Modulating Elastic Band Gap Structure in Layered Soft Composites Using Sacrificial Interfaces

Qianli Chen
Department of Civil and Environmental Engineering, University of Illinois at Urbana Champaign, Champaign, IL 61801

Ahmed Elbanna
Department of Civil and Environmental Engineering, University of Illinois at Urbana Champaign, Champaign, IL 61801

A wide range of engineered and natural composites exhibit a layered architecture whereby individual building blocks are assembled layer by layer using cohesive interfaces. We present a novel mechanism for evolving acoustic band gap structure in a model system of these composites through patterning the microstructure in a way that triggers nonplanar interfacial deformations between the layers as they are stretched. Through the controlled deformation and growth of interlayer channels under macroscopic tension, we observe the emergence of multiple wide band gaps due to Bragg diffraction and local resonance. We describe these phenomena in details for three example microstructures and discuss the implications of our approach for harnessing controlled deformation in modulating band gap properties of composite materials. [DOI: 10.1115/1.4034537]

1 Introduction

Layered composites are frequently found as building blocks of tough biological structures [1–4]. Among those, bone is a typical example exhibiting remarkable combination of stiffness and toughness [5]. The basic building block of bone at the microscale is the mineralized collagen fibril (MCF) in which the soft collagen matrix is reinforced by stiff hydrated calcium phosphates [6]. The MCFs are glued together using interfaces of noncollagenous proteins with sacrificial bonds and hidden length to form a layered structure [7–10]. Another example of a layered structure is sea-shell nacre which endows dramatic improvement of stiffness and toughness compared to its constituent phases independently [11]. The enhancement of toughness in those biological materials is partially attributed to wavy surfaces and cohesive interaction along the interfaces between bulk materials [12–14]. These interfaces are sacrificial in the sense that they represent weak spots where energy gets dissipated by progressive accumulation of damage while the rest of the composite remains intact and elastic. The naturally optimized properties of stiffness, strength, and toughness, suggest that there is a link between geometric patterning, sacrificial interfaces, and improved mechanical performance. More recently, it has also been hypothesized that the origin of these improved properties, in a composite like bone, for example, may be linked to the ability of generating multiple band gaps [15].

Composite materials with periodic microstructure are capable of generating a band gap structure through which elastic and acoustic wave propagation may be controlled [16–20]. Waves with frequencies falling into the band gap are barred by the periodic structure. The band gap phenomenon in composite material is caused by two mechanisms: Bragg diffraction and local resonance [21,22]. The Bragg diffraction occurs when the elastic wavelength is comparable to the periodicity of the microstructure. The position and the width of the band gap may be controlled by careful design of the microstructure materials [23–26]. Moreover, mechanically triggered large deformation [27] and instability-induced interfacial wrinkling [28,29] are found of capacity to tune the evolution of band gap profile. Local resonance happens when the phases of composite material have strong elastic properties contrast. Banded frequencies caused by local resonance are generally lower than those caused by Bragg diffraction [30] and may exist even in the absence of periodicity and symmetry [21,31]. Designing such band gap structures enables the application in wave filtering, wave guiding, acoustic mirrors and vibration isolators [32–38].

We showed in an earlier paper that a bone-inspired composite, with patterned heterogeneity, exhibits the capacity of generating tunable corrugation under externally applied concentric tension [39]. By stacking 1D fibers, with the designed microstructure, to form layered composites, these corrugations collectively lead to the formation of interlayer channels with shapes and sizes tunable by the level of stretch (Fig. 1). In this paper, we demonstrate an application of harnessing this design in evolving the elastic band gap structure in these composites. A unique feature of our design is the dynamic evolution of the structural composition as a function of stretch and inclusion distribution. In particular, an additional phase, namely voided channels, gradually emerge (disappear) with increasing (decreasing) stretch despite being absent at zero stretch.

2 Model and Results

We consider layered composites made up of stacks of fibrils that are glued along their longer dimension as shown in Fig. 1. We choose fibril thickness \( t = 30 \mu m \), length of inclusion \( L = 75 \mu m \), inclusion thickness \( t = 7.5 \mu m \), inclusion spacing \( S = 40 \mu m \), and inclusion eccentricity from center line of fibril \( c = 4.5 \mu m \) [39]. Three examples of inclusion patterns are discussed: (a) nonstaggered aligned inclusions (Fig. 1(a)), (b) staggered identical inclusions (Fig. 1(b)), and (c) staggered symmetric inclusions (Fig. 1(c)). An extensive analysis of the effect of geometry and material properties on the response of these composites under longitudinal (along \( x \)-axis in Fig. 1) stretch are reported in our previous paper [39]. In general, the corrugation amplitude increases with the stiffness of inclusion and its eccentricity from the local tension axis.

The unit cell is discretized using eight-node bi-quadrilateral elements (Q8). We run the basic stretch analysis and band gap calculations in an in-house MATLAB code for finite-deformation elasticity. The dynamic wave propagation verification simulation is run by the commercial finite-element software ABAQUS. The two phases are modeled using Neo-Hookean hyperelastic material model. The silicon inclusion has Young’s modulus of \( E_s = 170 \text{ GPa} \), Poisson’s ratio \( \nu_s = 0.064 \), and density \( \rho_s = 2300 \text{ kg/m}^3 \). The matrix material is modeled as polydimethylsiloxane (PDMS) with initial
Young’s modulus of $E_m = 750$ kPa, Poisson’s ratio of 0.495, and density $\rho_m = 1000$ kg/m$^3$. This combination of materials were used in our previous experiment [40]. Reduced integration is applied for quadrature and the nonlinear problem is solved with full Newton Raphson method. Elastic band structure calculations are executed for a unit cell in the deformed configuration, and thus, the dimensions of the Brillouin zone are updated accordingly with Craig–Bampton mode decomposition, and Bloch boundary conditions are then applied [41]. The formulas for finite element method (FEM) and block wave calculations are summarized in the Appendix.

The interaction between two composite fibrils is simulated by a traction–separation law with equivalent Young’s modulus of $E_{coh} = 1$ kPa, Poisson’s ratio $\nu_{coh} = 0.495$, and initial thickness $t_{coh} = 1$ mm. Then, we have equivalent normal stiffness $K_n = E_{coh}t_{coh}/t_{coh}$ and shear stiffness $K_s = E_{coh}t_{coh}/[2t_{coh}(1 + \nu_{coh})]$, where $t_{coh}$ is the out-of-plane thickness of fibril. In this paper, we use the bilinear law (Eq. (A7)) for simplicity but the qualitative nature of the results depends weakly on the specific form and properties of the cohesive law. To investigate the influence of the interfaces, the responses of both monolithic (i.e., no interfaces) and layered systems (with interfaces) under uniaxial stretch along x-axis in Fig. 1 are simulated and compared.

Three monolithic composites with inclusions are modeled and served as reference groups for comparisons. Unlike the layered system there are no interfaces in the monolithic case. The monolithic nature of matrix material stiffens the overall composite response. The Bloch wave analysis reveals that no elastic band-structure behavior is found except in case (c) where a narrow band gap of width 0.008 MHz appears near 0.26 MHz (Fig. 2).

The introduction of interfaces enables more complex deformation patterns and richer elastic band gap structure. In the case of the nonstaggered inclusion pattern (case a), the fibrils shrink in
the transverse direction, within the region of pure PDMS, more than in the regions where the silicon inclusions exist. In cases (b) and (c), corrugation develops due to the eccentricity of inclusions. Channels, of different shapes and orientations, form as stretch level increases because of different stacking patterns. All three cases show deformed wavy surface under uniaxial stretch along x-axis in Fig. 1, and this alters the dispersion property of unit cell. Unlike in the monolithic cases, the layered composites have band gaps at the undeformed state and are able to develop richer behavior after stretch.

2.1 Case (a) Composite With Nonstaggered Inclusions. Figure 3(a) reveals that there exist multiple wide elastic band gaps at zero strain. As stretch increases, some of the smaller bandgaps disappear and other bandgaps become even wider (Fig. 4(a)). To understand the origin of the band gaps in this case, it is illuminating to analyze the eigenmode deformation. For that purpose, selected eigenmodes are plotted to the right of the dispersion curves. Most of these eigenmodes suggest that the deformation is mainly concentrated within soft matrix material representing a local resonance behavior. Few exceptions exist. For example modes D, F, and D' show distributed deformations where the inclusions also vibrate due to Brag scattering. While in mode F' the deformation is localized in the matrix but the influence of the channel is apparent: the deformation is concentrated close to the channel tips. Furthermore, the dispersion lines along the vertical propagation direction Y – Γ are almost flat signifying very low group velocities. This is due to the existence of the horizontal cohesive interfaces with low stiffness values that slow down wave propagation across them. Finally, eigenmodes of the composite in this inclusion pattern keep their general shape as stretch grows but the corresponding eigenfrequencies change.

2.2 Case (b) Composite With Identical Staggered Inclusions. Figure 3(b) shows examples of the band gap structure in this case. Fewer band gaps exist compared to case (a) and they mostly arise due to local resonance in the PDMS matrix. Once again, the effect of channel development is apparent where deformations are banded parallel and normal to their locations. Furthermore, the dispersion relations are altered significantly by deformation, unlike in case (a). This is primarily due to the complex growth of the interfacial channels.

2.3 Case (c) Composite With Symmetrically Staggered Inclusions. Figure 3(c) shows examples of the band gap structure in this case. Unlike the previous cases, no band gaps develop at zero strain. Also the dispersion lines along the vertical propagation direction Y – Γ are not as flat as in cases (a) and (b) above. This is attributed to the development of contact between the layers upon bending. The composite is thus continuous through contact region and waves may propagate across the horizontal interfaces at the speed allowed by the matrix material. We also note that the eigenmode analysis reveals that the deformation at the boundaries of the band gap is localized near the nonplanar features of the channels, signifying the influence of the complex evolution of the interfacial separation.

The band gap evolution as a function of stretch is shown in Fig. 4. As previously discussed, multiple band gaps develop as stretch level increases. The composite with nonstaggered inclusions (case (a)), shows multiple wide band gaps above 0.13 MHz at all levels of stretch. For case (b), four clusters of band gaps initially exists near frequencies 0.16, 0.23, 0.33, and 0.35 MHz, respectively. As stretch increases, the band gap near 0.16 MHz becomes wider and moves to higher frequency while the other three close. Near stretch levels of 1.15 and 1.17, two band gaps open at frequency 0.26 and 0.28 MHz, respectively, but they are generally smaller than the lower frequency band gap. For case (c), a band gap appears after stretch of 1.05 near 0.2 MHz and opens up to width of 0.04 MHz as the stretch level increases.

The opening and closure of band gaps as a function of deformation may be explained as follows. Due to the hyperelastic nature of the matrix material, the matrix material undergoes stiffness softening as stretch grows. Stiffness changes nonuniformly among the bulk constituents with stretch since the matrix experiences the most changes while the silicon inclusion remains almost linear elastic with constant stiffness. The variability of the band gap width is due to the competition between stiffness changes as the hyperelastic material is changed and the evolving geometry due to the nonuniform deformation of the interfaces which lead to complex channel shapes and scattering response.

As a verification of band gap behavior, we examine the transmission plots for the composite with staggered inclusion pattern (case (b)) as an example. Nine unit cells are connected together in the longitudinal direction, and periodic boundary condition is applied to the upper and lower boundaries of those cells to create...
a semifinite composite system. We connect one end of the composite system to infinite elements to absorb waves and apply stretch and vibration at the other end. The finite-element analysis proceeds as follows. We first stretch the composite to the required level. Then, we apply a small amplitude vibration (less than 1% of the stretch amplitude) at the stretched end. We compute the transmission ratio as the ratio of the vibration amplitude at the interface of the composite with the infinite elements to the applied
vibration amplitude at the stretched end. Two scenarios are presented in Fig. 5, one at stretch of 1.10 where no band gap has shown up between 0.2 MHz and 0.3 MHz, and one at stretch of 1.30, where there are two band gaps near 0.26 MHz and 0.28 MHz. From Fig. 5(b), we may observe that for both stretch levels, shear waves are attenuated above 0.25 MHz. However, for the longitudinal waves (Fig. 5(a)), the attenuation is most noticeable below 0.24 MHz and above 0.29 MHz for the stretch level of 1.10 but it is coincident with the band gap region at stretch level of 1.30. That is, while longitudinal and shear waves may each attenuate at frequencies outside the band gap, it is only within the band gap that the amplitudes of both types of waves are significantly reduced simultaneously.

3 Discussion

We have numerically demonstrated the capability of modulating band gap structure in soft composites using sacrificial interfaces. While several approaches have been used previously to achieve this purpose, including designing of hierarchical composite structure [23,37], triggered instabilities in monolithic periodic material [27,42], and instability-induced interfacial wrinkling [28,29], this is the first time, to the best of our knowledge, that sacrificial interfaces with controlled damage behavior is used to tune the band gap behavior.

The introduction of interfaces to a monolithic composite enriches the deformability of the system and provides a mean to create and alter the band gap structure. The interfacial deformation along composite fibrils is controlled by the inclusion pattern. Nonstaggered (case a) and staggered symmetrical (case c) inclusion patterns result in the formation of parallel horizontal array of holes in aligned and staggered manners, respectively, while the staggered inclusion pattern (case b) leads to oblique orientation of holes. In all cases, the composite geometry is evolving gradually. The layered nature of the composite makes the group velocity of vertical wave approach zero in case (a) and (b). The contact between the fibrils promote relatively faster group velocities.

The eigenmodes of unit cell indicate that the band gap evolution in our system is facilitated by both Bragg diffraction and local
resonance. The interfacial channels represent a new periodic inclusion of degrading stiffness and irregular boundary geometry. The periodicity of the channels provides additional diffraction paths for wave propagations. Moreover, wave reflection and refraction at the channel/matrix interface is opposite in polarity to wave propagations. Furthermore, even if the interface remains damaged, the channels nucleate and grow to complex irregular shapes that interfere with the wave propagation and cause more complex behavior and possibly more frequency band gaps than composites with regular holes or cuts [42,45,46].

In general, band gaps of the composite fibril system shows rich and controllable band gap behavior than the monolithic composite where no band gap shows up even with the same inclusion pattern as the layered composite (except for a tiny band gap in case (c)). It is the interaction between the inclusion pattern and the sacrificial interfaces which manipulate wave diffraction and interference leading to the creation of multiple frequency band gaps. For the cases considered in this paper, we show that the band gaps exist at initial stretch-free state and can be modulated through stretch level. Multiple wide band gaps are observed in nonstaggered inclusion pattern (case a) making it very efficient for wave attenuation. For the other two cases, band gap are also wide but not as rich as the case (a). For all three cases, the introduction of interfaces and deformation-caused stiffness redistribution plays essential roles in the evolution of these band gaps.

Future extension of this study will involve investigation of further applications and optimization of the tunable band gap structure. For example, the emergence of multiple band gaps under large stretch may have applications in wave filtering, sound isolation, and vibration damping. Furthermore, the width of the band gaps may be maximized through topology optimization so that the tunable band gaps, observed in the current study, may extend over wider regions of frequencies. Finally, the connection between band gap structure and the effective toughness of the composite material is a topic that requires further exploration. In particular, it may be possible, through careful designing of the inclusion pattern and sacrificial interfaces, to be able to control crack nucleation and propagation by varying the band gap structure in the composite as a function of deformation.

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Appendix: Constitutive Laws

The material deformation is described as a mapping from reference configuration $X$ to the deformed configuration $x$

$$x = \gamma(X,t)$$  \hspace{1cm} (A1)

The displacement of a material point form is

$$u = x - X = \gamma(X,t) - X$$ \hspace{1cm} (A2)

The deformation gradient tensor is defined as

$$F = \frac{\partial x}{\partial X} = I + \frac{\partial u}{\partial X}$$ \hspace{1cm} (A3)

where $I$ is the identity matrix, and its Jacobian is $J = \det(F)$.

Two different soft materials are building up the composite (Fig. 1). Each material is assumed to be homogeneous and isotropic with hyperelastic response. We use the generalized Neo-Hookean solid [47,48] model with strain energy density proposed by

$$W = \frac{\mu}{2} (I_1 - 3) + \frac{K}{2} (J - 1)^2$$ \hspace{1cm} (A4)

where $I_1 = I_1/J^{2/3}$ making it more convenient for nearly incompressible materials, $\mu$ and $K$ are the shear modulus and bulk modulus of the material, respectively.

The stress–strain relation and tangent stiffness follow as

$$\sigma = \frac{\mu}{J^{5/3}} \left( B - \frac{1}{3} I_1 I \right) + K (J - 1) I$$ \hspace{1cm} (A5)

and

$$C_{ijkl} = \frac{\mu}{J^{3/2}} \left[ \delta_{ij} B_{kl} + \delta_{kl} B_{ij} - \frac{2}{3} (\delta_{il} B_{kj} + \delta_{lj} B_{ik}) + \frac{2}{3} I_1 \delta_{ij} \delta_{kl} \right] + K (2J - 1) I \delta_{ij} \delta_{kl}$$ \hspace{1cm} (A6)

Cohesive Interaction for the Layered Composite. The interaction between two composite fibrils is simulated by a traction–separation relation. In this paper, we use the bilinear law for simplicity but the qualitative nature of the results depends weakly on the specific form of the cohesive law. The two-dimensional bilinear cohesive law is defined by [49,50]

$$T_{n,i} = \begin{cases} K_{n,i} \delta_n, & \delta \leq \delta_t, \\ K_{n,i} \delta_n - \frac{1}{2} \delta_t \frac{\delta_n}{\delta_t} \delta_t, & \delta_t \leq \delta \leq \delta_f, \\ 0, & \delta \geq \delta_f \end{cases}$$ \hspace{1cm} (A7)

where $T_{n,i}, K_{n,i}, \delta_t, \delta_f$ is the normal or tangent traction, stiffness, and separation, respectively. $\delta$ is the magnitude of total separation given by $\delta = \sqrt{\delta^2 + \delta_t^2}$, and $\delta_t$ and $\delta_f$ determine the damage initialization and complete failure, respectively (Fig. 6).

Figure 7 shows the effect of varying the cohesive interface equivalent Young’s modulus on the band gap profile of the composite with the nonstaggered inclusion pattern (Case a) at a stretch-free state. In this case of zero elongation, since the cohesive material remains intact along the whole interface, the band gap profile is only affected by the elastic normal and shear stiffness of the layer and not its softening response. The results in Fig. 7 suggest that the band gap width decreases as the equivalent Young’s modulus of the cohesive interface increases. The dispersion lines plot converges to the monolithic composite case (Fig. 2(a)) as the modulus increases. Indeed, when $E_{coh}$ is infinitely

![Fig. 6 Bilinear cohesive law of inter-fibril interaction](image-url)
large (which is equivalent to imposing a rigid constraint between the two points on the opposite side of the interface), we will get exactly the same result in Fig. 2(a) where interface no longer exists.

Wave Propagation. The equations of motion are given by

\[ \frac{\partial \sigma}{\partial x} = \rho \frac{\partial^2 u}{\partial t^2} \]  \hspace{1cm} (A8)

in absence of body force, where \( \sigma \) is the Cauchy stress, and \( \rho \) is the density which varies for different material in composite.

The propagation of elastic wave in periodic composites may be analyzed by Bloch’s theorem [51] and further developed in the following way [52]. We start by decomposing the solution as

\[ u(X,t) = U(X) e^{-i\omega t} \]  \hspace{1cm} (A9)

where \( U(X) \) is a complex valued function of \( X \). Accordingly, we also have the following decomposition for stress

\[ \sigma(X,t) = \Sigma(X) e^{-i\omega t} \]  \hspace{1cm} (A10)

Equation (A8) now becomes

\[ \frac{\partial \Sigma}{\partial x} - \rho \omega^2 U \]  \hspace{1cm} (A11)

Due to periodicity, the displacement is constrained by

\[ U(X) = U(X+L)e^{-i\kappa L} \]  \hspace{1cm} (A12)

where \( L \) is the vector connecting equivalent points in periodic structure, \( \kappa \) is the wave vector contain the information of wavelength and direction.

Similarly, the stress also satisfies

\[ \Sigma(X) = \Sigma(X+L)e^{-i\kappa L} \]  \hspace{1cm} (A13)

which is satisfied by applying the constrain of displacement under FEM discretization.

The wave vector is chosen from the first Brillouin zone in reciprocal lattice for the representative unit cell as shown in Fig. 7. The reciprocal lattice is defined by base vectors \( \mathbf{R}_1 \) and \( \mathbf{R}_2 \) and

\[ R_1 = \frac{2\pi}{a} \frac{A_2 \times e}{a}, \quad R_2 = \frac{2\pi}{a} \frac{e \times A_1}{a} \]  \hspace{1cm} (A14)

where \( A_1 \) and \( A_2 \) are base vector in direct lattice (Fig. 1), \( a = ||A_1 \times A_2|| \), and \( e = (A_1 \times A_2)/a \) so that

\[ R_i A_j = 2\pi \delta_{ij} \]  \hspace{1cm} (A15)

It is suggested in the literature that the band gap information may be obtained by surfing only the points along boundaries of this zone [53]. While this is not rigorously proven, we adopt the same procedure in the current paper (Fig. 8).

The wave propagation response is analyzed by solving the eigenvalue problem of

\[ K - \omega^2 M = 0 \]  \hspace{1cm} (A16)

The matrices \( K \) and \( M \) are the tangent stiffness and mass matrices generated from the standard finite-element nonlinear analysis at different stretch level. The displacement constrain of Eq. (A12) should be applied to both \( K \) and \( M \) before solving the eigenvalue problem. Mode decomposition can then be used to accelerate the computation process [41].

References


