



Closed-form solutions to the effective properties of magnetoelectric composites

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Abstract

Magnetoelectric coupling is of interest for a variety of applications, but is weak in natural materials. Strain-coupled fibrous composites of piezoelectric and piezomagnetic materials are an attractive way of obtaining enhanced effective magnetoelectricity. This paper studies the effective magnetoelectric behaviors of two-phase multiferroic composites with periodic array of inhomogeneities. For a class of microstructures called periodic E-inclusions, we obtain a rigorous closed-form formula of the effective magnetoelectric coupling coefficient in terms of the shape matrix and volume fraction of the periodic E-inclusion. Based on the closed-form formula, we find the optimal volume fractions of the fiber phase for maximum magnetoelectric coupling and correlate the maximum magnetoelectric coupling with the material properties of the constituent phases. Based on these results, useful design principles are proposed for engineering magnetoelectric composites.

Model

We consider a composite consisting of a periodic array of parallel and separated prismatic cylinders as sketched in Figure 1. The cylinders and the matrix are made of two distinct phases: transversely isotropic piezoelectric or piezomagnetic materials. New physical property of magnetoelectricity arises from interactions between two phases mediated by strain.

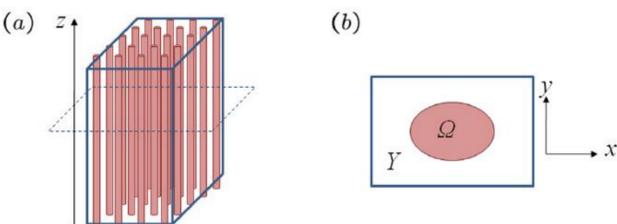


Figure 1: Configuration of the fibrous composite: (a) the overall composite and (b) a unit cell in the xy -plane with Ω being one phase and $Y \setminus \Omega$ being the other phase.

Problem Statement

The composite is assumed to be invariant for any translation in \mathbf{e}_z -direction and subjected to anti-plane shear. The local magneto-electro-elastic state is described by

$$\begin{aligned} \text{out-of-plane displacement: } u_z &= w(x, y), \\ \text{electrostatic potential: } \varphi &= \varphi(x, y), \\ \text{magnetostatic potential: } \psi &= \psi(x, y). \end{aligned}$$

Define vector field $\mathbf{u} = [w, \varphi, \psi]$. Then the unit cell problem for determining the local fields and effective properties can be written as

$$\begin{cases} \nabla \cdot [\mathbf{L}(\mathbf{x})(\nabla \mathbf{u} + \mathbf{F})] = 0 & \text{on } Y, \\ \text{periodic boundary conditions on } \partial Y, \end{cases} \quad (1)$$

Where in (r) -phase (either matrix or inclusion) the components of tensor $\mathbf{L}(\mathbf{x})$ is given by

$$L_{piqj}^{(r)} = A_{pq}^{(r)} \delta_{ij}, \quad A_{pq}^{(r)} = \begin{pmatrix} C_{44} & e_{15} & q_{15} \\ e_{15} & -\kappa_{11} & -\lambda_{11} \\ q_{15} & -\lambda_{11} & -\mu_{11} \end{pmatrix}.$$

Closed-form solutions for periodic E-inclusions

Closed-form solutions to Eq. (1) for periodic E-inclusions are achieved by noticing a critical property of periodic E-inclusions, i.e., the Eshelby uniformity property persists for periodic E-inclusions in a finite unit cell with periodic boundary conditions. This can be conveniently shown by the method of Green's function or Fourier analysis. Then the classic equivalent inclusion method can be used to solve the inhomogeneous problem. Upon some algebraic calculations, the effective tensor for periodic composites of piezoelectric and piezomagnetic composites as illustrated in Figure 1 is given by

$$\mathbf{L}^e = \mathbf{L}^{(m)} + f[(1-f)\Delta\mathbf{L}\mathbf{R} - \mathbf{II}]^{-1}\Delta\mathbf{L}, \quad (3)$$

where f - volume fraction of the fibrous phase, \mathbf{II} - the identity tensor, $\mathbf{L}^{(m)}$ - material tensor of the matrix phase, $\Delta\mathbf{L} = \mathbf{L}^{(m)} - \mathbf{L}^{(i)}$ - difference between material tensors of the matrix and inclusion, and the components of tensor \mathbf{R} is given by

$$R_{piqj} = (\mathbf{A}^{(m)})_{pq}^{-1} Q_{ij}.$$

Periodic E-inclusions

Closed-form solutions to Eq. (1) are desirable but rare; an exception is when a) *the inclusion is an ellipsoid* and b) *the matrix phase is infinite*. Under these conditions, Eq. (1) admits a closed-form solution, namely, the celebrated *Eshelby's solution*. However, analysis based on the Eshelby's solution cannot account for interactions since it is a *single* inclusion model. Periodic E-inclusions are new shapes for which Eq. (1) admits a closed-form solution for finite unit cell Y . Examples of periodic E-inclusions are shown in Figure 2.

The letter "E" in the terminology "E-inclusions" arises from the associations with **E**llipsoids, **E**shelby, and **E**xtrimal properties. Rigorously, periodic E-inclusions are defined as domains such that the overdetermined problem

$$\begin{cases} \Delta\phi = f - \chi\Omega & \text{on } Y, \\ \nabla\nabla\phi = -(1-f)\mathbf{Q} & \text{on } \Omega, \\ \text{periodic bdry cond.} & \text{on } \partial Y, \end{cases} \quad (2)$$

admit a solution, where f - volume fraction, \mathbf{Q} - shape matrix, and Y - unit cell. The overdetermined condition in Eq. (2)₂ places strong restrictions on the shape. The existence can be proved by considering variational inequalities; in the dilute limit $f \rightarrow 0$, simply-connected periodic E-inclusions coincide with ellipsoids which implies the Eshelby conjecture.

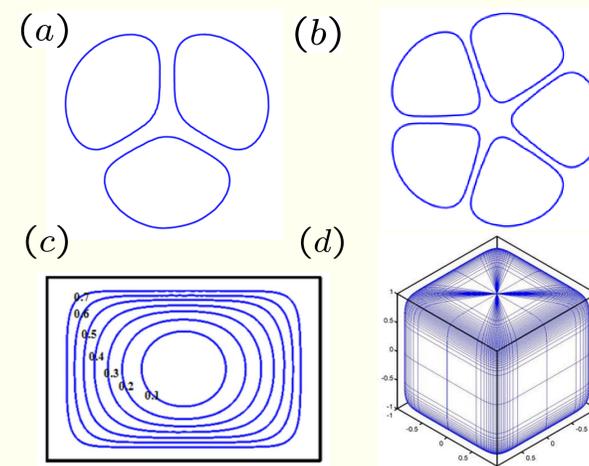


Figure 2: Examples of periodic E-inclusions: (a) a three-component E-inclusions, (b) a five-component E-inclusions, (c) 2D periodic E-inclusions in a rectangular unit cell, with isotropic shape matrix but different volume fractions. (d) a 3D periodic E-inclusion of volume fraction 0.7 and isotropic shape matrix.

Results

Once the closed-form formula Eq. (3) of the effective tensor is obtained, we can plot the interested magnetoelectric coupling coefficient against a number of design parameters including volume fraction, electric permittivity, magnetic permeability, elastic modulus, etc. The results are shown in the following Figure 3, 4, 5.

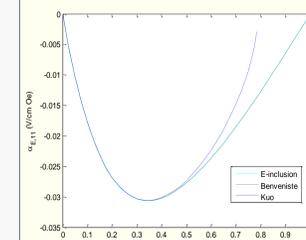


Figure 3: The predicted ME voltage coefficients versus volume fractions with BTO fibers in CFO matrix. We make two observations: (i) the closed-form prediction based on E-inclusion is consistent with previous models, and (ii) there is an optimal volume fraction for the desired maximum ME voltage coefficient.

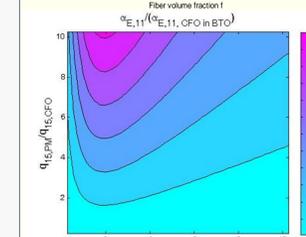


Figure 4: The contour plots of the maximum effective ME voltage coefficients. The unit for ME voltage coefficient is 0.0245 V/cmOe and the horizontal and vertical axes represent normalized piezoelectric coefficient of PE phase and normalized piezomagnetic coefficient of PM phase, respectively.

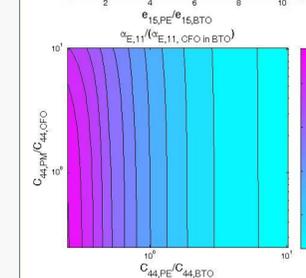


Figure 5: The contour plots of the maximum effective ME voltage coefficients. The unit for ME voltage coefficient is 0.0245 V/cmOe and the horizontal and vertical axes represent normalized elastic constants of the PE and PM phase, respectively.

Implied Design Principles

- There exists an optimal volume fraction for maximum ME voltage coefficient which can be obtained by maximizing the corresponding coefficients in Eq. (3) over volume fraction f .
- Softer materials are desirable for improving the ME voltage coefficient.
- The permittivity of PM phase has a much stronger effect on the ME voltage coefficient for composites of PM fibers in a PE matrix than for composites of PE fibers in a PM matrix and is preferably large.

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