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Mixed-variational formulation for phononic band-structure calculation of arbitrary unit cells

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ABSTRACT

This paper presents phononic band-structure calculation results obtained using a mixed variational formulation for 1-, and 2-dimensional unit cells. The formulation itself is presented in a form which is equally applicable to 3-dimensiomal cases. It has been established that the mixed-variational formulation presented in this paper shows faster convergence with considerably greater accuracy than variational principles based purely on the displacement field, especially for problems involving unit cells with discontinuous constituent properties. However, the application of this formulation has been limited to fairly simple unit cells. In this paper we have extended the scope of the formulation by employing numerical integration techniques making it applicable for the evaluation of the phononic band-structure of unit cells displaying arbitrary complexity in their Bravais structure and in the shape, size, number, and anisotropicity of their micro-constituents. The approach is demonstrated through specific examples.

1. Introduction

There has been a recent surge of research effort towards achieving exotic dynamic response through novel microstructural design of composites. Within mechanics and elastodynamics these responses can be categorized in two broad areas: phononics and metamaterials. Phononics is the study of stress wave propagation in periodic elastic composites, whereas, metamaterials builds upon the area of phononics with dynamic homogenization schemes and seeks to create periodic composites with overall dynamic properties that are not shared by common materials. The required first step to attain this is to evaluate the phononic band-structure of periodic composites.

The phononic band-structure (Martinezsala et al., 1995) results from the periodic modulation of stress waves, and as such has deep similarities with areas like electronic band theory (Bloch, 1928) and photonics (Ho et al., 1990). Such periodic modulations provide for very rich wave-physics and the potential for novel applications (Cervera et al., 2001; Yang et al., 2002; Khelif et al., 2003; Reed et al., 2003; Yang et al., 2004; Gorishnyy et al., 2005; Mohammadi et al., 2008; Sukhovich et al., 2008; Lin et al., 2009). These applications depend upon the ability of calculating the required phononic band-structure. In addition to the ability of calculating phononic band-structures, certain research areas such as phononic band-structure optimization (Sigmund and Jensen, 2003; Rupp et al., 2007; Bilal and Hussein, 2011; Diaz et al., 2005; Halkjær et al., 2006) and inverse problems in dynamic homogenization, also demand that the band-structure calculating algorithm possess speed, efficiency, accuracy, and versatility. There exist several techniques by which band-structures of photonic and phononic composites can be computed. These include the plane wave expansion (PWE) method (Ho et al., 1990; Leung and Liu, 1990; Zhang and

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Satpathy, 1990), the multiple scattering method (Kafesaki and Economou, 1999), the finite difference time domain method (Chan et al., 1995), the finite element method (White et al., 1989), variational methods (Goffaux and Sánchez-Dehesa, 2003) and more (see Hussein, 2009).

In this paper we elaborate upon a mixed variational formulation for phononic band-structure calculations which is based upon varying both the displacement and the stress fields (Nemat-Nasser, 1972; Nemat-Nasser et al., 1975; Minagawa and Nemat-Nasser, 1976; Nemat-Nasser et al., 2011). Since it is based on a variational principle, any set of approximating functions can be used for calculations, e.g., plane-waves Fourier series or finite elements (Minagawa et al., 1981). The mixe formulation yields very accurate results and the rate of convergence of the corresponding approximating series solution is greater than that of the Rayleigh quotient with displacement-based approximating functions (Babuska and Osborn, 1978). Although the mixed-formulation shows a fast convergence, it has not yet been used to evaluate the band-structures of complex 2-, and 3-dimensional unit cells. In this paper we extend the scope of the formulation by employing numerical integrations and describe clearly how it can be applied to 1-, 2-, and 3-dimensional unit cells of arbitrary complexity in their Bravais structure and in the shape, size, number, and anisotropicity of their micro-constituents. We present 1-, and 2-dimensional test cases which verify the results of the formulation with published results in literature (exact solution for 1-dimensional and plane wave approximation for 2-dimensional). For the 2-phase 2-dimensional case we note that acceptable convergence over the first 18 phononic branches is achieved when the displacement and stress fields are approximated by 121 Fourier terms each.

2. Statement of the problem

In the following treatment repeated Latin indices mean summation, whereas, repeated Greek indices do not. Consider the problem of elastic wave propagation in a general 3-dimensional periodic composite. The unit cell of the periodic composite is denoted by Ω and is characterized by 3 base vectors $\mathbf{h}^i$, $i = 1, 2, 3$. Any point within the unit cell can be uniquely specified by the vector $\mathbf{x} = H_i \mathbf{h}^i$ where $0 \leqslant H_i \leqslant 1, i = 1, 2, 3$. The same point can also be specified in the orthogonal basis as $\mathbf{x} = x_i \mathbf{e}^i$. The reciprocal base vectors of the unit cell are given by,

$$\mathbf{q}^1 = 2\pi \frac{\mathbf{h}^2 \times \mathbf{h}^3}{\mathbf{h}^1 \cdot (\mathbf{h}^2 \times \mathbf{h}^3)}; \quad \mathbf{q}^2 = 2\pi \frac{\mathbf{h}^3 \times \mathbf{h}^1}{\mathbf{h}^2 \cdot (\mathbf{h}^3 \times \mathbf{h}^1)}; \quad \mathbf{q}^3 = 2\pi \frac{\mathbf{h}^1 \times \mathbf{h}^2}{\mathbf{h}^3 \cdot (\mathbf{h}^1 \times \mathbf{h}^2)} \tag{1}$$

such that $\mathbf{q}^i \cdot \mathbf{h}^j = 2\pi\delta_{ij}$, where the denominators of the above vectors are the volume of the unit cell. Fig. 1 is the schematic of a 2-dimensional unit cell, indicating the unit cell basis vectors, the reciprocal basis vectors and the orthogonal basis vectors.

The wave vector for a Bloch-wave traveling in the composite are given as $\mathbf{k} = Q_i \mathbf{q}^i$ where $0 \leqslant Q_i \leqslant 1$, $i = 1, 2, 3$. The composite is characterized by a spatially varying stiffness tensor, $C_{jkmn}(\mathbf{x})$, and density, $\rho(\mathbf{x})$, which satisfy the following periodicity conditions:

$$C_{jkmn}(\mathbf{x} + n_i \mathbf{h}^i) = C_{jkmn}(\mathbf{x}); \quad \rho(\mathbf{x} + n_i \mathbf{h}^i) = \rho(\mathbf{x}), \tag{2}$$

where $n_i (i = 1, 2, 3)$ are integers.

2.1. Field equations and boundary conditions

For harmonic elastodynamic problems the equations of motion and kinematic relations at any point $\mathbf{x}$ in Ω are given by

$$\sigma_{jk,k} = -\lambda \rho u_j; \quad \varepsilon_{jk} = \frac{1}{2}(u_{j,k} + u_{k,j}), \tag{3}$$

where $\lambda = \omega^2$, and $\boldsymbol{\sigma} e^{-i\omega t}$, $\boldsymbol{\varepsilon} e^{-i\omega t}$, and $\mathbf{u} e^{-i\omega t}$ are the space and time dependent stress tensor, strain tensor, and displacement vector, respectively. The stress tensor is related to the strain tensor through the elasticity tensor, $\sigma_{jk} = C_{jkmn}\varepsilon_{mn}$. The traction and displacement at any point in the composite are related to the corresponding traction and displacement at another point, separated from the first by a unit cell, through Bloch relations. These relations serve as the homogeneous boundary conditions on $\partial\Omega$. If the Bloch wave vector is $\mathbf{k}$ then these boundary conditions are given by,

$$u_j(\mathbf{x} + \mathbf{h}^i) = u_j(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{h}^i}; \quad t_j(\mathbf{x} + \mathbf{h}^i) = -t_j(\mathbf{x}) e^{i\mathbf{k}\cdot\mathbf{h}^i}, \quad \mathbf{x} \in \partial\Omega, \tag{4}$$

where $t_j = \sigma_{jk} \nu_k$ are the components of the traction vector and $\boldsymbol{\nu}$ is the exterior unit normal vector on $\partial\Omega$.

2.2. Mixed-variational formulation

It has been shown (Nemat-Nasser et al., 1975; Minagawa and Nemat-Nasser, 1976) that the solution to (3) that satisfies the boundary conditions, (4), renders the following functional stationary:

$$\lambda_N = \frac{\langle \sigma_{jk}, u_{j,k} \rangle + \langle u_{j,k}, \sigma_{jk} \rangle + \langle D_{jkmn} \sigma_{jk}, \sigma_{mn} \rangle}{\langle \rho u_j, u_j \rangle}, \tag{5}$$

where $\mathbf{D}$ is the compliance tensor and the inner product is given by,

$$\langle u, v \rangle = \int_\Omega u v^* d\Omega, \tag{6}$$

where v^* is the complex conjugate of v.

2.3. Approximation with periodic test functions

Now we approximate the stress and displacement fields with the following test functions:

$$\bar{u}_j = \sum_{\alpha,\beta,\gamma} U_j^{\alpha\beta\gamma} f^{\alpha\beta\gamma}(\mathbf{x}), \quad \bar{\sigma}_{jk} = \sum_{\alpha,\beta,\gamma} S_{jk}^{\alpha\beta\gamma} f^{\alpha\beta\gamma}(\mathbf{x}), \tag{7}$$

where the test functions satisfy the boundary conditions, (4), and are orthogonal in the sense that $\langle f^{\alpha\beta\gamma}, f^{\theta\eta\xi} \rangle$ is proportional to $\delta_{\alpha\theta}\delta_{\beta\eta}\delta_{\gamma\xi}$, $\boldsymbol{\delta}$ being the Kronecker delta. Substituting from (7) to (5) and setting the derivative of λ_N with respect to the unknown coefficients, $(U_j^{\alpha\beta\gamma}, S_{jk}^{\alpha\beta\gamma})$, equal