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Micromechanics Analysis for Effective Properties of Piezocomposites

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Abstract— **In recent years, smart composite materials have been employed in various science and engineering applications such as aerospace structures, nondestructive testing devices, medical devices, and sensing and actuating applications. One of the most popular classes is a 1-3 piezocomposite that composes of homogeneous transversely isotropic piezoelectric cylinders embedded in an isotropic elastic material. The 1-3 piezocomposites can produce higher electro-mechanical coupling effects, more conformable and less brittle than pure piezoelectric materials. For optimal design of these composites to meet high requirements in practical science and engineering applications, it is essential to know the effective properties that couple electromechanical properties of the composites. This paper is concerned with the development of an efficient methodology to determine the effective properties of smart composite materials with special emphasis on 1-3 piezocomposites. A micromechanics theory based on a periodic microfield approach together with the boundary element method have been employed to calculate effective properties of the piezocomposites. A computer program has been developed based on the proposed solution scheme. Comparisons with the available existing solutions are performed to verify the accuracy of the developed solution scheme. Selected numerical examples are presented to demonstrate the capability of the present algorithm, and to show the influence of various parameters on the effective electro–mechanical properties of the composites.**

Keywords—**Smart materials, Piezocomposites, Effective properties, Micromechanics, Boundary element method, Periodic microfield.**

I. Introduction

Smart composites have drawn significant interest in recent years due to the rapid development in adaptive material system. There are many advantages to use composites over more traditional smart materials such as the possibility of weight or volume reduction, increase in ductility and enhanced coupling constant [1]. Because of increasing demands for extended application, smart composites have been developed to improve the material properties and overcome drawbacks of the bulk smart materials. The most popular class of smart composites is piezoelectric such as 1-3 piezocomposites that contain piezoelectric rods embedded in a polymer matrix and aligned through the thickness of the composite. Fig. 1 shows a typical 1–3 piezocomposite in which the piezoceramic constituent is continuous in one direction while the matrix material is connected in all 3 orthogonal directions. The 1-3 piezocomposites can produce higher electromechanical coupling effects, more conformable and less brittle that pure piezoelectric materials.

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For the optimal design of these composites to meet high requirements in practical engineering applications, it is essential to know the effective properties of coupled electro-mechanical properties. Research on piezoelectric composite materials has been developed for predicting and simulating linear coupled electro-mechanical behavior. The method of calculation can be categories as analytical e.g. self-consistent [2] and Mori-Tanaka [3]; and numerical method e.g. finite element method and boundary element method. Due to the complexity of the field equations of composite materials, semi-analytical or numerical approaches seem to be more capable than pure analytical counterparts. A finite modeling volume is a primary requirement to implement in numerical simulations and is generally referred as representative volume element (RVE) or a unit cell. Lee et al. [4] performed finite element analysis and micromechanics based averaging of a RVE to determine the effective properties of a coupled electro-magneto-elastic composite consisting of elastic matrix reinforced with piezoelectric and piezomagnetic fibers. Afterwards, Bondarev et al. [5] developed a special RVE to determine the piezoelectric composite properties containing tubular PZTs. Further, FEM was employed by Jafari et al. [6] for numerical simulations in study the overall properties of piezoelectric composite based on hierarchical multi-scale approach and study the influential parameters on the RVE concept.

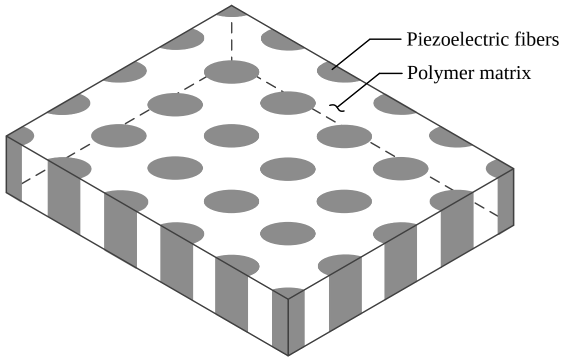


Figure 1. Schematic of a 1-3 piezocomposite

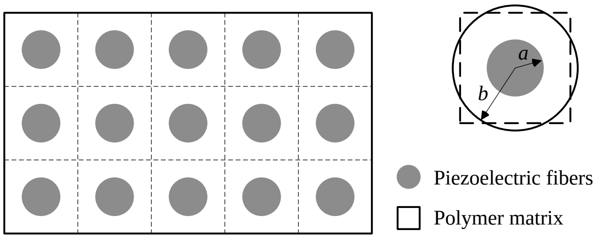
It should be mentioned that the FEM requires domain discretization in order to perform the analysis. In some cases, this results in both expensive computational demand and inaccurate numerical results, especially in solving fiber-matrix problems with high local fluctuations. On the other hand, the boundary element method (BEM) based micromechanical analysis only involves the boundary discretization of the unite cell since the governing differential equation is satisfied exactly within the domain leading to a relatively small system with a sufficient accuracy. Therefore, a simple, accurate and economic feature of BEM can make the prediction more effectively. Qin [7] developed a micromechanical boundary element algorithm to predict the effective material properties of a bulk piezoelectric material with holes. The algorithm based on two typical micromechanics model, the self-consistent and Mori-Tanaka methods, and the boundary element formulation. The algorithm was been growth to model a piezoelectric composite with inclusion of various shapes [8]. A micromechanics BEM algorithm was also applied to determine the effective properties electroelastic properties of transversely isotropic piezoelectric material containing randomly distributed voids by Wang et al. [9]. Recently, a periodic microfield micromechanics approach based on the BEM was proposed by Sapsathiarn and Senjuntichai [10] to calculate the effective properties of composite with periodic piezoelectric fibers. It was noted that the proposed BEM-based micromechanics scheme was an efficient tool for a plane strain problem.

The study of mechanics and effective properties of 1-3 piezocomposites is important to further development and application of this class of materials. To the author's knowledge, the determination of effective properties for the piezoelectric fiber-reinforced composites using BEM-based periodic microfield approach is currently not available in the literature for a complete set of coefficients for 3D problem. In this paper, an efficient methodology to determine the effective properties of smart composite materials with special emphasis on 1-3 piezocomposites is presented by employing the micromechanics theory and the boundary element method.

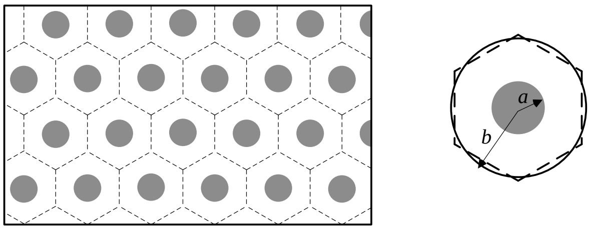
II. Micromechanics Theory

Micromechanics theory is a theory that relates macro and micro length-scale problems. The length-scales associated with macro and micro-levels are relative. At the macro-level, the material properties are usually assumed to be sufficiently homogeneous, whereas at the micro-level i.e. at the level of the constituents, the material properties are always heterogeneous and consist of distinguishable components such as inclusions, grains and cavities. The periodic microfield approach for a micromechanical analysis has a key assumption on periodicity of the microstructure, which suggests that the whole macroscopic specimen consists of periodically repeated unit cells. Therefore, the physical and geometrical properties of the microstructure can be identified by a representative volume element (RVE) or unit cell. Various types of RVEs are possible for unidirectionally fiber reinforced composites.

A typical unit cell of a 1-3 composite has a cross section that is either a square shape or a hexagonal shape as shown in Fig. 2(a) and 2(b) respectively that frequently employed in the literature [11]. To simplify the theoretical analysis of a unit cell, the square or hexagonal cross-section area is replaced by a circle of equal area and the height of the unit cell is equal to the thickness of the composites. Therefore, the unit cell of a 1-3 piezocomposite based on the concentric cylinder model is shown in Fig. 2 which consists of a piezoelectric solid cylindrical rod of radius a surrounded by a polymer annular cylinder of outer radius b and height $2h$. The basic and governing equations for the piezocomposite finite cylinder are presented in the next section.



(a) Square periodic unit cell



(b) Hexagonal periodic unit cell

Figure 2. The cross-section of piezocomposites and the RVE.

III. Basic and Governing Equation

Consider a piezocomposite cylinder of in radius a, outer radius b and height $2h$ under axisymmetric electromechanical loading applied to the boundary is shown in Fig. 3. The composite material consists of piezoelectric rods embedded in a polymer matrix and aligned through the thickness of the composite. The constitutive equations for piezoelectric material polarized in the z-direction without body force and electric charge can be written as

$$\sigma_{rr} = c_{11}\epsilon_{rr} + c_{12}\epsilon_{\theta\theta} + c_{13}\epsilon_{zz} - e_{31}E_z \quad (1)$$

$$\sigma_{\theta\theta} = c_{12}\epsilon_{rr} + c_{11}\epsilon_{\theta\theta} + c_{13}\epsilon_{zz} - e_{31}E_z \quad (2)$$

$$\sigma_{zz} = c_{13}\epsilon_{rr} + c_{13}\epsilon_{\theta\theta} + c_{33}\epsilon_{zz} - e_{33}E_z \quad (3)$$

$$\sigma_{rz} = 2c_{44}\epsilon_{rz} - e_{15}E_r \quad (4)$$

$$D_r = 2e_{15}\epsilon_{rz} + \varepsilon_{11}E_r \quad (5)$$

$$D_z = e_{31}\epsilon_{rr} + e_{31}\epsilon_{\theta\theta} + e_{33}\epsilon_{zz} + \varepsilon_{33}E_z \quad (6)$$

where σ_{ij}, ϵ_{ij}, D_i and E_i are the components of stress, strain, electric displacement and electric field, respectively. c_{11}, c_{12}, c_{13}, c_{33} and c_{44} are elastic constants under zero or constant electric field. e_{15}, e_{31} and e_{33} are piezoelectric coefficients. ε_{11} and ε_{33} are dielectric constants under zero or constant strain. The components of strain and electric field can be expressed as

$$\epsilon_{rr} = \frac{\partial u_r}{\partial r} \quad (7)$$

$$\epsilon_{\theta\theta} = \frac{u_r}{r} \quad (8)$$

$$\epsilon_{zz} = \frac{\partial u_z}{\partial z} \quad (9)$$

$$\epsilon_{rz} = \frac{1}{2}\left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}\right) \quad (10)$$

where $u_r(r,z)$ and $u_z(r,z)$ denote the mechanical displacements in the r and z -direction, respectively. In addition, the relationship between the electric field E_i ($i = r,\, z$) and the electric potential $\phi(r,z)$ is given by

$$E_r = -\frac{\partial \phi}{\partial r} \quad (11)$$

$$E_z = -\frac{\partial \phi}{\partial z} \quad (12)$$

The equilibrium equations for a piezoelectric cylinder subjected to axisymmetric end loading can be expressed as

$$\frac{\partial \sigma_{rr}}{\partial r} + \frac{\partial \sigma_{rz}}{\partial z} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0 \quad (13)$$

$$\frac{\partial \sigma_{rz}}{\partial r} + \frac{\partial \sigma_{zz}}{\partial z} + \frac{\sigma_{rz}}{r} = 0 \quad (14)$$

$$\frac{\partial D_r}{\partial r} + \frac{\partial D_z}{\partial z} + \frac{D_r}{r} = 0 \quad (15)$$

Combination the constitutive equations Equations. (1)-(12) with the equilibrium equations (13)-(14) results in the set of governing equations expressed in terms of the displacements and the electric potential. The potential function representation is introduced to uncouple the governing equations. The general solutions of finite solid and annular piezoelectric cylinders are given by Senjuntichai et al [12] and Rajapakse el al. [13] respectively. The case of a transversely isotropic elastic medium is obtained by setting e_{ij} and ε_{ij} in (1)-(6) to zero and dropping (15) from the equilibrium equation.

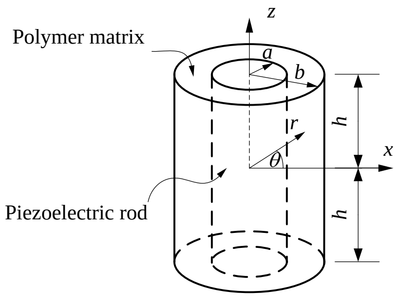


Figure 3. Idealized unit cell of 1-3 piezocomposite and coordinate system.

The boundary conditions for the composite cylinder under axsymmetric loading can be expressed as

$$\sigma^f_{zz}(r,\pm h) = \sigma^f_{zz}(r) \quad \text{for} \quad 0 \le r \le a \quad (16)$$

$$\sigma^f_{rz}(r,\pm h) = \sigma^f_{rz}(r) \quad \text{for} \quad 0 \le r \le a \quad (17)$$

$$D^f_z(r,\pm h) = D^f_z(r) \quad \text{for} \quad 0 \le r \le a \quad (18)$$

$$\sigma^m_{zz}(r,\pm h) = \sigma^m_{zz}(r) \quad \text{for} \quad a \le r \le b \quad (19)$$

$$\sigma^m_{zr}(r,\pm h) = \sigma^m_{rz}(r) \quad \text{for} \quad a \le r \le b \quad (20)$$

$$\sigma^m_{rr}(b,z) = \sigma^m_{rr}(z) \quad \text{for} \quad -h \le z \le h \quad (21)$$

$$\sigma^m_{rz}(b,z) = \sigma^m_{rz}(z) \quad \text{for} \quad -h \le z \le h \quad (22)$$

Note that superscripts f and m are used to denote the quantities associated with the piezoelectric fiber and polymer matrix respectively. Along the fiber-matrix interface which the bond between the fiber and matrix is perfect, the continuity of displacements and traction is required. Therefore,

$$\sigma^f_{rr}(a,z) = \sigma^m_{rr}(a,z) \quad \text{for} \quad -h \le z \le h \quad (23)$$

$$\sigma^f_{rz}(a,z) = \sigma^m_{rz}(a,z) \quad \text{for} \quad -h \le z \le h \quad (24)$$

$$D^f_r(a,z) = 0 \quad \text{for} \quad -h \le z \le h \quad (25)$$

$$u^f_r(a,z) = u^m_r(a,z) \quad \text{for} \quad -h \le z \le h \quad (26)$$

$$u^f_z(a,z) = u^m_z(a,z) \quad \text{for} \quad -h \le z \le h \quad (27)$$

where σ^f_{ij} and D^f_z are the traction and electric charge applied on the reinforced piezoelectric fiber respectively; σ^m_{ij} is the traction applied on the transverse isotropic elastic matrix. The boundary element method based periodic microfield approach is performed for evaluation of effective material properties. The boundary conditions of the periodic unit cell are discretized to determine the Green's function. The procedure for determination of the Green's function is presented in next section.

IV. Boundary Element Analysis of Unit Cell

The unit cell of 1-3 piezocomposite as shown in Fig. 3 consists of a two-domain i.e. a reinforced piezoelectric fiber domain Ω_1 with boundary Γ_1 and a transversely isotropic elastic matrix domain Ω_2 with Boundary Γ_2. The boundary integral equations for each sub-domain are performed. Thereafter, a global equation system for the whole domain of the unit cell is assembled by considering the interface continuity condition between fiber and matrix. The boundary integral equation for piezoelectric fiber with domain Ω_1 and boundary Γ_1 can be written as

$$c(\mathbf{x}')u_i(\mathbf{x}') = \int_{\Gamma_1}\left[G_{ji}(\mathbf{x};\mathbf{x}')\tau_j(\mathbf{x}) - \tilde{H}_{ji}(\mathbf{x};\mathbf{x}')u_j(\mathbf{x})\right]d\Gamma(\mathbf{x}) \quad (28)$$

where $i = r,z,q$ and the summation is implied on the index $j = r,z,q$; $\mathbf{x}$ and $\mathbf{x}'$ denote a field point and a load point respectively; G_{ji} and $\tilde{H}_{ji}$ denote the displacement and traction components respectively in the j -direction ($j = r,z$) due to a unit concentrated line load applied in the i -direction ($i = r,q$); G_{qi} and $\tilde{H}_{qi}$ denote the electric potential and electric charge respectively due to a unit concentrated line load applied in the i -direction; G_{jq} and $\tilde{H}_{jq}$ denote the displacement and traction components respectively in the j -direction due to a unit electric line charge; G_{qq} and $\tilde{H}_{qq}$ denote the electric potential and electric charge respectively due to a unit electric positive charge. Closed form Green's functions for line loads and a line electric charge can be determined as mention in the preceding section.

A similar boundary integral equation can be established for for transversely isotropic elastic matrix with domain Ω_2. The final boundary element equation for whole domain Ω of the unit cell can be obtained by assembling the sub-domain Ω_1 and Ω_2 together with the consideration the interface continuity conditions between the fibers and the matrix. The unknown terms and the known terms are then rearranged to the left-hand side and the right-hand side respectively. The numerical integrations for the functions G and H are carried out. The global equation system becomes a set of following linear algebraic equations

$$[\mathbf{A}]\{\mathbf{X}\} = \{\mathbf{B}\} \qquad (29)$$

where $\{\mathbf{X}\}$ is the vector unknown nodal displacements (or tractions), electric potential (or electric charge) at boundary nodes; $\{\mathbf{B}\}$ is the contribution to the equation system due to prescribed nodal boundary values; and $[\mathbf{A}]$ is the known coefficient matrix. Finally, the unknown nodal values of the displacements (or tractions), electric potential (or electric charge) can be obtained by solving (29).

V. Determination of Effective Coefficients

The macroscopic response of composites can be determined using the micromechanics theory based on the analysis of RVE and the multi-BEM formulation presented in the preceding section. The periodic microfield approach should be mention in this study to determine the effective material properties of electro-magneto-elastic composites. According to micromechanics theory, the macro-stress, $\bar{\boldsymbol{\sigma}}$, and macro strain, $\bar{\boldsymbol{\varepsilon}}$, of the composites can be defined as the volume average stress in a RVE as follows

$$\bar{\boldsymbol{\sigma}} = \frac{1}{V}\int_{\Omega}\boldsymbol{\sigma}\,d\Omega \qquad (30)$$

$$\bar{\boldsymbol{\varepsilon}} = \frac{1}{V}\int_{\Omega}\boldsymbol{\varepsilon}\,d\Omega \qquad (31)$$

where Ω is the domain of RVE and V is its volume. Similarly, the average electric displacement and electric are defined as follows:

$$\bar{\mathbf{D}} = \frac{1}{V}\int_{\Omega}\mathbf{D}\,d\Omega \qquad (32)$$

$$\bar{\mathbf{E}} = \frac{1}{V}\int_{\Omega}\mathbf{E}\,d\Omega \qquad (33)$$

The macroscopic constitutive relation of this composite can then be expressed in terms of the macro stress and the macro strain as

$$\begin{Bmatrix}\bar{\boldsymbol{\sigma}}\\ \bar{\mathbf{D}}\end{Bmatrix} = \begin{bmatrix}\mathbf{c}^* & \mathbf{e}^{*T}\\ \mathbf{e}^* & -\boldsymbol{\eta}^*\end{bmatrix}\begin{Bmatrix}\bar{\boldsymbol{\varepsilon}}\\ -\bar{\mathbf{E}}\end{Bmatrix} \qquad (34)$$

where the superscript asterisk (*) indicates the effective material properties of the composites. In order to determine the effective properties of three-phase electro-magneto-elastic composite, four independent uniaxial constant strain states and two independent uniaxial constant electric field state are individually applied to the RVE. By applying the six independent states to the RVE, six sets of the left-hand side vector in (34) can be performed as follow

$$\begin{Bmatrix}\bar{\boldsymbol{\sigma}}^*\\ \bar{\mathbf{D}}^*\end{Bmatrix} = \begin{bmatrix}\mathbf{c}^* & \mathbf{e}^{*T}\\ \mathbf{e}^* & -\boldsymbol{\eta}^*\end{bmatrix}\begin{bmatrix}\bar{\boldsymbol{\varepsilon}}^* & 0\\ 0 & -\bar{\mathbf{E}}^*\end{bmatrix} \qquad (35)$$

where $\bar{\boldsymbol{\sigma}}^*$ and $\bar{\mathbf{D}}^*$ denote six vector sets of $\bar{\boldsymbol{\sigma}}$ and $\bar{\mathbf{D}}$ respectively due to apply the uniaxial constant strain states $\bar{\boldsymbol{\varepsilon}}^*$ and uniaxial constant electric field states $\bar{\mathbf{E}}^*$. In addition, $\bar{\boldsymbol{\varepsilon}}^*$ and $\bar{\mathbf{E}}^*$ are diagonal matrixes. Therefore, the 6x6 effective matrix of the two-phase electro-elastic composites is easily determined.

VI. Conclusion

The micromechanics theory based on the periodic microfield approach and the boundary element method presented in this study have been proposed the appropriate and efficient method to determine a complete set of coefficients of 3D model in smart composites. The BEM-based micromechanics scheme is a productive tool for numerical evaluate of the effective properties due to the implementation of surface variable in the averaging process instead of volume averaging. Future work may present the influence of coupled electro/magneto/thermo-mechanical properties of the smart composite materials.

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