Negative effective dynamic mass-density and stiffness: Micro-architecture and phononic transport in periodic composites

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We report the results of the calculation of negative effective density and negative effective compliance for a layered composite. We show that the frequency-dependent effective properties remain positive for cases which lack the possibility of localized resonances (a 2-phase composite) whereas they may become negative for cases where there exists a possibility of local resonance below the length-scale of the wavelength (a 3-phase composite). We also show that the introduction of damping in the system considerably affects the effective properties in the frequency region close to the resonance. It is envisaged that this demonstration of doubly negative material characteristics for 1-D wave propagation would pave the way for the design and synthesis of doubly negative material response for full 3-D elastic wave propagation.

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I. INTRODUCTION

Rytov\textsuperscript{1} studied the Bloch-form\textsuperscript{2} or Floquet-type\textsuperscript{3} elastic waves propagating normal to layers in a periodic layered composite and produced the expression for the dispersion relation that gives the pass-bands and stop-bands in the frequency-wave number space. Because of the emergence of structural composite materials with application to aerospace and other technologies, the 1960’s witnessed considerable scientific activity mostly focused on estimating the effective static properties of composites, whereby elegant and rigorous bounds for their effective properties were established;\textsuperscript{4–11}\textsuperscript{,} The early effort to study the dynamic response of elastic composite materials was mostly limited to one-dimensional problems. To create a general numerical approach to solving elastic waves in composites, Kohn \textit{et al.}\textsuperscript{12} proposed using a modified version of the Rayleigh quotient in conjunction with the Bloch-form waves to calculate the dispersion curves. To directly account for the strong discontinuities that generally exist in the elastic properties of a composite’s constituents, Nemat-Nasser\textsuperscript{13–16} developed a mixed variational formulation to calculate the eigenfrequencies and modeshapes of harmonic waves in 1-, 2-, and 3-dimensional periodic composites.

Recent research in the fields of metamaterials and phononic crystals has opened up intriguing possibilities for the experimental realization of such exotic phenomena as negative refraction and super-resolution. The realization of such phenomena, using crystal anisotropy, has met with recent successes both in the fields of photonics\textsuperscript{17–20} and phononics.\textsuperscript{21–23} It is also possible to realize such anomalous wave propagation characteristics with the use of the so called doubly negative materials.\textsuperscript{24} It has long been understood that this double negative behavior is a result of local resonances existing below the length-scale of the wavelength. This physical intuition was used to realize such materials for electromagnetic waves.\textsuperscript{25–28} Analogous arguments and results have also been proposed for the elastodynamic case.\textsuperscript{29, 30} The central idea in this approach is that the traveling

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wave experiences the averaged properties of the microstructure. Therefore, it becomes imperative to define these averaged properties in a consistent manner in order to be able to explain and predict wave propagation characteristics in such materials. There has been recent interest in the field of dynamic homogenization which seeks to define the averaged material parameters which govern electromagnetic/elastodynamic mean wave propagation. \cite{31-36} Subsequent efforts have led to effective property definitions which satisfy both the averaged field equations and the dispersion relation of the composite. \cite{37-42} In the present paper, we show that the effective properties thus defined become negative in the presence of local resonances, thereby capturing the dynamic effect first anticipated by Veselago \cite{24} for the electromagnetic waves. Although the current treatment concerns 1-D composites, it is expected that the physical intuition gained will help to design 3-D composites with extreme material property profiles.

II. EFFECTIVE DYNAMIC PROPERTIES FOR LAYERED COMPOSITES

A brief overview of the effective property definitions is provided here for completeness (see \cite{39} for details). For harmonic waves traveling in a layered composite with a periodic unit cell $\Omega_1 = \{ x: -a/2 \leq x < a/2 \}$ the field variables (velocity, $\hat{u}$, stress, $\hat{\sigma}$, strain, $\hat{\epsilon}$, and momentum, $\hat{p}$) take the following Bloch form:

$$\hat{F}(x, t) = \text{Re} \left[ F(x) e^{i(qx - \omega t)} \right]$$

Field equations are

$$\frac{\partial \hat{\sigma}}{\partial x} + i\omega \hat{p} = 0; \quad \frac{\partial \hat{u}}{\partial x} + i\omega \hat{\epsilon} = 0$$

We define the averaged field variable as

$$\langle \hat{F} \rangle(x) = \langle F \rangle e^{i qx}; \quad \langle F \rangle = \frac{1}{a} \int_{-a/2}^{a/2} F(x) dx$$

where $F(x)$ is the periodic part of $\hat{F}(x, t)$. In general, the following constitutive relations hold

$$\langle \epsilon \rangle = D \langle \sigma \rangle + S_1 \langle \dot{u} \rangle; \quad \langle p \rangle = S_2 \langle \sigma \rangle + \rho \langle \dot{u} \rangle$$

with nonlocal space and time parameters. For Bloch wave propagation, the above can be reduced to

$$\langle \epsilon \rangle = D^{\text{eff}} \langle \sigma \rangle; \quad \langle p \rangle = \rho^{\text{eff}} \langle \dot{u} \rangle$$

$$D^{\text{eff}} = \frac{\tilde{D}}{1 + v_p S_1} = \frac{iq \langle \dot{u} \rangle}{\langle \sigma \rangle}; \quad \rho^{\text{eff}} = \frac{\tilde{\rho}}{1 + v_p S_2} = \frac{\langle p \rangle}{-i\omega \langle u \rangle}$$

where $v_p = \omega q = [D^{\text{eff}} \rho^{\text{eff}}]^{-1/2}$ defines the phase velocity and the dispersion relation. These effective properties satisfy the averaged field equations and the dispersion relation. These definitions have been extended to the full 3-D case using micromechanics. \cite{42}

III. EFFECTIVE PROPERTIES OF 2-PHASE COMPOSITES

A mixed-variational formulation is used to calculate the band-structure and modeshapes for the layered composites (see appendix) which are required to calculate the effective properties.

Fig. 1 shows the effective properties calculated for the first two pass-bands of a 2-phase layered composite. Each phase is 5mm thick and the material properties of the phases are

1. \( E_{P1} = 2 \times 10^9 \text{ Pa}; \quad \rho_{P1} = 1000 \text{ kg/m}^3 \)
2. \( E_{P2} = 200 \times 10^9 \text{ Pa}; \quad \rho_{P2} = 3000 \text{ kg/m}^3 \)

where $E$ is the stiffness, $\rho$ is the density, and $P1$ and $P2$ denote phases 1 and 2, respectively. It is seen that the static values (0 frequency) of the effective parameters emerge as the dominant averages of the material properties. The non-dispersive nature of the parameters in the low frequency regime is reflected by the fact that the long wavelength waves are not affected by the microstructure. While
both density and compliance are simultaneously real and positive in the pass-bands, one of these is negative in the stop-bands (not plotted), thereby precluding the existence of propagating waves for the associated frequency ranges. Even if we only consider the pass-bands, it is still possible to have complex effective density and compliance for purely elastic but asymmetric unit cells. It doesn’t seem possible, however, to obtain simultaneously negative properties without resorting to local resonances even for the cases where a great impedance mismatch exists between the two phases.

IV. EFFECTIVE PROPERTY OF 3-PHASE COMPOSITES

Consider a unit cell, built on the physical intuition suggested in. Fig. 2 shows the unit cell of a 3-phase composite. The central heavy and stiff phase can resonate locally if the second phase is sufficiently compliant. The total thicknesses of phase 1, 2, and 3 in the calculations which follow, are 2.9 mm, 1 mm, and 0.435 mm respectively.

A. Simultaneously negative density and compliance

Fig. 3 shows the effective properties calculated for the first two pass-bands of four different 3-phase unit cells, each with an increasingly compliant second phase. As the compliance of the second phase is increased, the first two branches move to the lower frequency regime and the effective properties become negative over a fraction of the second pass-band, which increases with increasing second-phase compliance. Since the calculated effective properties are real and negative in the pass-bands, they reflect the propagating nature of the bands, precisely satisfying the dispersion relation, \((\omega/q)^2 = 1/(D_{\text{eff}} \rho_{\text{eff}})\).
As expected, the existence of simultaneously negative parameters is highly sensitive to the density of $P_3$ and the compliance (stiffness) of $P_2$. The resonance is also contingent upon adequate stiffness mismatch between $P_2$ and $P_3$ whereas it is largely independent of the geometric and material parameters of $P_1$. These relations are more evident in the limiting regime where the definition of effective mass is easily established.

B. Limiting case of a spring-mass system

Consider the one-dimensional model of Fig. 4 where a cylindrical cavity has been carved out of a rigid bar of mass $M_0$. Another rigid body of mass $m$ is placed within the cavity and connected to the walls of the cavity by springs of a common stiffness $K$. 

A harmonic force with frequency $\omega$ is applied to the bar. The macroscopic force $F(t)$ is related to the macroscopic acceleration of the rigid bar with the effective mass of the system. This frequency-dependent effective mass is given by,

$$M_{\text{eff}} = M_0 + \frac{m\omega_0^2}{\omega_0^2 - \omega^2}$$

where $\omega_0 = \sqrt{2K/m}$ is the resonant frequency of the system. $M_{\text{eff}}$ increases with increasing frequency up to the resonant frequency, at which point it becomes infinite. Beyond the resonant frequency $M_{\text{eff}}$ begins at negative infinity and approaches $M_0$. Now consider again the unit cell of Fig. 2 and use the following material properties:

1. $E_{P1} = 870 \times 10^9 \text{ Pa}; \rho_{P1} = 2000 \text{ kg/m}^3$
2. $E_{P2} = 2 \times 10^8 \text{ Pa}; \rho_{P2} = 5 \text{ kg/m}^3$
3. $E_{P3} = 320 \times 10^9 \text{ Pa}; \rho_{P3} = 8000 \text{ kg/m}^3$

$P_1$ and $P_3$ are rigid compared to $P_2$, and $P_2$ can be assumed to be massless. The equivalent spring constant for $P_2$ is $E_{P2}/l_2$ where $l_2 = 1/2 = .5 \text{ mm}$ is the thickness of one layer of the phase. The mass of $P_3$ is $l_3\rho_{P3}$ where $l_3 = 0.435 \text{ mm}$ is the thickness of the central layer. With these values, the resonant frequency $f = \sqrt{2K/m}/2\pi$ of the system is approximately 76 kHz. Fig. 5 shows the effective density for the corresponding first two pass-bands. It is seen that the variation of $\rho_{\text{eff}}$ is essentially congruent to the variation of $M_{\text{eff}}$ for the ideal case. At approximately 76 kHz, $\rho_{\text{eff}}$ increases towards infinity. Beyond this frequency, starting from negative infinity, it approaches zero. There is a stop-band in Fig. 5 which is not present in Eq. (6) and reflects the fact that the system in Fig. 4 is a finite system, while the example of Fig. 5 corresponds to an infinite periodic composite.

### C. Inclusion of dissipation

We now consider the effect of including damping in the system on the negative characteristics of the 3-phase composite. Consider the example of Fig. 3(d) where damping has been introduced in the three phases. Damping is introduced as an additional imaginary part to the elastic modulus. Although sophisticated damping models may be used, we use a constant imaginary part (as a small percent of the real part) for the present purpose. Fig. 6 shows the effective property calculations for the damped layered composite. For the damped case, both the effective density and the effective compliance assume complex values, consistent with the fact that there are no clear pass-bands or stopbands. Fig. 6 shows the real parts of the effective properties. Comparing the results with Fig. 3 it may be verified that the effective properties calculated for the small damping case (1 percent) are very close to those of the undamped composite. Increasing the damping considerably affects the
FIG. 5. Effective density for the limiting case.

FIG. 6. Effective properties (real parts) for the damped layered composite. a. Effective density, b. Effective compliance

properties in the region close to the resonance. Away from the resonance, however, the effect of damping on the real parts of the properties are minimal.

V. DISCUSSION

Characterization of the effective dynamic properties of heterogeneous composites is more complex than of their static properties. The average dynamic properties are non-local in space and in time, and are generally non-unique. Still, for frequency-wavenumber pairs that satisfy the dispersion relations of 1-D composites, the non-unique constitutive relation can be transformed into a form with vanishing coupling parameters. The coefficients of this constitutive form ($D_{\text{eff}}$, $\rho_{\text{eff}}$ in this paper) are uniquely determined from the microstructure and satisfy the averaged field equations and the dispersion relations of the composite. For composites with symmetric unit cells,
these parameters in general are real-valued and positive on the pass-bands. They are complex-valued for composites which have an asymmetric unit cell. For these unit cells, it is generally not easy to achieve simultaneously real-valued and negative parameters. This paper explores the special cases which are expected to give rise to simultaneously negative effective values of density and stiffness (compliance), and shows that the constitutive form developed in\textsuperscript{39} adequately captures the physics of internal resonances.

Recent research has also led to the definition and computation of effective dynamic properties for the 3-D case.\textsuperscript{42} The exact nature of these effective tensors for composites with internal resonances remains to be studied. It is envisaged that the intuition gained from the present work would help to design real 3-D composites which would display extreme material properties at predicted frequencies.

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APPENDIX A: MIXED METHOD FOR CALCULATION OF EIGENMODES OF PERIODIC COMPOSITES

Consider harmonic waves in an unbounded periodic elastic composite consisting of a collection of unit cells, $\Omega$. In view of periodicity, we have $\rho(x) = \rho(x + m' I^\beta)$, and $C^{jkmn}(x) = C^{jkmn}(x + m' I^\beta)$, where $x$ is the position vector with components $x_j$, $j = 1, 2, 3$, $\rho(x)$ is the density and $C^{jkmn}(x)$, $(j, k, m, n = 1, 2, 3)$ are the components of the elasticity tensor in Cartesian coordinates. $m'$ is any integer and $I^\beta$, $\beta = 1, 2, 3$, denote the three vectors which form a parallelepiped enclosing the periodic unit cell.

For time harmonic waves with frequency $\omega$ ($\lambda = \omega^2$), the field quantities are proportional to $e^{\pm i \omega t}$. The field equations become

$$\sigma_{jk,k} + \lambda \rho u_j = 0; \quad \sigma_{jk} = C^{jkmn} u_{m,n} \tag{A1}$$

For harmonic waves with wavevector $q$, the Bloch boundary conditions take the form

$$u_j(x + I^\beta) = u_j(x)e^{i q I^\beta}; \quad t_j(x + I^\beta) = -t_j(x)e^{i q I^\beta} \tag{A2}$$

for $x$ on $\partial \Omega$, where $t$ is the traction vector.

To find an approximate solution of the field equations (Eq. (A1)) subject to the boundary conditions (Eq. (A2)), we consider the following expressions:

$$\bar{u}_j = \sum_{\alpha, \beta, \gamma = -M}^{+M} U^{(q_{\alpha\beta\gamma})} f^{(q_{\alpha\beta\gamma})}(x) \tag{A3}$$

$$\bar{\sigma}_{jk} = \sum_{\alpha, \beta, \gamma = -M}^{+M} S^{(q_{\alpha\beta\gamma})} f^{(q_{\alpha\beta\gamma})}(x) \tag{A4}$$

where the approximating functions $f^{(q_{\alpha\beta\gamma})}$ are continuous and continuously differentiable, satisfying the Bloch periodicity conditions. The eigenvalues are obtained by rendering the following functional stationary:

$$\lambda_N = (\langle \sigma_{jk}, u_{j,k} \rangle + \langle u_{j,k}, \sigma_{jk} \rangle - (D^{jkmn}\sigma_{jk}, \sigma_{mn})) / \langle \rho u_j, u_j \rangle \tag{A5}$$

where $\langle gu_j, v_j \rangle = \int_{\Omega} g u_j v_j^* dV$, with star denoting complex conjugate, and $D^{jkmn}$ are the components of the elastic compliance tensor, the inverse of the elasticity tensor $C^{jkmn}$.

Substituting Eq. (A3) and (A4) into Eq. (A5) and equating to zero the derivatives of $\lambda_N$ with respect to the unknown coefficients $U^{(q_{\alpha\beta\gamma})}$ and $S^{(q_{\alpha\beta\gamma})}$, we arrive at the following set of linear
homogeneous equations:

\[ \langle \bar{\sigma}_{jk} + \lambda N \rho \bar{u}_j, f^{(\alpha\beta\gamma)} \rangle = 0; \quad \langle D_{jkmn} \bar{\sigma}_{mn} - \bar{u}_j, f^{(\alpha\beta\gamma)} \rangle = 0 \]  

(A6)

There are \(6M_p^3\) \((M_p = 2M + 1)\) equations in Eq. (A6)\(^2\) for a general 3-directionally periodic composite. They may be solved for \(S^{(\alpha\beta\gamma)}\) in terms of \(U^{(\alpha\beta\gamma)}\) and the result substituted into Eq. (A6)\(^1\). This leads to a system of \(3M_p^3\) linear equations. The roots of the determinant of these equations give estimates of the first \(3M_p^3\) eigenvalue frequencies. The corresponding eigenvectors are \(U_j^{(\alpha\beta\gamma)}\) from which the displacement field within the unit cell is reconstituted. The stress variation in the unit cell is obtained from Eq. (A6)\(^2\).

1. Example: A 2-layered composite

To evaluate the effectiveness and accuracy of the mixed variational method, consider a layered composite (Fig. 7) with harmonic longitudinal stress waves traveling perpendicular to the layers. The displacement, \(u\), and stress, \(\sigma\), are approximated by

\[ \bar{u} = \sum_{a=-M}^{+M} U^{(a)} e^{i(q_a + 2\pi nx/a)}, \quad \bar{\sigma} = \sum_{a=-M}^{+M} S^{(a)} e^{i(q_a + 2\pi nx/a)} \]  

(A7)

In the above equations, \(a\) is the periodicity length. Substituting these into Eq. (A6)\(^2\) we obtain \(S^{(a)}\) in terms of \(U^{(a)}\). The resulting equations are then substituted into Eq. (A6)\(^1\), providing a set of \(M_p\) linear homogeneous equations, the roots of whose determinant give the first \(M_p\) eigenvalue frequencies for a given wavenumber \(q\).

The exact dispersion relation for 1-D longitudinal wave propagation in a periodic layered composite has been given by Rytov:

\[ \cos(qa) = \cos(\omega h_1/c_1) \cos(\omega h_2/c_2) - \Gamma \sin(\omega h_1/c_1) \sin(\omega h_2/c_2) \]  

(A8)

\[ \Gamma = (1 + \kappa^2)/(2\kappa); \quad \kappa = \rho_1 c_1/\rho_2 c_2 \]  

(A9)

where \(h_i\) is the thickness, \(\rho_i\) is the density, and \(c_i\) is the longitudinal wave velocity of the \(i\)th layer \((i = 1, 2)\) in a unit cell. In Fig. 8 we compare the frequency-wavenumber dispersion relations obtained by this mixed variational method and the exact solution.

The first five modes calculated from the mixed variational formulation are shown in Fig. 8. The accuracy of the results calculated from the mixed method depend upon the number of the Fourier terms used in the approximation \((M_p)\). For the case of Fig. 8, they are very close to the exact solution. Since the exact dispersion relations are available for only fairly simple geometries like layered composites, the mixed variational formulation provides an attractive and effective method.
FIG. 8. Frequency-wavenumber dispersion relations calculated from the mixed variational formulation. \( M_p = 21 \) terms are used in Fourier expansion.

to calculate the eigenfrequencies and eigenvectors associated with three-dimensionally periodic composites.