SOFT MODES IN NONLINEAR COMPOSITES ON THE EDGE OF ELASTIC INSTABILITY

Pavel I. Galich and Edwin L. Thomas

Department of Materials Science and NanoEngineering, Rice University, Houston, TX, US
email: pg28@rice.edu

Nonlinear composites, allowing large reversible geometry changes, have already been shown to have remarkable deformation-induced phononic properties, such as negative group velocity, asymmetric transmission, and distinct types of band gaps. The emergence of advanced electro- and magneto-elastic materials have also enabled control of the propagation of phonons by application of electric and magnetic fields, respectively, to induce symmetry changes that enhance the functionality spectrum of nonlinear composites. While many researchers have investigated the phononic properties of composites after the onset of elastic instability, there are very few studies analyzing the propagation of phonons in the nearly unstable (but still stable) composites. To the best of our knowledge, thus far, only layered and fiber composites on the edge of elastic instability have been investigated. We extend previous numerical studies to more complex periodic composites possessing p4mm plane group. Using 2D periodic geometries, we demonstrate that nearly unstable nonlinear composites possess an exciting potential for tuning phonon propagation. Specifically, in the vicinity of the elastic instability, the lowest phononic mode starts to “soften”, i.e. the frequency of this mode tends to zero for a particular wavenumber, with increased strain. In the physics of crystals, a “soft mode” is a precursor to a second-order phase transition due to, for example, a change in temperature. Similarly, in continuum mechanics a “soft mode” is a forerunner of elastic instability, usually accompanied by ensuing symmetry changes in the geometry of the composite. Here, in the periodic composites, mode “softening” leads to a drastic decrease of the phase velocities and negative group velocities of elastic shear waves.

Keywords: nonlinear phononic crystal, elastic instability, soft modes, finite deformation, p4mm

1. Introduction

In the physics of crystals, “soft mode” is a precursor to a structural phase transition (i.e. ferroelectric transition) due to, for example, a change in temperature [1]. A soft mode is usually defined as collective excitation whose frequencies decrease anomalously in the vicinity of the transition point (e.g., transition temperature). Interestingly, a second-order transition is accompanied by vanishing of the eigenfrequency with certain critical wavenumber, while a first-order transition occurs prior to the vanishing of the eigen-frequency [1]. In continuum mechanics, a soft mode is a forerunner of elastic instability [2,3], usually accompanied (beyond the instability) by symmetry changes in the geometry of the composite. Similarly
to the second-order phase transition, the eigenfrequency of a certain wavelength vanishes at the onset of elastic instability [2,3]; however, in general, an elastic instability can be either a first- or second-order mechanical buckling transition, depending on the contrast in elastic moduli [4]. Mode “softening” leads to a drastic decrease of the phase velocities and negative group velocities of elastic shear waves [2,3]. While many researchers have investigated the phononic properties (i.e. band gaps) of various 2D composites in the post-buckling regime [5–8], there are very few studies analyzing the propagation of phonons in the nearly unstable (but still stable) composites. To the best of our knowledge, thus far, only layered and fiber composites on the edge of elastic instability have been investigated [2,3]. We extend these numerical studies to more complex periodic composites possessing symmetries of the p4mm plane group. Using simple 2D geometries, we demonstrate that nearly unstable nonlinear composites possess an exciting potential for tuning phonon propagation.

2. Numerical analysis

2.1 Problem description

Let us consider a 2D periodic composite comprised of a stiff square lattice with elements of length $a$ and width $d$ ($d \ll a$), and a soft matrix (Figure 1 (a)). The area fractions of the stiff (lattice) and soft (matrix) phases are $s_l = d(2a - d)/a^2$ and $s_m = 1 - s_l$, respectively. Here and after, $(\cdot)_l$ and $(\cdot)_m$ refer to the lattice and matrix, respectively. The considered composite possesses p4mm plane group symmetry [9].

Composite constituents are described by the neo-Hookean strain energy density function integrated in COMSOL Multiphysics 5.4 as

$$ W(\mathbf{F}_{\xi}) = \frac{\mu_{\xi}}{2} (\mathbf{F}_{\xi} \cdot \mathbf{F}_{\xi} - 3) - \mu_{\xi} \ln(J_{\xi}) + \frac{\Lambda_{\xi}}{2} (\ln J_{\xi})^2, \tag{1} $$

where $\mu_{\xi}$ is the shear modulus, $\Lambda_{\xi}$ is the first Lame parameter, $\mathbf{F}_{\xi}$ is the deformation gradient, and $J_{\xi} = \det(\mathbf{F}_{\xi})$; $\xi$ stands for $m$ (matrix) or $l$ (lattice). In this paper, we consider in-plane equibiaxial contraction of the composite (Figure 1 (b)), which can be described by the following macroscopic deformation gradient

Figure 1: (a) Illustration of the periodic composite with a square lattice ($d/a = 0.02$) and its primitive cell. (b) Schematic representation of the equibiaxially compressed composite and the corresponding primitive cell after the onset of elastic instability.
\[ \mathbf{F} = \lambda \mathbf{e}_1 \otimes \mathbf{e}_1 + \lambda \mathbf{e}_2 \otimes \mathbf{e}_2, \]  
where \( \lambda \) is the stretch ratio, and \((\mathbf{e}_1, \mathbf{e}_2)\) is the orthonormal basis.

### 2.2 Bloch-Floquet analysis superimposed on a finite deformation

To obtain the dispersion relations for the elastic waves propagating in a finitely deformed composite, we employ the numerical Bloch-Floquet analysis [10] superimposed on the finite deformation in COMSOL Multiphysics 5.4. A unit cell used for simulations is shown in Figure 1 (a). The numerical analysis has two steps: (Step 1) in-plane equibiaxial deformation is imposed through the periodic conditions shown in Eq. (3); (Step 2) Floquet periodic conditions are imposed on a deformed state (Eq. (4)). Then, by solving the corresponding eigenvalue problems for a range of Bloch wave vectors [5], the dispersion relations for finitely deformed periodic composites are calculated.

**Step 1. Equibiaxial deformation.**

\[
\begin{align*}
\mathbf{u}|_{\text{right}} &= \mathbf{u}|_{\text{left}} + (\lambda - 1)\mathbf{a} \\
\mathbf{v}|_{\text{right}} &= \mathbf{v}|_{\text{left}}, \\
\mathbf{u}|_{\text{top}} &= \mathbf{u}|_{\text{bottom}} + (\lambda - 1)a, \\
\mathbf{v}|_{\text{top}} &= \mathbf{v}|_{\text{bottom}}, \\
\mathbf{u}|_{A} = \mathbf{v}|_{A} = 0
\end{align*}
\]  
\[ (3) \]

where \( u \) and \( v \) are displacements in \( \mathbf{e}_1 \) and \( \mathbf{e}_2 \) directions, respectively; the subscripts right, left, top and bottom denote the sides of the primitive cell, and the letter “A” denotes the node at the right bottom corner of the unit cell (Figure 1 (a)).

**Step 2. Floquet periodic conditions.**

\[
\begin{align*}
\mathbf{u}|_{\text{right}} &= \mathbf{u}|_{\text{left}}e^{-iK_x a} \\
\mathbf{v}|_{\text{right}} &= \mathbf{v}|_{\text{left}}e^{-iK_x a}, \\
\mathbf{u}|_{\text{top}} &= \mathbf{u}|_{\text{bottom}}e^{-iK_y a} \\
\mathbf{v}|_{\text{top}} &= \mathbf{v}|_{\text{bottom}}e^{-iK_y a}
\end{align*}
\]  
\[ (4) \]

where \( K_x \) and \( K_y \) are the components of the Bloch wave vector \( \mathbf{K} \) in the undeformed (reference) configuration. Recall that the Bloch wave vector in the deformed (current) configuration can be calculated as \( \mathbf{k} = \mathbf{F}^{-T} \cdot \mathbf{K} \).

### 3. Results and Discussion

We investigate nonlinear bi-phase composites with different \( \frac{d}{a} \) ratios (or area fractions) and fixed contrast in shear moduli \( \mu_l/\mu_m = 1000 \), where in all simulations \( \mu_m = 1 \) MPa, \( \Lambda_m = 24 \) MPa, \( \Lambda_l = 4 \) GPa and \( \rho_m = \rho_l = 1000 \) kg/m³; the corresponding Poisson’s ratios are \( \nu_m = 0.48 \) and \( \nu_l = 0.4 \). The composites with similar elastic moduli of the constituents can be fabricated by multi-material 3D printing, for example, on Objet260 Connex3 3D printer by Stratasys [11,12]. The frequency is normalized as \( f_n = f_a/\overline{\epsilon}_{sw} = f_a/\sqrt{\overline{\mu}/\overline{\rho}} \), where \( \overline{\mu} = (s_l/\mu_l + s_m/\mu_m)^{-1} \) is the weighted harmonic mean shear modulus and \( \overline{\rho} = s_l\rho_l + s_m\rho_m \) is the weighted arithmetic mean density. Recall that the basis vectors for the square reciprocal lattice are \((1,0)2\pi/a\) and \((0,1)2\pi/a\), and the high symmetry points of the irreducible Brillouin zone (IBZ) for the p4mm plane group are \( \Gamma(0,0) \), \( X(1/2,0)2\pi/a \) and \( M(1/2,1/2)2\pi/a \) (Figure 2 (b)). The point groups at the \( \Gamma, X \) and \( M \) points are 4mm, mm2 and 4mm, respectively [13].

#### 3.1 Phononic mode softening at M point of IBZ

Figures 2 (c-e) show evolution of the band structure in an equibiaxially contracted composite with p4mm symmetry. In the undeformed composite (\( \lambda = 1 \)), the lowest mode along the \( \Gamma-M \) path has positive slope (Figure 2 (c)). Under equibiaxial stretch of \( \lambda = 0.992 \) (compression) the slope becomes negative, and the lowest eigenfrequency at the M point becomes very sensitive to small increases in loading (compare the lowest blue and red dispersion curves along the \( \Gamma-M \) path in Figure 2 (e)). This susceptibility of the lowest dispersion curve signals the onset of elastic instability. Remarkably, the eigenmode of the eigenfrequency that first hits zero (Figure 2 (f)) resembles the buckling shape of the composite after the onset of the elastic instability. It should be noted that the prominent mode softening in the
vicinity of elastic instability is a neat phenomenon, because it is usually observed in the small range of deformation (e.g., $\Delta \lambda \cdot 100\% = 0.006\%$ for the composite in Figure 2); however, by a proper choice of composite constituents (i.e. elastic moduli and area/volume fractions) the range of deformation with prominent mode softening can be widened up to 1.5% [3]. Interestingly, even a relatively small change

Figure 2: Mode softening at the M point of IBZ in the vicinity of the elastic instability in the equibiaxially compressed composite with the plane group p4mm. (a) Schematic representation of the equibiaxial compression. (b) IBZ. (c-e) Evolution of band structure. (f) Eigenmode at the M point in the vicinity of elastic instability. The critical stretch for $d/a = 0.02$ is $\lambda_{cr} = 0.99189$. 

vicinity of elastic instability is a neat phenomenon, because it is usually observed in the small range of deformation (e.g., $\Delta \lambda \cdot 100\% = 0.006\%$ for the composite in Figure 2); however, by a proper choice of composite constituents (i.e. elastic moduli and area/volume fractions) the range of deformation with prominent mode softening can be widened up to 1.5% [3]. Interestingly, even a relatively small change
in the area fraction of the lattice elements (i.e. from $s_l = 0.04$ to $s_l = 0.10$, which corresponds to a considerable change in the thickness of the lattice elements from $d/a = 0.02$ to $d/a = 0.05$) can significantly influence the mode softening phenomenon (Figure 3). Specifically, for the composite with $d/a = 0.05$ the major mode softening occurs along the $\Gamma$–$X$ path, and the eigenfrequency right next to the $\Gamma$ point first becomes zero, not at the M point (compare Figure 2 (e) and Figures 3 (c-d)). Thus, in this case, the composite exhibits the so-called long-wave ($K_{cr} \to 0$) or macroscopic instability [14]. Note that the lowest dispersion curve also “softens” at the M point with increase in compressive deformation, however, the vanishing of the mode is much slower than in the composite with $d/a = 0.02$. Hence, mode softening can occur simultaneously in various regions of IBZ. Moreover, the position of mode softening is not uniquely defined by the plane group of the composite, but by the area fraction of the stiffer phase in the considered example. It is worth noting also that the pressure mode is barely affected by the equibiaxial compression, while the shear mode prominently softens (compare Figures 3 (a) and (d)).

Figure 3: Mode softening in the vicinity of the elastic instability in the equibiaxially compressed composite with increased thickness of the lattice elements, i.e. $d/a = 0.05$, corresponding to increased area fraction of the stiffer phase $s_l = 0.10$. (a) Band structure in the undeformed composite. (b) Band structure in the composite subject to the equibiaxial stretch of $\lambda = 0.994$ (blue). (c-d) Evolution of the band structure in the composite (black to blue to red) compressed towards the critical stretch $\lambda_{cr} = 0.992$ (red).
4. Conclusions

The lowest phononic modes in bi-phase composites with p4mm plane group symmetry “soften” in the vicinity of an elastic instability, following the mode softening scenario usually observed during a second-order structural phase transition (e.g., ferroelectric transition). The position of the softening within the IBZ strongly depends on the geometrical and material parameters of the composite. In particular, the composite comprised of stiff square lattice and soft matrix can exhibit mode softening either at the Γ or the M points of IBZ depending on the area fraction of the stiff phase (Figure 2 and Figure 3). Equibiaxially contracted bi-phase composites with plane group p4mm can exhibit mode softening by 2 different scenarios (see Figures 2-3).

AKNOWLEDGEMENTS

We acknowledge the financial support from the Air Force Office of Scientific Research via a Multi-University Research Initiative (Contract no. FA9550-14-1-0037).

REFERENCES
