



Overall properties of piezoelectric composites with spring-type imperfect interfaces using the mechanics of structure genome

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ABSTRACT

In this study, the mechanics of structure genome has been extended to piezoelectricity problem of composite materials with spring-type imperfect interfaces model. This full field micromechanics approach is applied to predict the effective electro-elastic properties of piezoelectric composite materials containing imperfect contact between the matrix and the reinforcements. Examples of long fibers and spherical particles reinforced piezoelectric composite materials are used to demonstrate the robustness and accuracy of the proposed micromechanics theory. The size-dependency of the overall electro-elastic properties shows the importance of imperfect interfaces in modeling the electro-elastic behavior of composite materials.

1. Introduction

In a great number of engineering composite materials, the interface between the dissimilar phases are imperfect due to the atomic lattices mismatch, phonons scattering, poor mechanical or chemical adherence, surface contamination, oxide and interphase diffusion/reaction layers, debonding, etc [1]. This can significantly affect the local field distribution and effective properties of these composite materials and make them size-dependent [2–4] and must therefore be taken into account in a rigorous predictive model.

In the piezoelectricity problems, the imperfect contact condition between the reinforcements and the surrounding matrix is typically described by three interface models: two special interface models (membrane-type [5] and spring-type [6] interface models) and one general interface model [7,8]. According to the membrane-type model, the displacement and electric fields are continuous across the interface, while the traction vector field and the normal electric displacement exhibit interfacial jumps which are proportional to certain surface derivatives of the displacement and electric fields. The spring-type interface model assumes that the traction vector and the normal electric displacement are continuous across the interface, whereas the displacement vectors and the electric field suffer interfacial jumps proportional to the traction vector and the normal electric displacement. The general piezoelectric interface model was derived in Refs. [7,8] with the idea of replacing an interphase by an imperfect interface and performing an asymptotic analysis. In this general interface model, the displacement vector, the electric field, the traction vector and the

normal electric displacement field are discontinuous across the interface. Important progress has been made in studying the effects of imperfect interfaces on the effective electro-elastic properties of piezoelectric composite materials by theoretical analysis [9–15], numerical simulations [6,16–18] and experimental efforts [11,19–21] and references cited therein.

The objective of this study is to use the mechanics of structure genome (MSG) [22], a multiscale constitutive modeling framework, to develop an efficient micromechanics approach for predicting the effective electro-elastic properties of piezoelectric composite materials containing spring-type imperfect interfaces. The MSG micromechanics approach will be applied to piezoelectricity problem with the spring-type imperfect interfaces model reported in Ref. [8]. Using the variational asymptotic method for unit cell homogenization (VAMUCH) [23–31], MSG has been recently developed to provide a unified theory for constitutive modeling of heterogeneous materials and structures [3,4,22,32–37]. MSG unifies micromechanics and structural mechanics to provide a single approach to model all types of composite structures. MSG is based on the concept of Structure Genome (SG), which is defined as the smallest mathematical building block of the material. The advantages of the MSG approach in comparison to existing computational homogenization methods such as the representative volume element (RVE) analysis [38–40] and the mathematical homogenization theories (MHT) [41] are given in Refs. [3,22]. MSG is able to predict structural properties in terms of microstructures without unnecessary scale separation and is based on the principle of minimum information loss (PMIL) to minimize the information loss between the original

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model and the homogenized model. It minimizes the loss of information during homogenization of anisotropic, heterogeneous solid media by the variational asymptotic method (VAM) [42] which is applicable to any solid mechanics problem admitting a variational structure where one or more relatively small parameters are involved. The “smallness” of these parameters is exploited by using an asymptotic expansion structure of the functional of the problem (and not of the unknown field quantities as done in conventional asymptotic methods). VAM combines the advantages of both variational and asymptotic methods so that the models constructed using VAM can be directly implemented using the well established finite element method (FEM).

In comparison to existing computational homogenization theories [39,40], as far as a solid heterogeneous material featuring a 3D RVE with periodic boundary conditions is concerned, RVE analysis, MHT and MSG will provide exactly the same results for both effective properties and local fields. As far as efficiency is concerned, computing for e.g. the complete elastic stiffness matrix of an elastic composite material, RVE analysis requires solving six static problems because the coupled equation constraints used to apply the periodic boundary conditions affect the coefficient matrix of the linear system. MHT and MSG can be implemented using the finite element method so that the linear system will be factorized once and solve for six load steps. Theoretically, MHT and MSG could be six times more efficient than RVE analysis. However, such equivalence does not exist for situations when one cannot apply periodic boundary conditions. MHT is not applicable for general aperiodic materials unlike MSG [43]. RVE analysis and MSG can still use appropriate boundary conditions but the results could differ from each other. For solid materials featuring lower-dimensional heterogeneities such as binary composites or unidirectional continuous fiber reinforced composites, RVE analysis and MHT can only obtain properties and local fields with the same dimensionality as that of the RVE, while MSG can still obtain the complete set of 3D properties and local fields out of a 1D or 2D analysis. The main reason is that numerical implementations of MHT and RVE are based on a weak form converted from the strong form of a boundary value problem whereas MSG directly solves a variational statement based on energetic considerations. Finally yet importantly, MSG has the capability to construct directly models for beams/plates/shells based on the same principle of minimum information loss, which is different from the RVE analysis and MHT although it is possible to modify RVE analysis and MHT to construct models for beams/plates/shells. More details on the MSG approach can be found in Ref. [22] and related papers [32–34,36,43].

The paper is organized as follows. Section 2 presents the governing fields equations of linear piezoelectricity problem and the interfacial jump relations of the spring-type imperfect interfaces model. Section 3 gives the theoretical formulation of the MSG with the spring-type imperfect interfaces model for piezoelectric composites. Section 4 presents some numerical examples to show the accuracy of the predictions of the proposed MSG based micromechanics approach. Finally, conclusions are given in section 5. The results presented in this work are obtained using GetFEM++ [44] as the finite element library and Gmsh [45] as the pre-processing tool.

2. Piezoelectric composite with imperfect interfaces: general setting

2.1. Governing fields equations

The constitutive model for linear polarized piezoelectric material is given as

$$\sigma_{ij} = C_{ijkl}^E \varepsilon_{kl} - e_{kij} E_k, \tag{1}$$

$$D_i = e_{ikl} \varepsilon_{kl} + \kappa_{ik}^E E_k, \tag{2}$$

where the field variables are the stress σ_{ij} , the strain ε_{ij} , the electric field E_k , and the electric flux (electric displacement) D_i . The material

properties are the elastic stiffness measured at constant electric field, C_{ijkl}^E , the piezoelectric stress constant, e_{ijk} , the permittivity constant measured at fixed strain, κ_{ij}^E . When the stress and electric field are taken as the independent field variables, an alternative expression of the constitutive model is given as

$$\varepsilon_{ij} = S_{ijkl}^E \sigma_{kl} + d_{kij} E_k, \tag{3}$$

$$D_i = d_{ikl} \sigma_{kl} + \kappa_{ik}^E E_k, \tag{4}$$

where the elastic compliance under constant electric field S_{ijkl}^E , the piezoelectric strain constant d_{ijk} , the permittivity constant measured at fixed stress κ_{ij}^E , are given as follows

$$S_{ijkl}^E = (C^E)_{ijkl}^{-1}, \tag{5}$$

$$d_{ijk} = e_{imn} S_{mnjk}^E, \tag{6}$$

$$\kappa_{ij}^E = \kappa_{ij}^E + e_{imn} d_{jmn}, \tag{7}$$

The strain and the electric field are related to the elastic displacement, u_i , and the electric potential, ϕ , by the following relations

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \tag{8}$$

$$E_i = -\phi_{,i}, \tag{9}$$

where the subscript comma denotes the partial differentiation. The piezoelectric effect is governed by coupled mechanical equilibrium and electric flux conservation equations

$$\sigma_{ij,j} = 0, \tag{10}$$

$$D_{i,i} = 0, \tag{11}$$

which are defined in the absence of body forces and body charges. The quasi-static behavior of linear piezoelectric material is characterized by Eqs. (1), (2) and (8)–(11).

For convenience, the linearized constitutive equations (1) and (2) are written in a compact form as

$$\Sigma_{i\alpha} = L_{i\alpha j\beta} \Psi_{j\beta} \tag{12}$$

where

$$\Sigma_{i\alpha} = \begin{cases} \sigma_{i\alpha}, & i, \alpha = 1,2,3, \\ D_i, & i = 1,2,3, \quad \alpha = 4, \end{cases} \tag{13}$$

$$\Psi_{i\alpha} = \begin{cases} \varepsilon_{i\alpha}, & i, \alpha = 1,2,3, \\ \phi_{,i}, & i = 1,2,3, \quad \alpha = 4, \end{cases} \tag{14}$$

$$L_{i\alpha j\beta} = \begin{cases} C_{i\alpha j\beta}^E, & i, \alpha, j, \beta = 1,2,3, \\ e_{j\alpha}, & i, j, \alpha = 1,2,3, \quad \beta = 4, \\ e_{ij\beta}, & i, j, \beta = 1,2,3, \quad \alpha = 4, \\ -\kappa_{ij}^E, & i, j = 1,2,3, \quad \alpha = \beta = 4. \end{cases} \tag{15}$$

From now on, Latin indices are space indices assuming the values 1 to 3 while and Greek indices are fields indices assuming the values 1 to 4 and repeated indices are summed over their range except where explicitly indicated. With this convention, the displacement field and electric potential (called potential fields in the subsequent sections) are written as

$$U_\alpha = \begin{cases} u_\alpha, & \alpha = 1,2,3 \\ \phi, & \alpha = 4. \end{cases} \tag{16}$$

Through this paper, *pseudo-tensors* are represented by letters in bold face, i.e. \mathbf{L} is used for $L_{i\alpha j\beta}$ while Σ, \mathbf{U} and Ψ are used for $\Sigma_{i\alpha}, U_\alpha$ and $\Psi_{i\alpha}$, respectively. We use the term, *pseudo-tensor*, since, strictly speaking, \mathbf{L} is not a tensor even if its components ($C^E, \mathbf{e}, \kappa^E$) are tensors. Therefore, the tensor transformation rules have to be applied separately to each *component* of the pseudo-tensor. This holds true for Σ, \mathbf{U} and Ψ . In what

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