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AN ALGORITHM FOR STUDYING WAVE PROPAGATION IN PHONONIC CRYSTALS COMPOSED OF VISCOELASTIC MATERIAL

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Abstract

In order to deal with the viscoelasticity of constituents in phononic crystals, an algorithm based on the finite-difference-time-domain method and the numerical approximation of fractional derivative are proposed. It is validated with transfer matrix method which takes the viscosity into account by complex modulus with frequency dependence. Although the viscoelasticity of host material does not influence the frequency position of gaps, a wide transmission gap is found even for very weak viscosity, which gives new idea to design phononic crystals with wide transmission gaps.

1. INTRODUCTION

The propagation of elastic waves in periodic heterogeneous materials known as phononic crystals (PCs) has received much attention in recent years. Because of the periodicity of elasticity in PCs, there exist frequency band gaps within which wave propagation is forbidden, giving rise of prospective applications such as elastic/acoustic filters, noise/ vibration isolations, as well as improvements in design of transducers.

Several theoretical methods have been developed for investigating the frequency gaps of PCs, which include the plane wave expansion (PWE) method [1], the multiple-scattering theory (MST) method [2], and the Finite-difference-time-domain (FDTD) method [3-10]. The PWE method has the convergence problem when dealing with systems of either very high or very low filling ratios, or of large elastic mismatch, especially for the systems with mixing solid and fluid components. The MST and FDTD methods overcome those difficulties. But the approach based on MST is effective only for the systems containing spherical or cylindrical scatters. The FDTD approaches are suitable for nonspherical or complicated scatters. The advantages of adopting the FDTD methods include less calculation time than PWE, more material-selecting flexibility, and inclusion shape variation. But it requires enough discretization of time and spatial domain to guarantee its convergence and accuracy, therefore is generally rather time consuming. Fortunately computers become faster and cheaper enough to counteract FDTD's disadvantage. Moreover, FDTD methods are very suitable for parallelism computation realized with massage passing interface (MPI) on a personal computer cluster system [8], which makes them more applicable and efficient. Usually, FDTD methods are used to deal with the transmission problem of finite size phononic crystals, such as two-dimensional (2D) PCs consisting of liquid cylinders in aluminum host [3], or solid (hollow) cylinders in air [6], or steel cylinders in epoxy matrix [5,8], and three-dimensional (3D) PCs consisting of lead spheres forming FCC lattice in epoxy [4,7]. Tanaka [9] proposed an approach to calculate the band structures of 3D PCs using FDTD method. Cao [10] improved Tanaka's approach by introducing Bloch initial conditions and Bloch boundary conditions and dealt with 2D PCs.

In all of above mentioned works, the viscoelasticity of constituents like oil, air, polyethylene or epoxy are not taken into account. In fact most of the research works on PCs in open literature did not take the viscoelasticity of constituents into account due to the lack of available method. However, in an experiment, finite-size slabs are dealt with and the measured quantities are usually the transmission and reflection coefficients. Apart from that, realistic materials, especially polymers and liquids, are dispersive and dissipative. In order to obtain wide gaps in low frequencies, materials with small elastic modulus such as rubber and polymer are often used as one constituent in PCs. I.E. Psarobas [11] had proposed a method for 3D PCs based on multiple scattering theory and Kelvin-Voigt viscoelastic model, which suffers the inherited disadvantage of scatters shape limitation. To our best knowledge, there is no algorithm reported earlier accounting for viscoelasticity in 2D PCs.

In this paper, we propose an algorithm for calculating wave propagation in 2D PCs with viscoelastic host based on FDTD approach. The viscoelasticity is accounted for by means of the fractional derivative model (known as RTG model) which is chosen for its accuracy in wide frequency ranges and fewness of parameters. The method for calculating the transmission coefficients of finite slab of 2D PCs is formulized by integrating the RTG model into FDTD method, which is called RTG-FDTD method in this paper. The proposed method can be degenerated to traditional FDTD method by setting the parameters of RTG model to zeros. In section 2, the RTG model of viscoelastic materials and the elastic wave equations with RTG model of 2D PCs are described in detail. Then the proposed RTG-FDTD method is outlined in section 3. In section 4, several examples of solid/solid PCs are numerically simulated to illustrate the viscoelastic effects on wave transmission and the results are discussed in detail. Section 5 summarizes the discussions and the whole paper as conclusions.

2. FRACTIONAL DRIVATIVE MODEL OF VISCOELASTIC MATERIALS

Viscoelastic materials are largely used to provide damping to structures or to absorb underwater sound waves. In the past the rheological model for viscoelastic materials was based on the classical concept of derivatives with integer order, which led to constitutive equations with too many parameters to be identified. Over the last two decades, the fractional derivative has gained the reputation of an extremely adequate tool to model viscoelastic materials and resulted in the development of the so-called fractional derivative models [12].

2.1 The constitutive equation for viscoelastic materials in fractional derivatives

The generalized one-dimensional constitutive equation in fractional derivatives is

$$\sigma(t)+\sum_{m=1}^{M} b_m D^{\beta_m}\left[\sigma(t)\right]=E_0\varepsilon(t)+\sum_{n=1}^{N} E_n D^{\alpha_n}\left[\varepsilon(t)\right] \tag{1}$$

where $\sigma(t)$ and $\varepsilon(t)$ stand for strain and stress respectively. b_m, E_0, E_n are constants related to the concerned material. α_n and β_m are fractional orders of the derivatives usually with the values between 0 and 1. The exact definition of fractional derivatives $D^{\alpha}\left[f(t)\right]$ and its numerical appropriation will be given in next section.

Lots of research works indicate that equation (1) with neither M or N more than 1 is accurate enough to represent the dynamic behavior of viscoelastic materials. Therefore there are five parameters when $M, N = 1$ which is called five-parameter fractional derivative models. The four-parameter and three-parameter fractional derivative models are widely used in open literature. In this paper we use Kelvin-Voigt type fractional derivative model with only three parameters. The constitutive equation reads

$$\sigma(t) = E_0 \varepsilon(t) + E_0 \eta D^{\alpha}\left[\varepsilon(t)\right] \tag{2}$$

The concept of the complex modulus of elasticity is widely used in acoustics to characterize the dynamic elastic and damping properties of solid materials in the linearity range. By applying Fourier transformation to equation (2), one readily obtains (3) which relate the complex modulus to the fractional derivative model of Kelvin-Voigt type.

$$E_c(j\omega) \triangleq \frac{\sigma(j\omega)}{\varepsilon(j\omega)} = \left[E_0 + E_0\eta\omega^{\alpha}\cos\frac{\alpha\pi}{2}\right] + j\left[E_0\eta\omega^{\alpha}\sin\frac{\alpha\pi}{2}\right] \tag{3}$$

The constitutive equations of the Kelvin-Voigt fractional derivative model for three dimensional viscoelastic materials are

$$\begin{cases} S_{ij}(t) = 2G\left(1+\eta D^{\alpha}\right)e_{ij}(t) \\ \sigma_{kk}(t) = 3K\varepsilon_{kk}(t) \end{cases} \tag{4}$$

Where $S_{ij}(t)$ and $e_{ij}(t)$ are the deviatoric tensor of stress and strain respectively. $\sigma_{kk}(t)$ and $\varepsilon_{kk}(t)$ are the principal stress and strain. K and G are the bulk modulus and shear modulus.

2.2 Elastic wave equations of 2D PCs with viscoelasticity in fractional derivatives

The equations governing the motion of displacement $u_i(\boldsymbol{r},t)$ in inhomogeneous solids are given by

$$\rho(\boldsymbol{r})\ddot{u}_i(\boldsymbol{r},t) = \partial_j\left[\sigma_{ij}(\boldsymbol{r},t)\right] \tag{5}$$

$$\varepsilon_{ij}(\boldsymbol{r},t) = \frac{1}{2}\left\{\partial_j\left[u_i(\boldsymbol{r},t)\right] + \partial_i\left[u_j(\boldsymbol{r},t)\right]\right\} \tag{6}$$

where $\boldsymbol{r} = (x, y, z)$ and the summation convention over repeated indices is assumed.

In the 2D PC case, cylindrical scatters are paralleled to z axis and infinite long. The system has translational symmetry along z axis thus the material parameters do not depend on z. By assuming wave propagation in the *x*-*y* plane, the wave equation can split into two independent equations [3]. We study the XY mode in this paper which involves both longitudinal and transverse waves. Substitute equations (6) into (4), and rewrite equations (4) and (5) in components, we obtain the elastic wave equations of 2D PCs with viscoelasticity in fractional derivates, which reads as (7). The displacement and stress components like $u_x(x, y, t)$ are shortened as u_x for simplicity. ρ is the mass density of constituents, which varies with the periodicity. η is the loss factor of the viscoelastic material. If $\eta = 0$, equations (7) degenerate to the classical wave equations without viscoelasticity.

$$\begin{cases} \rho \dfrac{\partial^2 u_x}{\partial t^2} = \dfrac{\partial \tau_{xx}}{\partial x} + \dfrac{\partial \tau_{xy}}{\partial y} \\ \rho \dfrac{\partial^2 u_y}{\partial t^2} = \dfrac{\partial \tau_{xy}}{\partial x} + \dfrac{\partial \tau_{yy}}{\partial y} \\ \tau_{xx} = \left(K + \dfrac{4}{3}G\right)\dfrac{\partial u_x}{\partial x} + \left(K - \dfrac{2}{3}G\right)\dfrac{\partial u_y}{\partial y} + \dfrac{4}{3}G\eta D^\alpha\left(\dfrac{\partial u_x}{\partial x}\right) - \dfrac{2}{3}G\eta D^\alpha\left(\dfrac{\partial u_y}{\partial y}\right) \\ \tau_{yy} = \left(K - \dfrac{2}{3}G\right)\dfrac{\partial u_x}{\partial x} + \left(K + \dfrac{4}{3}G\right)\dfrac{\partial u_y}{\partial y} - \dfrac{2}{3}G\eta D^\alpha\left(\dfrac{\partial u_x}{\partial x}\right) + \dfrac{4}{3}G\eta D^\alpha\left(\dfrac{\partial u_y}{\partial y}\right) \\ \tau_{xy} = G\dfrac{\partial u_y}{\partial x} + G\dfrac{\partial u_x}{\partial y} + G\eta D^\alpha\left(\dfrac{\partial u_y}{\partial x}\right) + G\eta D^\alpha\left(\dfrac{\partial u_x}{\partial y}\right) \end{cases} \tag{7}$$

3. RTG-FDTD METHOD FOR 2D PCS WITH VISCOELASTICITY

In order to investigate the transmission property of 2D PCs with viscoelasticity, it is necessary to solve the wave equations (7). Since numerical approximation of fractional derivatives performed in time domain is more generally applicable than the Laplace transform solution [13], the equations (7) are integrated by means of a finite-difference time-domain scheme which is very convenient to be integrated with the numerical approximation of fractional derivatives.

3.1 Caputo fractional derivative

The Caputo fractional derivative is defined as equation (8) [14], where $\Gamma(\bullet)$ is gamma function. $f^{(n)}(t)$ is the classical nth order derivative. $\lceil \alpha \rceil$ is the ceiling function giving the smallest integer greater than or equal to α. $f(t)$ must be continuous and $\lceil \alpha \rceil$ times differentiable in t.

$$^{C}D^{\alpha} f(t) \triangleq \frac{1}{\Gamma(\lceil \alpha \rceil - \alpha)} \int_0^t \frac{f^{(\lceil \alpha \rceil)}(\tau)}{(t-\tau)^{1+\alpha-\lceil \alpha \rceil}} d\tau, \quad \alpha, t \in \mathbb{R}^+ \tag{8}$$

The Caputo differential operator is a linear operator. If $f^{(\lceil \alpha \rceil)}(t)$ exists and is continuous, and if $f^{(n)}(0) = 0$, $n = 1, 2, \cdots, \lceil \alpha \rceil$, the Caputo fractional derivative is equivalent to the Riemann- Liouville definition which is more popular in modeling viscoelastic materials. Such conditions are satisfied in the FDTD scheme, which will be seen later. One of the advantages of Caputo derivatives is that the initial conditions to produce a unique solution of fractional differential equations are akin to those of classical ODEs.

3.2 Numerical approximation of Caputo fractional derivatives

Unlike ordinary derivatives, which are point functionals, fractional derivatives are hereditary functionals possessing a total memory of past states. Since it is a fading memory effect, only the nearest memory with finite duration is used in practice. A numerical algorithm for computing Caputo derivatives has been derived by Diethelm [14].

$$ {}^{C}D^{\alpha} f(t_n) \approx \frac{h^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=0}^{n} a_{j,n} \left\{ f(t_{n-j}) - \sum_{k=0}^{[\alpha]} \left[(t_n - t_j)^k / k! \right] f^{(k)}(t_{0^+}) \right\} \quad (9a) $$

$$ a_{j,n} = \begin{cases} 1 & j=0 \\ (j+1)^{1-\alpha} - 2j^{1-\alpha} + (j-1)^{1-\alpha} & 0<j<n \\ (1-\alpha)n^{-\alpha} - n^{1-\alpha} + (n-1)^{1-\alpha} & j=n \end{cases} \quad (9b) $$

The authors have compared several numerical algorithms of fractional derivatives. $D^{\alpha}\left[\sin(\omega t)\right] = \omega^{\alpha} \sin\left(\omega t + \frac{\alpha\pi}{2}\right)$ is used as an benchmark. Figure 1 present the errors of different numerical approximations using the latest three periods as the history data. One can readily finds that the algorithm mentioned above gives the best approximation, which is the reason that Caputo fractional derivatives are chosen.

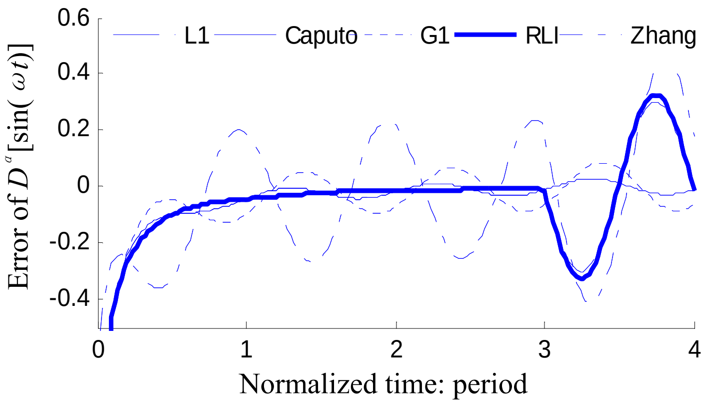

Figure 1. Comparison of several numerical algorithms for calculating fractional derivatives. Algorithms L1 and G1 are from [13]. RLI is the algorithm 2 in [14]. Zhang is referred to [15].

3.3 Finite-difference-time-domain scheme

In order to numerically solve the equations (7), we discretize them in both the spatial and time domains, set appropriate boundary conditions, and explicitly calculate the evolutions of u_x and u_y in the time domain. More specifically, real space is discretized into a rectangular grid where the variables are defined. u_x and u_y, τ_{xx}/τ_{yy} and τ_{xy} are spatially interlaced by half a grid cell. The elastic wave equations are approximated by center differences in both space and time. For example, the first and last equation in (7) will be discretized as (10a) and (10b).

$$ \begin{aligned} \tau_{xy}^{k}\left(l,m+\tfrac{1}{2}\right) &= \mu\left(l,m+\tfrac{1}{2}\right) \cdot \left[\frac{u_x^k(l,m+1) - u_x^k(l,m)}{d_y} + \frac{u_y^k\left(l+\tfrac{1}{2},m+\tfrac{1}{2}\right) - u_y^k\left(l-\tfrac{1}{2},m+\tfrac{1}{2}\right)}{d_x} \right] \\ &+ \mu\left(l,m+\tfrac{1}{2}\right)\eta \cdot \left\{ \frac{D^{\alpha}\left[u_x^k(l,m+1)\right] - D^{\alpha}\left[u_x^k(l,m)\right]}{d_y} + \frac{D^{\alpha}\left[u_y^k\left(l+\tfrac{1}{2},m+\tfrac{1}{2}\right)\right] - D^{\alpha}\left[u_y^k\left(l-\tfrac{1}{2},m+\tfrac{1}{2}\right)\right]}{d_x} \right\} \end{aligned} \quad (10a) $$

$$ \begin{aligned} u_x^{k+1}(l,m) &= 2u_x^k(l,m) - u_x^{k-1}(l,m) \\ &+ \frac{d_t^2}{\rho(l,m)} \left[\frac{\tau_{xx}^k\left(l+\tfrac{1}{2},m\right) - \tau_{xx}^k\left(l-\tfrac{1}{2},m\right)}{d_x} + \frac{\tau_{xy}^k\left(l,m+\tfrac{1}{2}\right) - \tau_{xy}^k\left(l,m-\tfrac{1}{2}\right)}{d_y} \right] \end{aligned} \quad (10b) $$

The computational region contains a slab of the composite medium sandwiched in homogenous host material. Mur's first order absorbing boundary conditions are used at the boundaries of the computational region perpendicular to the wave propagation direction. At the other two boundaries, periodic boundary conditions are used. The modulated Gaussian pulse is launched in the homogeneous region and propagates along the y axis through the composite. The components of the displacement vector as a function of time are collected on the other side. The time series collected are converted into the frequency domain using the fast Fourier transform. By normalizing these results relative to the incident wave, one can find the frequency response of the PC slab.

4. NUMERICAL EXAMPLES AND DISCUSSIONS

4.1 One dimensional PCs

Since there is no example of 2D PCs available in literature while counting on the damping and dispersion, a 1D PC is considered for validation because the well known transfer matrix (TM) method for 1D PCs can deal with the viscoelasticity on the basis of complex modulus with frequency dependence.

The 1D PC example is composed of Aluminum and epoxy layered alternatively. Each layer is 10mm thick which results in the lattice constant of 20mm. The elastic parameters used in the calculation are listed in table 1, and the fractional order is arbitrarily fixed to 0.5. The complex modulus with frequency dependence is determined with equation (3).

Table 1. Material parameters used in examples

	Aluminum	Epoxy
Mass density ρ (kg/m^3)	2730	1180
Lame constant λ (Pa)	6.89e10	4.43e9
Lame constant μ (Pa)	2.87e10	1.59e9

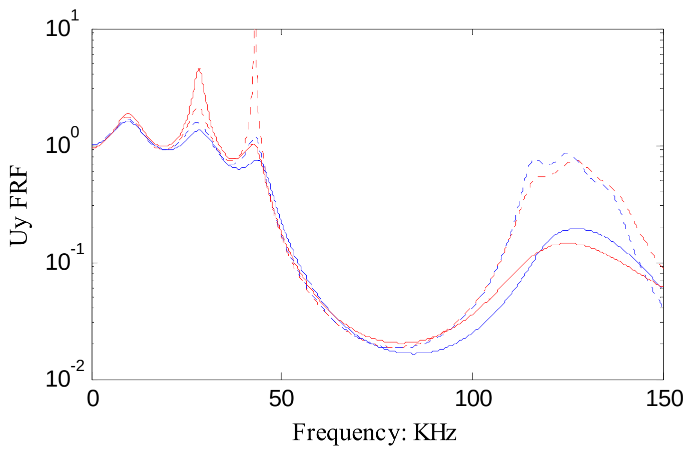

Figure 2. Transmission of 1D PC composed of aluminum and epoxy layered alternatively. Blue lines are calculated with 2D RTG-FDTD and red lines with TM method. η=0.0001 for solid lines and η=0.0005 for dotted lines.

The calculated transmission property for four periods with both TM and RTG-FDTD methods are presented in figure 2 with red and blue lines respectively. Two levels of viscosity are considered which are indicated with dotted lines for low viscosity and solid lines for medium viscosity. For both cases, the outlines of the transmissions calculated with TM and RTG-FDTD method are in very good agreement. In quantity, they reasonably agree to each other in most frequencies except some peaks and very high frequencies. The discrepancy in high frequency is understandable because the convergency of FDTD scheme becomes poor in higher frequency [3, 4] with given temporal and spatial grids, while the TM method does not suffer such a problem. But the reason of discrepancies about the peaks in low frequencies is still not clear for the authors. Comparing the transmissions with different level of viscosity, one can find larger attenuation in high frequencies for higher viscosity, which is reasonable and as expected.

4.2 Two dimensional PCs

The second example is a 2D PC consisting of aluminium cylinder embedded in epoxy matrix forming square lattice. The lattice constant is 20mm and the radius of the scatter is 8mm. The band structure is calculated with PWE method and illustrated in figure 3 on left panel. The longitudinal and transverse wave modes are indicated with solid and dotted lines respectively. As for the longitudinal waves, there are three gaps in ΓX direction below 150 kHz. The longitudinal wave transmission property with and without viscoelasticity are calculated with the proposed RTG-FDTD method, which is presented in the right panel of figure 3. The frequency ranges of the three gaps in both panels are in very good agreements, which validate our FDTD scheme in 2D cases. Comparing the transmission with to without viscosity, one readily sees the viscosity slightly widen each individual gap to higher frequency because of its dispersive effects. More important, the transmission peaks between gaps are largely attenuated, which results in a wide combined transmission gap. The attenuation is related to the wave modes. Flat bands will be largely attenuated when the host material is dissipative, which implied a new idea to design PCs with wide transmission gaps.

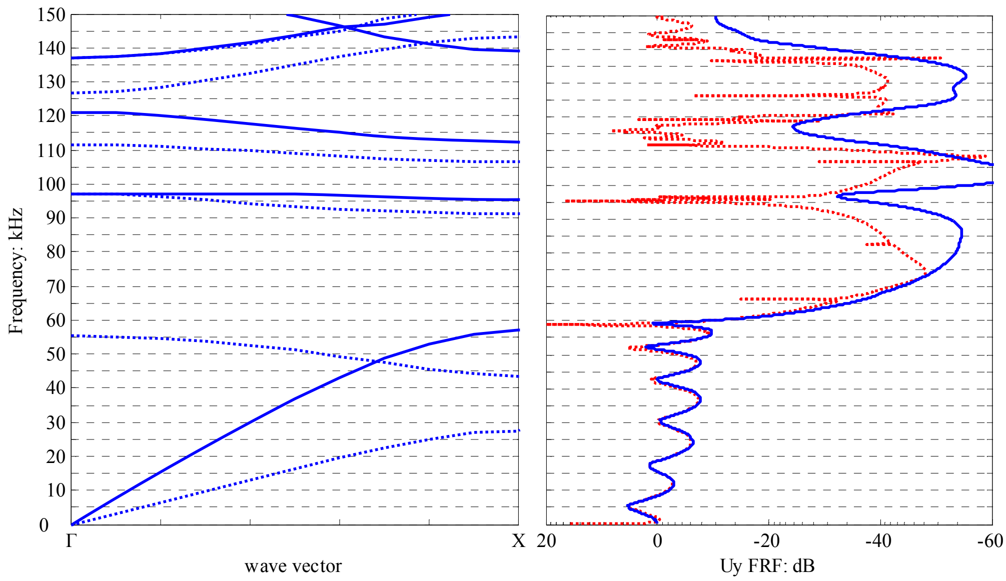

Figure 3. Band structure (left) and transmission (right) of 2D PC composed of aluminum cylinders squarely embedded in epoxy host calculated with 2D RTG-FDTD method. Solid line (blue) is for η=0.0001 and dotted line for η=0.

Although the examples are limited in the same constituent materials, the proposed RTG-FDTD method is generally applicable for even larger mismatch of elastic parameters.

More examples will be put in the presentation on the conference because of limitations on the length of papers.

5. CONCLUSIONS

An algorithm (RTG-FDTD) for calculating the transmission property of 2D PCs with viscoelastic constituents is proposed based on the FDTD scheme and the fractional derivatives. The transmission of a 1D PC is calculated with the transfer matrix method which takes the viscosity into account by complex modulus with frequency dependence for validation, which shows reasonable agreement to the results of the RTG-FDTD method and justifies the proposed algorithm. The effects of viscoelasticity of host material of 2D PC on its transmission property are investigated with the proposed method. It is noted that the dispersion of host material widens the gaps. Moreover, the damping effects evidently attenuate the flat bands between gaps and result in a wide transmission gap, which implied a new idea to design PCs with wide transmission gaps.

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