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Materials Today: Proceedings 3 (2016) 167 – 172

Advances in Functional Materials (Conference 2015), AFM 2015

Micromechanical modeling of piezoelectric-piezomagnetic composites using Computational Piezo-Grains (CPGs)

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Abstract

Accurate micromechanical modeling of particle and fibrous composite samples with large number of defects (inclusions, voids, cracks, etc.) using regular finite elements is expensive because of the mesh-refinement used around each defect. Based on Lekhnitskii formulation, we develop new type of elements (named "Computational Piezo-Grains" (CPGs)) with two important features: (1) each element can have an arbitrarily polygonal shape to mimic the shape of grains in the microscale, (2) each element may contain a void or inclusion embedded in its domain. The materials of the matrix and inclusions could be elastic, piezoelectric, or piezomagnetic, allowing for modeling various composite types.

Keywords: Finite elements; inclusion; composite; piezoelectric; piezomagnetic; Lekhnitskii; Trefftz; multiferroic.

1. Introduction

Because of the large amount of applications of piezo-composites [1], several types of finite elements with embedded defects were formulated recently for micromechanical modeling of such composites (see [2]-[3] for instance). This work extends the elements developed in [2] for piezoelectric composites to the case of piezoelectric-piezomagnetic composites.

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2214-7853 © 2016 Published by Elsevier Ltd.
Selection and peer-review under responsibility of Conference Committee Members of Advances in Functional Materials (Conference 2015).
doi:10.1016/j.matpr.2016.01.052

2. Computational Piezo-Grains (CPGs) formulation

In order to model an arbitrary polygonal shaped material grain with an inclusion or a void with only one "finite element", the proposed element geometry is shown in Fig. 1. The outer boundary of the element can take any arbitrary polygonal shape with any number of sides. An arbitrarily oriented ellipse is embedded in the element in order to model a void or an inclusion in the element's domain.

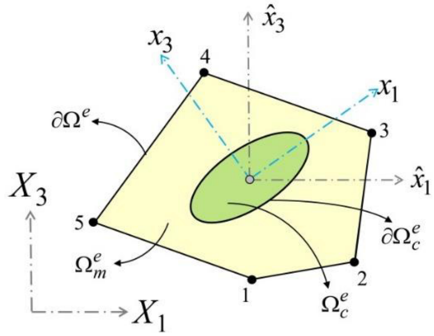

Fig. 1. 2D Computational Piezo-Grain (CPG) with an arbitrarily oriented elliptical void/inclusion and its local coordinates ($x_1 - x_3$) as well as the global ($X_1 - X_3$), and grain local ($\hat{x}_1 - \hat{x}_3$) Cartesian coordinate systems.

In order for these grains -or elements- to be able to model variety of piezo-composites, the material of the matrix or the inclusion in each element could be piezoelectric, piezomagnetic, or elastic with no couplings. Mathematically the following equations should be enforced in the non-conducting matrix domain (Ω^e_m) and inclusion domain (Ω^e_c):

1- Stress equilibrium and the electric and magnetic forms of Gauss's equations:

$$\partial_{\mathbf{u}}^T \boldsymbol{\sigma}^\alpha + \bar{\mathbf{b}}_f^\alpha = \mathbf{0}; \quad \boldsymbol{\sigma}^\alpha = (\boldsymbol{\sigma}^\alpha)^T, \quad \partial_{\mathbf{e}}^T \mathbf{D}^\alpha - \bar{\rho}_f^\alpha = 0, \quad \partial_{\mathbf{e}}^T \mathbf{B}^\alpha = 0 \tag{1}$$

2- Strain-displacement (for infinitesimal deformations), Electric field-electric potential, Magnetic field-magnetic potential relations:

$$\boldsymbol{\varepsilon}^\alpha = \partial_{\mathbf{u}} \mathbf{u}^\alpha, \quad \mathbf{E}^\alpha = -\partial_{\mathbf{e}} \varphi^\alpha \quad \mathbf{H}^\alpha = -\partial_{\mathbf{e}} \psi^\alpha \tag{2}$$

where $\partial_{\mathbf{u}} = \begin{bmatrix} \frac{\partial}{\partial x_1} & 0 & \frac{\partial}{\partial x_3} \\ 0 & \frac{\partial}{\partial x_3} & \frac{\partial}{\partial x_1} \end{bmatrix}^T \qquad \partial_{\mathbf{e}} = \begin{bmatrix} \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_3} \end{bmatrix}^T$

3- Constitutive laws:

$$\begin{Bmatrix} \boldsymbol{\sigma}^\alpha \\ \mathbf{D}^\alpha \\ \mathbf{B}^\alpha \end{Bmatrix} = \begin{bmatrix} \mathbf{C}^\alpha & \mathbf{e}^{\alpha T} & \mathbf{d}^{\alpha T} \\ \mathbf{e}^\alpha & -\mathbf{h}^\alpha & -\mathbf{n}^{\alpha T} \\ \mathbf{d}^\alpha & -\mathbf{n}^\alpha & -\mathbf{m}^\alpha \end{bmatrix} \begin{Bmatrix} \boldsymbol{\varepsilon}^\alpha \\ -\mathbf{E}^\alpha \\ -\mathbf{H}^\alpha \end{Bmatrix} \quad \text{or,} \quad \begin{Bmatrix} \boldsymbol{\varepsilon}^\alpha \\ -\mathbf{E}^\alpha \\ -\mathbf{H}^\alpha \end{Bmatrix} = \begin{bmatrix} \mathbf{S}^\alpha & \mathbf{g}^{\alpha T} & \mathbf{b}^{\alpha T} \\ \mathbf{g}^\alpha & -\boldsymbol{\beta}^\alpha & -\boldsymbol{\kappa}^{\alpha T} \\ \mathbf{b}^\alpha & -\boldsymbol{\kappa}^\alpha & -\boldsymbol{\upsilon}^\alpha \end{bmatrix} \begin{Bmatrix} \boldsymbol{\sigma}^\alpha \\ \mathbf{D}^\alpha \\ \mathbf{B}^\alpha \end{Bmatrix} \tag{3}$$

In the previous three equations the superscript $\alpha = m$ or c indicates whether we are talking about the matrix (*m*) or the inclusion (*c*) if any. $\mathbf{u}^\alpha$ (m), $\boldsymbol{\varepsilon}^\alpha$ (m/m) and $\boldsymbol{\sigma}^\alpha$ (Pa or N/m^2) denote mechanical displacement vector, strain and stress tensors written in vector form respectively, φ^α (V), $\mathbf{E}^\alpha$ (V/m or N/C) and $\mathbf{D}^\alpha$ (C/m^2) denote scalar electric potential, electric field & electric displacement vectors respectively, and ψ^α (A or C/s), $\mathbf{H}^\alpha$ (A/m or C/ms) and $\mathbf{B}^\alpha$ (N/Am or Vs/m^2) denote scalar magnetic potential, magnetic field & magnetic induction (magnetic flux density) vectors respectively. $\bar{\mathbf{b}}_f^\alpha$ is the body force vector, and $\bar{\rho}_f^\alpha$ is the electric free charge density. $\mathbf{C}^\alpha$ (Pa or N/m^2), $\mathbf{h}^\alpha$ (C/Vm), $\mathbf{m}^\alpha$ (N/A^2), $\mathbf{S}^\alpha$ (m^2/N), $\boldsymbol{\beta}^\alpha$ (Vm/C) and $\boldsymbol{\upsilon}^\alpha$ (A^2/N) are, respectively, the elastic stiffness tensor, dielectric permittivity tensor, magnetic permeability tensor, elastic compliance tensor, inverse of the permittivity tensor, and reluctivity tensor. $\mathbf{e}^\alpha$ (C/m^2) and $\mathbf{g}^\alpha$ (m^2/C) are piezoelectric tensors, $\mathbf{d}^\alpha$ (N/Am) and $\mathbf{b}^\alpha$ (Am/N) are piezomagnetic tensors, and $\mathbf{n}^\alpha$ (N/AV) and $\boldsymbol{\kappa}^\alpha$ (AV/N) are electromagnetic tensors. The diagonal matrices in eq. (3) are positive definite. If the material of the matrix or the inclusion is not piezoelectric, then the coupling piezoelectric matrices vanish $\mathbf{e}^\alpha = \mathbf{g}^\alpha = \mathbf{0}$ in eq. (3) and if the material is not piezomagnetic, then $\mathbf{d}^\alpha = \mathbf{b}^\alpha = \mathbf{0}$. Commercially available monolithic piezoelectric and piezomagnetic materials have very small or no electromagnetic coupling, hence $\mathbf{n}^\alpha = \boldsymbol{\kappa}^\alpha = \mathbf{0}$.

The following natural and essential boundary conditions should be enforced on the outer element (or grain) boundaries ($\partial\Omega^e = S_u^e \cup S_t^e \cup S_g^e = S_\varphi^e \cup S_Q^e \cup S_g^e = S_\psi^e \cup S_B^e \cup S_g^e$), and inclusion or void boundary $\partial\Omega_c^e$:

$$\mathbf{n}_\sigma \boldsymbol{\sigma}^m = \bar{\mathbf{t}} \quad \text{at } S_t^e, \qquad \mathbf{u}^m = \bar{\mathbf{u}} \quad \text{at } S_u^e, \tag{4}$$

$$\mathbf{n}_\mathbf{e} \mathbf{D}^m = \bar{Q} \quad \text{at } S_Q^e, \qquad \varphi^m = \bar{\varphi} \quad \text{at } S_\varphi^e, \tag{5}$$

$$\mathbf{n}_\mathbf{e} \mathbf{B}^m = \bar{Q}_M \quad \text{at } S_B^e, \qquad \psi^m = \bar{\psi} \quad \text{at } S_\psi^e, \tag{6}$$

$$\text{where} \quad \mathbf{n}_\sigma = \begin{bmatrix} n_1 & 0 & n_3 \\ 0 & n_3 & n_1 \end{bmatrix}, \qquad \text{and} \qquad \mathbf{n}_\mathbf{e} = \begin{bmatrix} n_1 & n_3 \end{bmatrix}, \tag{7}$$

$$\mathbf{u}^{m+} = \mathbf{u}^{m-}, \qquad \varphi^{m+} = \varphi^{m-}, \qquad \psi^{m+} = \psi^{m-} \qquad \text{at } S_g^e \tag{8}$$

$$(\mathbf{n}_\sigma \boldsymbol{\sigma}^m)^+ + (\mathbf{n}_\sigma \boldsymbol{\sigma}^m)^- = 0, \quad (\mathbf{n}_\mathbf{e} \mathbf{D}^m)^+ + (\mathbf{n}_\mathbf{e} \mathbf{D}^m)^- = 0, \quad (\mathbf{n}_\mathbf{e} \mathbf{B}^m)^+ + (\mathbf{n}_\mathbf{e} \mathbf{B}^m)^- = 0 \qquad \text{at } S_g^e \tag{9}$$

$$\mathbf{u}^m = \mathbf{u}^c, \qquad \varphi^m = \varphi^c, \qquad \psi^m = \psi^c \qquad \text{at } \partial\Omega_c^e \text{ (inclusion)} \tag{10}$$

$$-\mathbf{n}_\sigma \boldsymbol{\sigma}^m + \mathbf{n}_\sigma \boldsymbol{\sigma}^c = 0, \qquad \mathbf{n}_\mathbf{e} \mathbf{D}^m = \mathbf{n}_\mathbf{e} \mathbf{D}^c, \qquad \mathbf{n}_\mathbf{e} \mathbf{B}^m = \mathbf{n}_\mathbf{e} \mathbf{B}^c \qquad \text{at } \partial\Omega_c^e \text{ (inclusion)} \tag{11}$$

$$\mathbf{t}^m = \mathbf{n}_\sigma \boldsymbol{\sigma}^m = \mathbf{0}, \qquad Q^m = \mathbf{n}_\mathbf{e} \mathbf{D}^m = 0, \qquad Q_M^m = \mathbf{n}_\mathbf{e} \mathbf{B}^m = 0 \qquad \text{at } \partial\Omega_c^e \text{ (void)} \tag{12}$$

where $\bar{\mathbf{t}}$ is the specified boundary traction vector, $\bar{Q}$ is the specified surface charge density (or electric displacement) and $\bar{Q}_M$ is the specified surface magnetic flux density (or magnetic induction). n_1 and n_3, the two components present in $\mathbf{n}_\sigma$ and $\mathbf{n}_\mathbf{e}$, are the components of the unit outward normal to the boundaries S_t^e, S_Q^e, or S_B^e respectively. $\bar{\mathbf{u}}$ is the specified mechanical displacement vector at the boundary S_u^e, $\bar{\varphi}$ is the specified electric potential at the boundary S_φ^e, and $\bar{\psi}$ is the specified magnetic potential at the boundary S_ψ^e. S_g^e is the grain boundary shared with neighboring grains.

We assume linear primal fields along each grain boundary in terms of the nodal values of the mechanical displacements $\mathbf{q}_{\mathbf{u}i}$, electric potential $\mathbf{q}_\varphi$, and magnetic potential $\mathbf{q}_\psi$, as:

$$\tilde{\underline{\mathbf{u}}} = \tilde{\mathbf{N}} \mathbf{q} \qquad \text{at } \partial\Omega^e \tag{13}$$

where $\tilde{\mathbf{N}}$ are linear shape functions, $\tilde{\underline{\mathbf{u}}} = \begin{bmatrix} \tilde{u}_1 & \tilde{u}_3 & \tilde{\varphi} & \tilde{\psi} \end{bmatrix}^T$ and $\mathbf{q}^T = \left\{ \mathbf{q}_\mathbf{u}^T \quad \mathbf{q}_\varphi^T \quad \mathbf{q}_\psi^T \right\}$.

We also assume the following fields in the matrix and inclusion domain of each element:

$$\underline{\mathbf{u}}^\alpha = \mathbf{N}^\alpha \mathbf{c}^\alpha, \qquad \underline{\boldsymbol{\sigma}}^\alpha = \mathbf{M}^\alpha \mathbf{c}^\alpha, \qquad \text{in } \Omega^e \tag{14}$$

$\mathbf{c}^{\alpha}$ denotes the unknown real coefficients, $\underline{\tilde{\mathbf{u}}} = \begin{bmatrix} u_1 & u_3 & \varphi & \psi \end{bmatrix}^T$, $\underline{\boldsymbol{\sigma}}^{\alpha T} = \begin{bmatrix} \boldsymbol{\sigma}^{\alpha T} & \mathbf{D}^{\alpha T} & \mathbf{B}^{\alpha T} \end{bmatrix}$. $\mathbf{N}^{\alpha}$ and $\mathbf{M}^{\alpha}$ are Trefftz functions based on Lekhnitskii formulation [4] for interior/exterior fields which satisfy eqs. (1)-(3). For the case of impermeable elliptical voids, a special solution set which satisfies the void *stress-free* and *vanishing surface charge and magnetic flux densities* boundary conditions (eqs. (12)) can be used instead. For more details about Ttrefftz-Lekhnitskii functions used, readers are referred to [5] where the functions are written as general expressions that account for the material type whether it is piezoelectric, piezomagnetic, or elastic.
Then we can write:

$$\underline{\mathbf{t}}^{\alpha} = \underline{\mathbf{n}}\underline{\boldsymbol{\sigma}}^{\alpha} \qquad \text{at } \partial\Omega^e \text{ or } \partial\Omega_c^e, \tag{15}$$

where $\underline{\mathbf{t}}^{\alpha T} = \begin{bmatrix} \mathbf{t}^{\alpha T} & Q^{\alpha} & Q_M^{\alpha} \end{bmatrix}$, $\quad \underline{\mathbf{n}} = \begin{bmatrix} \mathbf{n}_{\boldsymbol{\sigma}} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{n}_{\mathbf{e}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{n}_{\mathbf{e}} \end{bmatrix}$

Now we can use the following multi-field boundary variational principle to enforce all the required conditions at the grain boundary and at the inclusion boundary:

$$\Pi_1(\underline{\mathbf{u}}^m, \underline{\mathbf{u}}^c, \underline{\tilde{\mathbf{u}}}) = \sum_{e=1}^{N} \left\{ \begin{aligned} & -\int_{\partial\Omega^e + \partial\Omega_c^e} \frac{1}{2}\underline{\mathbf{t}}^m \cdot \underline{\mathbf{u}}^m dS + \int_{\partial\Omega^e} \underline{\mathbf{t}}^m \cdot \underline{\tilde{\mathbf{u}}} dS + \int_{\partial\Omega_c^e} \underline{\mathbf{t}}^m \cdot \underline{\mathbf{u}}^c dS \\ & + \int_{\partial\Omega_c^e} \frac{1}{2}\underline{\mathbf{t}}^c \cdot \underline{\mathbf{u}}^c dS - \int_{S_t^e} \bar{\mathbf{t}} \cdot \tilde{\mathbf{u}} dS - \int_{S_Q^e} \bar{Q}\tilde{\varphi} dS - \int_{S_B^e} \bar{Q}_M \tilde{\psi} dS \end{aligned} \right\} \tag{16}$$

This will lead to the following element equation:

$$\mathbf{Kq} = \mathbf{Q} \tag{17}$$

where

$$\mathbf{K} = \mathbf{G}_{\mathbf{mq}}^T \mathbf{H}_{\mathbf{mm}}^{-1} \mathbf{G}_{\mathbf{mq}} + \mathbf{G}_{\mathbf{mq}}^T \mathbf{H}_{\mathbf{mm}}^{-1} \mathbf{G}_{\mathbf{mc}} \left(\mathbf{G}_{\mathbf{mc}}^T \mathbf{H}_{\mathbf{mm}}^{-1} \mathbf{G}_{\mathbf{mc}} + \mathbf{H}_{\mathbf{cc}} \right)^{-1} \mathbf{G}_{\mathbf{mc}}^T \mathbf{H}_{\mathbf{mm}}^{-1} \mathbf{G}_{\mathbf{mq}} \tag{18}$$

$$\begin{gathered} \mathbf{H}_{\mathbf{mm}} = \int_{\partial\Omega^e + \partial\Omega_c^e} \mathbf{M}^{mT} \underline{\mathbf{n}}^T \mathbf{N}^m dS, \quad \mathbf{G}_{\mathbf{mc}} = \int_{\partial\Omega_c^e} \mathbf{M}^{mT} \underline{\mathbf{n}}^T \mathbf{N}^c dS, \quad \mathbf{H}_{\mathbf{cc}} = \int_{\partial\Omega_c^e} \mathbf{M}^{cT} \underline{\mathbf{n}}^T \mathbf{N}^c dS \\ \mathbf{G}_{\mathbf{mq}} = \int_{\partial\Omega^e} \mathbf{M}^{mT} \underline{\mathbf{n}}^T \tilde{\mathbf{N}} dS, \quad \mathbf{Q}^T = \left[\int_{S_t^e} \bar{\mathbf{t}}^T \tilde{\mathbf{N}}_{\mathbf{u}} dS \quad \int_{S_Q^e} \bar{Q} \tilde{\mathbf{N}}_{\varphi} dS \quad \int_{S_B^e} \bar{Q}_M \tilde{\mathbf{N}}_{\psi} dS \right] \end{gathered} \tag{19}$$

Alternatively, the conditions on the outer grain boundary and the inclusion boundary can be enforced using collocation or least squares method. This will lead to relating the unknown coefficients, $\mathbf{c}^{\alpha}$, to the nodal variables:

$$\mathbf{c}^m = \mathbf{Z}^m \mathbf{q}, \quad \mathbf{c}^c = \mathbf{Z}^c \mathbf{q} \tag{20}$$

Then a simple variational principle can be used to enforce the natural boundary conditions:

$$\Pi_2(\underline{\mathbf{u}}^m) = \sum_{e=1}^{N} \left\{ \int_{\partial\Omega^e} \frac{1}{2}\underline{\mathbf{t}}^m \cdot \underline{\mathbf{u}}^m dS - \int_{S_t^e} \bar{\mathbf{t}}^m \cdot \mathbf{u}^m dS - \int_{S_Q^e} \bar{Q}\varphi^m dS - \int_{S_B^e} \bar{Q}_M \psi^m dS \right\} \tag{21}$$

which will give:

$$\mathbf{K} = \mathbf{Z}^{mT} \mathbf{H}_{\mathbf{mm}} \mathbf{Z}^m \tag{22}$$

where $\mathbf{H}_{\mathbf{mm}} = \int_{\partial\Omega^e} \mathbf{M}^{mT} \underline{\mathbf{n}}^T \mathbf{N}^m dS$ here.

We denote these two types of grains as "CPG-BVP" and "CPG-C" respectively. The derived stiffness matrices simplify when the grain includes a void instead of an inclusion, and simplify more when the grain includes no defect.

3. Numerical Examples

Any number of grains can be assembled exactly as regular finite elements are assembled to form a microstructure. Loads and essential BCs can then be prescribed on the outer boundary and the FE equations can be solved for nodal values, and then secondary fields can be calculated anywhere in the microstructure. Here we show sample results. All material properties are listed in [5]. Considering a domain with piezomagnetic $CoFe_2O_4$ matrix and piezoelectric $BaTiO_3$ inclusion subjected to traction loading in the vertical direction, only one CPG grain can be used to model this domain. Sample results (electric potential and vertical stress distributions) are shown in Fig. 2. The effective material properties of this piezo-composite for various volume fractions can also be estimated using a unit cell of any number of grains. A sample result (estimation of piezoelectric coefficients) can be seen in Fig. 3 (left) compared to the results in [6]. Finally a microstructure of 30 grains with polymer matrix and piezo-inclusions (PZT-4) in some grains, voids in other grains, and no defects in the remaining grains, can be modeled simply using 30 CPGs. The strain energy density distribution is presented in Fig. 3 (right) as a sample result.

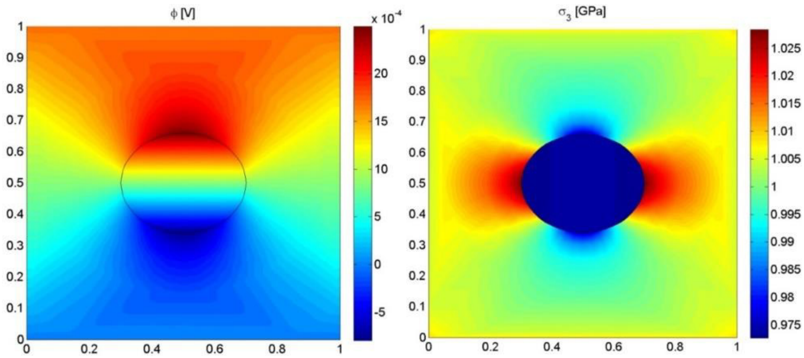

Fig. 2. Electric potential (left) and σ_{33} (right) distributions

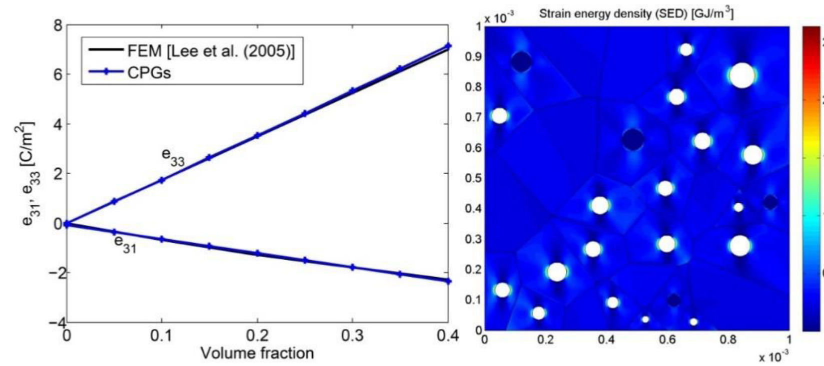

Fig. 3. (left) Effective piezoelectric coefficients of $BaTiO_3/CoFe_2O_4$ piezo-composite as functions of inclusions' volume fraction, (right) Strain energy density distribution in a microstructure of 30 grains

4. Summary and Conclusions

In order to model material microstructures with large number of defects (voids, inclusions, cracks), regular finite elements will definitely lead to very large system of equations that renders the analysis inefficient. Accordingly advanced finite elements with embedded defects are being developed to alleviate this problem. In this work, new multi-physics finite elements (named Computational Piezo-Grains (CPGs)) are developed to model piezo-composites in the micro-scale. Each element (or computational grain) can have the shape of a material grain with embedded elliptical void or inclusion. In order to enforce all governing equations and boundary conditions, the formulation of these grains relies on (1) Trefftz-Lekhnitskii functions for interior/exterior fields, (2) a multi-field boundary variational principle (BVP) or collocation method with simple primal boundary variational principle. Stiffness matrices can be derived and assembled exactly as regular finite elements are assembled. CPGs are successful in modeling piezo-composites with any number and distribution of voids or inclusions, and to estimate the effective material properties of piezoelectric-piezomagnetic composites.

Acknowledgment

This work was supported by a collaborative research agreement between the Army Research Lab's Vehicle Technology Division and University of California, Irvine. This support is gratefully acknowledged. The generous support of Saint Martin's University and California State University, Northridge to the first author are thankfully acknowledged.

References

[1] C-W Nan, M. I. Bichurin, S. Dong, D. Viehland, G. Srinivasan. J. Appl. Phys. 103 (2008), 031101.
[2] P. L. Bishay, S. N. Atluri, Comput. Mat. Sci. 83 (2014) 235–249.
[3] P. L. Bishay, L. Dong, S. N. Atluri, Comput. Mech. 54 (2014), 5, 1129-1139.
[4] S. G. Lekhnitskii, Theory of elasticity of an anisotropic body. Mir Publishers, Moscow, 1981.
[5] P. L. Bishay, S. N. Atluri, Eur. J. Mech. A: Solids 53 (2015) 311-328.
[6] J. Lee, J.G. Boyd IV, D.C. Lagoudas, Int. J. Eng. Sci. 43 (2005) 790-825.