Composite Structures 151 (2016) 70–80

Contents lists available at ScienceDirect

Composite Structures

journal homepage: www.elsevier.com/locate/compstruct

Different interface models for calculating the effective properties in piezoelectric composite materials with imperfect fiber–matrix adhesion

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ARTICLE INFO

Article history:
Available online 11 February 2016

Keywords:
Piezoelectric composites
Effective properties
Imperfect interface
Interface model
Finite Element Method

ABSTRACT

Piezoelectric materials are able to produce an electrical response when mechanically stressed (sensors) and inversely high precision motion can be obtained with the application of an electrical field (actuators). The macroscopic properties of piezoelectric composites depend upon the properties and the interfacial bonding conditions of the constituent phases, and the microstructures of the composites. In the present work, a new imperfect interface model for a thin elastic interface is derived. Square unit cell model was used to calculate all coefficients of the material tensor. The calculation was performed via FE package ABAQUS™. A computational procedure, based on Python language, was developed to systematically calculate all RVE effective coefficients. Comparisons to classical Hashin's and Nairn's interface model show very accurate agreement for debonding and perfect boding interface.

1. Introduction

Piezoelectric materials are able to produce an electrical response when mechanically stressed (sensors) and inversely high precision motion can be obtained with the application of an electrical field (actuators). Sensitivity analysis [1] and optimization techniques [2–4] are applied to maximize the piezoelectric actuator efficiency.

The macroscopic properties of piezoelectric composites depend upon the properties and the interfacial bonding conditions of the constituent phases, and the microstructures of the composites. Thus the effect of the interfacial bonding conditions on the mechanical and physical properties of various composites has attracted a lot of attention of researchers in many fields, especially, in physics, materials science and technology, and mechanics. The prediction of the effective moduli taking into account interface effect is one of the fundamental problems in mechanics of composites [5–10].

Modeling interface, which are often finite-thickness interphases, in composite materials is difficult. Interfaces play an important role in determining the performance of structural materials on a wide variety of dimension scales, from grain boundaries in metals, to inter-laminar bonds in composites and adhesive bonds in a large variety of structures. In all cases, a basic goal of nondestructive evaluation is the determination of the integrity of bonds. In fact, several properties of materials, such as, just to make a couple of examples, the mechanical behavior under stress [11] or the ultrasonic reflection coefficient of the interface [12], are very sensitive to boundary imperfections [13].

Regarding analytical models, different approaches have been proposed. Broutman and Agarwal [14], Theocaris et al. [15] and Sideridis [16] have considered the interphase as a layer between fiber (on inclusion) and matrix, of specified thickness and of elastic constants different from those of the matrix and the fiber. For an alternate model, a very thin interfacial zone of unspecified thickness has been considered. In that model, it is assumed that the radial and the tangential tractions are continuous across the interphase, but the displacements may be discontinuous from fiber to matrix due to the presence of the interphase. The tractions are assumed to be proportional to the corresponding displacement discontinuities. The proportionality constants then characterized the stiffness of the interphase, which is represented by spring layer model. Lene and Leguillar [17], Benveniste [18], Aboudi [19], Steif and Hoysan [20], Achenbach and Zhu [21], and Hashin [22–24] are some works related to spring layer model.

One way to model interphases is to abandon attempts for explicit modeling and instead replace 3D interphases with 2D interfaces [22]. The interphase effects are reduced for modeling the response of 2D interfaces due to tractions normal and tangential to the

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http://dx.doi.org/10.1016/j.compstruct.2016.02.003
0263-8223/

interfacial surface, which can be modeled by interface traction laws. Elimination of 3D interphases removes the resolution problem. The use of interface traction laws replaces numerous unknown and potentially unmeasurable interphase properties with a much smaller number of interface parameters. If interface traction laws can be determined, one can potentially model interphase effects well. That approach for interphase modeling was developed for analytical modeling of interface effects in composite materials [25–28], and for wave transmission in damage planes [29].

In the present work, a new imperfect interface model for a thin elastic interface is derived. A three dimensional (3D) representative volume element (RVE) model was developed for analyzing effective properties of piezoelectric fiber embedded in a non-piezoelectric matrix composite with imperfect interface using suitable interface models (including a new one), which were compared in terms of their capability to determine the effective coefficients. Square unit cell model was used to calculate all coefficients of the material tensor. The calculation was performed via FE package ABAQUS™. A computational procedure, based on Python language, was developed to systematically calculate all RVE effective coefficients. It is important to highlight that Tita et al. [30] presented the numerical approach to evaluate the effective properties of different volume fractions for piezoelectric fibers (with circular and square cross section) embedded in a non-piezoelectric matrix using only a Hashin's modified interface model. However, in the present work, the proposed interface model is more generalized than Hanshin's and Nairn's interface model, and it was used for determining the effective properties of different volume fractions for piezoelectric fibers (with only circular cross section) embedded in a non-piezoelectric matrix. Therefore, Nairn's interface model can be considered as a particular case of the proposed model. Comparisons to classical Hashin's and Nairn's interface model show very accurate agreement for debonding and perfect boding interface.

2. Constitutive equations, Finite Element Method and representative volume element (FEM–RVE)

Considering that, the piezoelectric materials respond linearly to changes to mechanical and electrical fields. A three-phase reinforced piezoelectric composite is studied here, in which the fiber has homogeneous and transversely isotropic properties. In addition, the matrix and the interface have homogeneous and isotropic properties. Three standard notation systems are commonly used to describe the constitutive modeling of linear-piezoelectric materials. Using the conventional indicial notation in which repeated subscripts are summed over the range of $i, j, k, l = 1, 2, 3$, the constitutive equations can be written as follow:

$$\begin{aligned} \sigma_{ij} &= C^{E}_{ijkl}\varepsilon_{kl} - e_{kij}\,E_{k,} \\ D_i &= e_{ikl}\,\varepsilon_{kl} + \kappa^{S}_{ij}\,E_{j,} \end{aligned} \tag{1}$$

where σ_{ij} and ε_{ij} are respectively the stress and infinitesimal strain tensors, D_i and E_i are the electric displacement and electric field vectors. The elastic tensor C^E_{ijkl}, the piezoelectric tensor e_{ijk} and the dielectric tensor κ^S_{ij} possess the following symmetry properties $C^E_{ijkl} = C^E_{ijlk} = C^E_{jikl} = C^E_{klij}$, $e_{ijk} = e_{ikj}$, $\kappa^S_{ij} = \kappa^S_{ji}$. In addition, the superscript E indicates constant electric field, while the superscript S indicates constant strain.

For a transversally isotropic piezoelectric material, the constitutive equation can be written in terms of the following expanded matrix form:

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{31} \\ D_1 \\ D_2 \\ D_3 \end{Bmatrix} = \begin{bmatrix} C^E_{11} & C^E_{12} & C^E_{13} & 0 & 0 & 0 & 0 & 0 & -e_{13} \\ C^E_{13} & C^E_{11} & C^E_{13} & 0 & 0 & 0 & 0 & 0 & -e_{13} \\ C^E_{13} & C^E_{13} & C^E_{33} & 0 & 0 & 0 & 0 & 0 & -e_{33} \\ 0 & 0 & 0 & C^E_{66} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & C^E_{44} & 0 & 0 & -e_{15} & 0 \\ 0 & 0 & 0 & 0 & 0 & C^E_{44} & -e_{15} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & e_{15} & \kappa^S_{11} & 0 & 0 \\ 0 & 0 & 0 & 0 & e_{15} & 0 & 0 & \kappa^S_{11} & 0 \\ e_{13} & e_{13} & e_{33} & 0 & 0 & 0 & 0 & 0 & \kappa^S_{33} \end{bmatrix} \begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{12} \\ \varepsilon_{23} \\ \varepsilon_{31} \\ E_1 \\ E_2 \\ E_3 \end{Bmatrix}, \tag{2}$$

where the contracted Voigt notation is used. In Eq. (2), the 3-axis is aligned with the principle direction of polarization.

In classical lamination theory, the composite lamina is modeled as a homogeneous orthotropic medium with certain effective moduli that describe the 'average' material properties of the composite. For micromechanical analysis, composites can be studied using representative volume element (RVE) or unit cell. The RVE is the smallest portion of the actual composite, which has same elastic, dielectric and piezoelectric constants and fiber volume fraction of the investigated material. It is a microstructural model of a material, which can be used to obtain the response of the corresponding homogenized macroscopic continuum in a macroscopic material point. Thus, the proper choice of the RVE determines largely the accuracy of the modelling of a heterogeneous material. In present work, the RVE are assumed as combinations of piezoelectric fibers embedded in a polymer matrix, including an interface, obeying a specified fiber volume fraction. This representative volume element (RVE) is modeled by solid finite elements. Thus, the numerical model is used to determine a homogeneous medium equivalent to the original composite and, as commented earlier, comprises the smallest portion of the piezoelectric composite, which keeps the most representative combination of its main materials. Thus, it is assumed that the average mechanical and electrical properties of a unit cell are equal to the average properties of the composite material as follow:

$$\begin{aligned} \bar{\sigma}_{ij} &= \langle\sigma_{ij}\rangle = \frac{1}{|V|}\int_V \sigma_{ij}\,dV, \quad \bar{\varepsilon}_{ij} = \langle\varepsilon_{ij}\rangle = \frac{1}{|V|}\int_V \varepsilon_{ij}\,dV, \\ \bar{D}_i &= \langle D_i\rangle = \frac{1}{|V|}\int_V D_i\,dV, \quad \bar{E}_i = \langle E_i\rangle = \frac{1}{|V|}\int_V E_i\,dV, \end{aligned} \tag{3}$$

where $|V|$ is the unit cell volume.

Discretizing Eq. (3) using the Finite Element Method (FEM), the average values can be calculated by:

$$\begin{aligned} \bar{\sigma}_{ij} &= \frac{1}{|V|}\sum_{n=1}^{nel}\sigma^{(n)}_{ij}\;V^{(n)}, \quad \bar{\varepsilon}_{ij} = \frac{1}{|V|}\sum_{n=1}^{nel}\varepsilon^{(n)}_{ij}\;V^{(n)}, \\ \bar{D}_i &= \frac{1}{|V|}\sum_{n=1}^{nel}D^{(n)}_{i}\;V^{(n)}, \quad \bar{E}_i = \frac{1}{|V|}\sum_{n=1}^{nel}E^{(n)}_{i}\;V^{(n)}, \end{aligned} \tag{4}$$

where nel is the number of finite elements of the complete unit cell, $V^{(n)}$ is the volume of the nth element, and $\sigma^{(n)}_{ij}$, $\varepsilon^{(n)}_{ij}$, $D^{(n)}_i$ and $E^{(n)}_i$ are the respective tensors evaluated in the nth element.

For a complete description of a differential problem in order to determine effective material properties, it is necessary to formulate appropriate boundary conditions. Since periodic structures are investigated so called periodic boundary conditions are applied to the considered RVE. Considering of the composite as a periodical array of the RVEs, the periodic boundary conditions must be applied to the RVE models. This implies that each RVE in the composite has the same deformation mode and there is no separation or overlap between the neighboring RVEs. For any parallelepiped