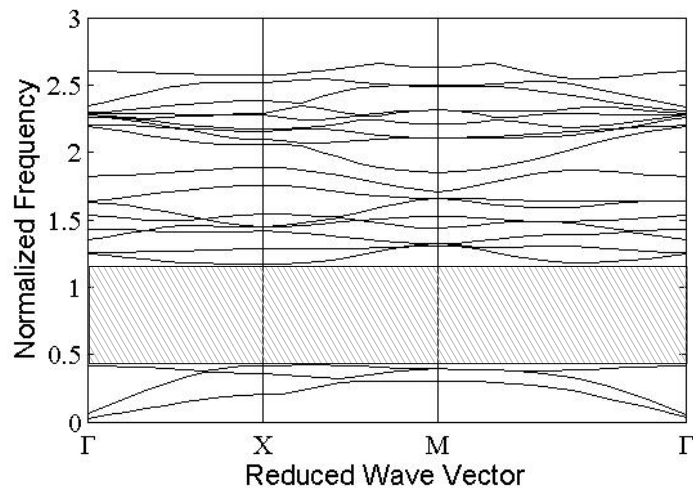
Figure 5. Dispersion curve (cooper and resin).

The same steps are described to analyse alumina and aluminium. In that case, the first band gap normalized frequencies are 0.443 and 0.523, which are smaller than the band gap provided by cooper and resin.

4.2 Gradation analysis

Comparing Fig. (5) with Fig. (9) it is observed the gradation material influence in the band gap width by applying a continuous gradation between the two materials (cooper and resin), after 10 iterations, first band gap normalized frequencies equal to 0.492 and 0.524 is obtained (Fig. 9). Besides, in this case, the unit cell presents intermediate pseudo density values (Fig. 8).

5. Conclusion

From the preliminary results it is observed that a carefully choice of the materials is relevant. In the first case (copper and resin) band gap width is 0.745 (normalized value). On the other hand, in the second case the band gap is 0.08. Thus the first one is more than eight times bigger. It is important to notice that the difference between copper and resin constituent material properties is much bigger than between alumina and aluminium. For example, the ration between the density and the Young's modulus regard cooper and resin is, respectively, 7.57 and 36. Nevertheless, by applying the same thought to alumina and aluminium the same ratio is equal to 1.48 and 5,71, respectively. Thus, higher is the difference between constituent materials compounding, wider is the PC band gap.

Another important factor is the influence of the gradation between materials. It is observed that applying a smooth gradation the band gap width (cooper and resin) is reduced to 0.032 (normalized frequency), it means 4.3% of the band gap width obtained by applying a discrete gradation for the same materials in Section 4.1.

For the further studies it will be discussed the influence of the symmetry condition of the unit cell.
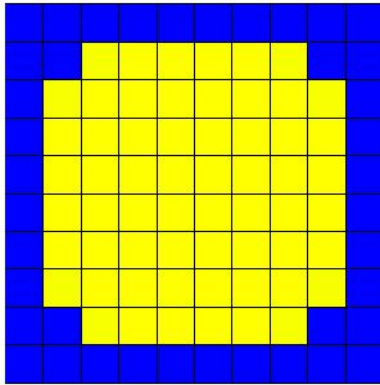
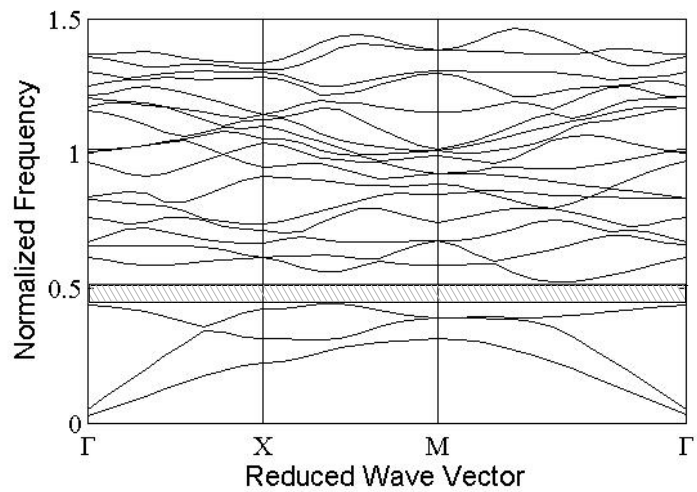Figure 6. Unit cell designed (alumina and aluminium.
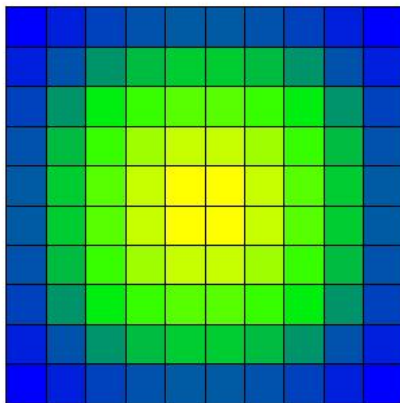

Figure 7. Dispersion curve (alumina and aluminium).

Figure 8. Unit cell designed (cooper and aluminium.
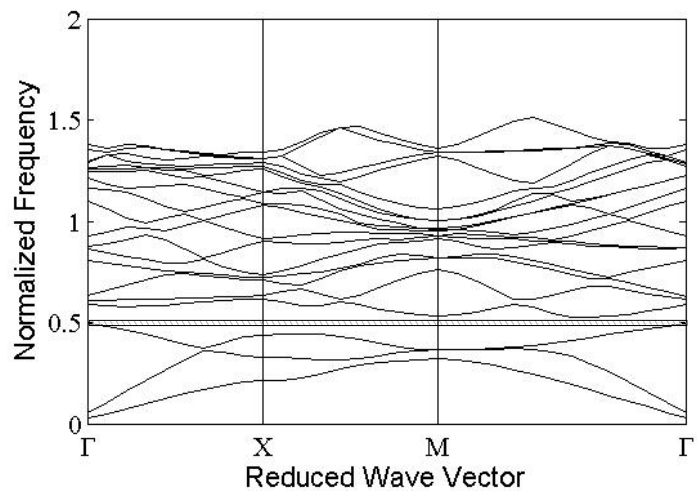

Figure 9. Dispersion curve (cooper and aluminium).

6. ACKNOWLEDGEMENTS

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