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Material properties of piezoelectric composites by BEM and homogenization method

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Abstract

Applications of boundary element method (BEM) to piezoelectric composites in conjunction with homogenization approach for determining their effective material properties are discussed in this paper. The composites considered here consist of inclusion and matrix phases. The homogenization model for composites with inhomogeneities is developed and introduced into a BE formulation to provide an effective means for estimating overall material constants of two-phase composites. In this model, a representative volume element (RVE) is used whose volume average stress and strain are calculated by the boundary tractions and displacements of the RVE. Thus BEM is suitable for performing calculations on average stress and strain fields of the composites. Numerical results for a piezoelectric plate with circular inclusions are presented to illustrate the application of the proposed micromechanics—BE formulation.

Keywords: Piezoelectric; Effective property; BEM; Micromechanics

1. Introduction

The determination of effective properties for piezoelectric composite consisting of inclusion and matrix phases has received considerable attention during the past decades. It is well known that the effective properties of such composites depend on the physics and geometry of the two phases. For estimating the overall properties of the composite, the equivalent inclusion method is a popular approach. It is based on Eshelby's eigenstrain solution for single inclusions embedded into infinite matrix [1] and the effective properties can be expressed in terms of the volume fraction and geometries of the inclusion as well as the properties of the components. Over recent years various methods have been developed based on this approach and have been used widely in determining the overall properties of various composite materials [2–4]. Among them most typical approaches are the dilute scheme [5], the self-consistent method [6], the generalized self-consistent method [7], the Mori–Tanaka method [8,9] and the differential method [10]. Common to each of these micromechanics theories is the use of the well-known stress and strain concentration factors obtained through an analytical solution of a single crack, or void, or inclusion embedded in an infinite medium. However, for a problem with complexity in the aspects of geometry and mechanical deformation, a combination of these approaches and numerical methods such as finite element method (FEM) and boundary element method (BEM) presents a powerful computational tool for estimating effective material properties. It should be mentioned that the main disadvantage of the FEM is that domain discretization is required to perform the analysis. Moreover, in some cases it results in both an inaccurate and an expensive technique, especially in solving crack or some special inclusion problems. On the other hand, the BE method involves discretization of the boundary of a structure only, because the governing differential equation is satisfied exactly inside the domain, leading to a relatively smaller system size with sufficient accuracy. Moreover, in the present micromechanics model, the average strain and electric field (SEF) are calculated through the boundary displacement and electric

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potential (DEP) of the solid only. Therefore, BE approach is very suitable for performing this type of calculation. In this paper, a BEM based micromechanics algorithm is proposed for analyzing overall properties of piezoelectric material with inclusions or voids of various shapes. The algorithm is based on two typical micromechanics models (self-consistent and Mori–Tanaka methods) and boundary element formulation. An iterative scheme is designated for the self-consistent BE method. Numerical results of effective material constants are obtained by the proposed formulation for a piezoelectric solid with circular inclusions.

2. Homogenization approach

2.1. Basic formulations

Let us consider a piezoelectric composite in which the inclusions or holes are in cylindrical shape. In this case both the matrix and the inclusion can be viewed as transversely isotropic and coupling between in-plane stresses and in-plane electric fields takes place. For a Cartesian coordinate system *Oxyz*, choose the *z*-axis as the poling direction, and denote the coordinates *x* and *z* by x_1 and x_2 in order to get a compacted notation. The plane strain constitutive equations are expressed by [9]

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \\ D_1 \\ D_2 \end{Bmatrix} = \begin{bmatrix} c_{11} & c_{12} & 0 & 0 & e_{21} \\ c_{12} & c_{22} & 0 & 0 & e_{22} \\ 0 & 0 & c_{33} & e_{13} & 0 \\ 0 & 0 & e_{13} & -\kappa_{11} & 0 \\ e_{21} & e_{22} & 0 & 0 & -\kappa_{22} \end{bmatrix} \begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \\ -E_1 \\ -E_2 \end{Bmatrix} \tag{1}$$

or inversely

$$\begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ 2\varepsilon_{12} \\ -E_1 \\ -E_2 \end{Bmatrix} = \begin{bmatrix} f_{11} & f_{12} & 0 & 0 & p_{21} \\ f_{12} & f_{22} & 0 & 0 & p_{22} \\ 0 & 0 & f_{33} & p_{13} & 0 \\ 0 & 0 & p_{13} & -\beta_{11} & 0 \\ p_{21} & p_{22} & 0 & 0 & -\beta_{22} \end{bmatrix} \begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \\ D_1 \\ D_2 \end{Bmatrix} \tag{2}$$

and simply, in matrix form

$$\mathbf{\Pi} = \mathbf{CZ}, \quad \mathbf{Z} = \mathbf{F\Pi}, \tag{3}$$

where σ_{ij}, ε_{ij}, D_j and E_j are stress, strain, electric displacement, and electric field, respectively; c_{ij} is elastic stiffness; f_{ij} elastic compliance; e_{ij} and p_{ij} are piezoelectric constants; κ_{ij} and β_{ij} dielectric permittivity; $\mathbf{F} = \mathbf{C}^{-1}$; and

$$\begin{aligned} \mathbf{\Pi} &= \{\Pi_i\}^{\mathrm{T}} = \{\sigma_{11} \quad \sigma_{22} \quad \sigma_{12} \quad D_1 \quad D_2\}^{\mathrm{T}}, \\ \mathbf{Z} &= \{Z_i\}^{\mathrm{T}} = \{\varepsilon_{11} \quad \varepsilon_{22} \quad 2\varepsilon_{12} \quad -E_1 \quad -E_2\}^{\mathrm{T}}, \end{aligned} \tag{4}$$

$$\varepsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i}), \quad (-E_i) = \phi_{,i} \tag{5}$$

with u_i being elastic displacement and ϕ the electric potential.

2.2. The representative volume element

In our analysis, a representative volume element (RVE) Ω is chosen so as to be statistically representative of the two-phase composite. In particular, the characteristic size of the heterogeneities is supposed to be small with respect to the dimension of the RVE, which in turn is supposed to be small compared to the wavelength of the macroscopic structure.

In order to understand the key point of the homogenization procedure, let us consider a RVE consisting of the matrix material and inclusion phase (see Fig. 1). As a RVE is comprised of different materials, the microconstitutive law that governs each material or phase in a RVE is given by the standard constitutive law. On the other hand, the macro-SED and macro-SEF on the macro-level are directly associated with the global analysis of a two-phase composite. On the macro-level, a RVE is regarded just as a point with a homogenized constitutive law. The macro-SED, $\overline{\Pi}_i$, is usually defined as the volume average of SED in a RVE, $\langle \Pi_i \rangle$, as follows:

$$\overline{\Pi}_i = \langle \Pi_i \rangle_\Omega = \frac{1}{V}\int_\Omega \Pi_i \,\mathrm{d}\Omega, \tag{6}$$

where Ω is the domain of the RVE and V is its volume. Similarly, the volume average of SEF $\overline{Z}_i$ and the volume average of free energy density $\overline{W}$ in a RVE is defined by

$$\overline{Z}_i = \langle Z_i \rangle_\Omega = \frac{1}{V}\int_\Omega Z_i \,\mathrm{d}\Omega, \tag{7}$$

$$\begin{aligned} \overline{W} &= \frac{1}{V}\int_\Omega W \,\mathrm{d}\Omega = \frac{1}{2V}\int_\Omega \Pi_i Z_i \,\mathrm{d}\Omega \\ &= \frac{1}{2V}\int_\Omega C_{ij} Z_i Z_j \,\mathrm{d}\Omega = \frac{1}{2V}\int_\Omega F_{ij} \Pi_i \Pi_j \,\mathrm{d}\Omega, \end{aligned} \tag{8}$$

where $(\mathbf{C})_{ij} = C_{ij}$ and $(\mathbf{F})_{ij} = F_{ij}$ are, respectively, local stiffness and local compliant coefficients which are different from phase to phase. Moreover, the macroscopic strain energy should satisfy

$$\overline{W} = \frac{1}{2}\overline{\Pi}_i \overline{Z}_i. \tag{9}$$

The effective properties represented by effective stiffness C^*_{ij} or compliancy F^*_{ij} of the piezoelectric composites can be defined by the average SED and SEF as

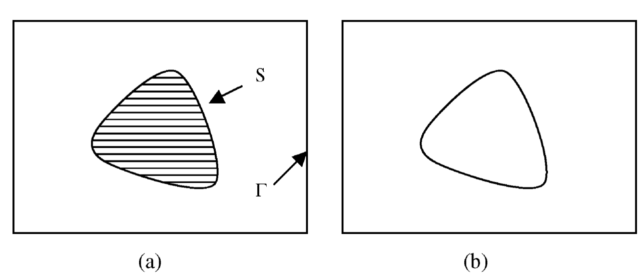

Fig. 1. RVE model used in FE and BE analysis: (a) RVE with an inclusion; (b) RVE with a void.

$$\overline{\Pi}_i = C^*_{ij}\overline{Z}_j, \quad \overline{Z}_i = F^*_{ij}\overline{\Pi}_j \tag{10}$$

or by the equivalence of the free strain energy

$$\frac{1}{2}\overline{\Pi}_i\overline{Z}_i = \frac{1}{2V}\int_{\Omega}\Pi_i Z_i\,\mathrm{d}\Omega \tag{11}$$

or

$$\frac{1}{2}\overline{C}_{ij}\overline{Z}_i\overline{Z}_j = \frac{1}{2V}\int_{\Omega}C_{ij}Z_iZ_j\,\mathrm{d}\Omega. \tag{12}$$

The linearity of stress–strain relation for elastic body leads to

$$\overline{C}_{ij} = \frac{\partial^2\overline{W}}{\partial\overline{Z}_i\partial\overline{Z}_j}. \tag{13}$$

Then an explicit form of the effective stiffness components can be evaluated as below.

2.3. Homogenization model

The homogenization method for a composite with defects has been discussed elsewhere [2,11]. For the reader's convenience we describe the method here briefly.

For piezoelectric materials with inclusions or microcavities, the homogenization theory may be established based on some fundamental results in the theory of two-phase linear piezoelectric media. In the case of two-phase materials, the volume average of SED and SEF tensors is defined by

$$\langle\mathbf{\Pi}\rangle = v^{(1)}\langle\mathbf{\Pi}^{(1)}\rangle + v^{(2)}\langle\mathbf{\Pi}^{(2)}\rangle,$$
$$\langle\mathbf{Z}\rangle = v^{(1)}\langle\mathbf{Z}^{(1)}\rangle + v^{(2)}\langle\mathbf{Z}^{(2)}\rangle, \tag{14}$$

where superscripts "(1)" and "(2)" denote the matrix and inclusion phases, $v^{(1)}$ and $v^{(2)}$ their volume fractions. Substituting Eq. (14) into Eq. (10) and noting that $\mathbf{\Pi}^{(i)} = \mathbf{C}^{(i)}\mathbf{Z}^{(i)}$, we have

$$\mathbf{C}^* = \mathbf{C}^{(1)} + (\mathbf{C}^{(2)} - \mathbf{C}^{(1)})\mathbf{A}^{(2)}v^{(2)},$$
$$\mathbf{F}^* = \mathbf{F}^{(1)} + (\mathbf{F}^{(2)} - \mathbf{F}^{(1)})\mathbf{B}^{(2)}v^{(2)} \tag{15}$$

in which the symmetric tensors $\mathbf{A}^{(2)}$ and $\mathbf{B}^{(2)}$ are defined by the linear relations

$$\langle\mathbf{Z}^{(2)}\rangle = \mathbf{A}^{(2)}\mathbf{Z}^0, \quad \langle\Pi^{(2)}\rangle = \mathbf{B}^{(2)}\Pi^0 \tag{16}$$

with $\mathbf{Z}^0$ and $\mathbf{\Pi}^0$ being remote SEF and SED fields applied on the effective medium. The interpretation of $\langle\mathbf{Z}^{(2)}\rangle$ in Eq. (16) follows from the average strain theorem [12]:

$$\langle Z^{(2)}_{ij}\rangle = \frac{1}{2\Omega_2}\int_{\partial\Omega_2}\{[1 + H(i-3)]U_in_j\} + U_jn_i\,\mathrm{d}\Omega, \tag{17}$$

where Ω_2 and $\partial\Omega_2$ are the total volume and boundary of the inclusion or void, $H(i)$ is the Heaviside step function, $\mathbf{n} = \{n_1, n_2, 0\}^{\mathrm{T}}$ is the normal local to inclusion surface, and

$$\{Z_{11}, Z_{22}, 2Z_{12}, Z_{31}, Z_{32}\} = \{\varepsilon_{11}, \varepsilon_{22}, 2\varepsilon_{12}, -E_1, -E_2\},$$
$$\{U_i\} = \{u_1, u_2, \phi\}. \tag{18}$$

We consider now the case when inclusions become voids which are thought of as being filled with air. This implies that $\mathbf{C}^{(2)} \to 0, \mathbf{F}^{(2)} \to \infty$. Thus we assume $\mathbf{C}^{(2)} = 0$, where $\mathbf{C}^{(2)}$ stands for stiffness constants of the void-phase. Then Eq. (15) become

$$\mathbf{C}^* = \mathbf{C}^{(1)}(\mathbf{I} - \mathbf{A}^{(2)}v^{(2)}), \quad \mathbf{F}^* = \mathbf{F}^{(1)}(\mathbf{I} + \mathbf{B}^{(0)}v^{(2)}), \tag{19}$$

where $\mathbf{I}$ is the unit tensor and $\mathbf{B}^{(0)}$ is defined by

$$\langle\mathbf{Z}^{(2)}\rangle = \mathbf{F}^{(1)}\mathbf{B}^{(0)}\mathbf{\Pi}^0. \tag{20}$$

Therefore, the estimation of integral (17) and thus, $\mathbf{A}^{(2)}$ is the key to predicting the effective electroelastic moduli $\mathbf{C}^*$. The calculation of integral (17) through use of boundary element method is the subject of subsequent section.

3. Boundary element equations

In this section, a two domain boundary element model is introduced for DEP and SED on the boundary of each domain. The two subdomains are separated by the interfaces between fiber and matrix (see Fig. 1). Each subdomain can be separately modelled by a direct BEM. A global assembly of the boundary element subdomains is then performed by enforcing continuity of the DEP and SED at the subdomain interface.

In two-dimensional piezoelectric composite, the BE formulation takes the form [13]

$$c^{(\alpha)}(\xi)U^{(\alpha)}_i(\xi) = \int_{S^{(\alpha)}}[U^{*(\alpha)}_{ij}(\mathbf{x},\xi)T^{(\alpha)}_j(\mathbf{x}) - T^{*(\alpha)}_{ji}(\mathbf{x},\xi)U^{(\alpha)}_j(\mathbf{x})]\,\mathrm{d}S(\mathbf{x}), \tag{21}$$

where the superscript "(α)" stands for the quantity associated with the αth phase ($\alpha = 1$ being matrix and $\alpha = 2$ being fiber) $T_i = \sigma_{ij}n_j$ $(i = 1, 2)$, $T_3 = D_in_i$ and

$$S^{(\alpha)} = \begin{cases} S + \Gamma, & \alpha = 1, \\ S, & \alpha = 2, \end{cases}$$
$$c^{(\alpha)}(\xi) = \begin{cases} 1 & \text{if } \xi \in \Omega^{(\alpha)}, \\ 0.5 & \text{if } \xi \in S^{(\alpha)} \ (S^{(\alpha)} \text{ smooth}), \\ 0 & \text{if } \xi \notin \Omega^{(\alpha)} \cup S^{(\alpha)}, \end{cases} \tag{22}$$

$$[U^*_{ij}] = \begin{bmatrix} u^*_{11} & u^*_{12} & -\phi^*_1 \\ u^*_{21} & u^*_{22} & -\phi^*_2 \\ u^*_{31} & u^*_{32} & -\phi^*_3 \end{bmatrix},$$
$$[T^*_{ij}] = \begin{bmatrix} t^*_{11} & t^*_{12} & -\omega^*_1 \\ t^*_{21} & t^*_{22} & -\omega^*_2 \\ t^*_{31} & t^*_{32} & -\omega^*_3 \end{bmatrix} \tag{23}$$

in which Γ and S are the boundaries of the RVE and inclusions, respectively (see Fig. 1), u_{ij}^* and t_{ij}^* $(i,j=1,2)$ denote, respectively, the displacement and traction component in the jth direction at a field point $\mathbf{x}$ due to an unit point force acting in the ith direction at source point $\boldsymbol{\xi}$, u_{3i}^* and t_{3i}^* $(i=1,2)$ represent the ith displacement and traction at $\mathbf{x}$ due to an unit electric charge at $\boldsymbol{\xi}$, ϕ_i^* and ω_i^* $(i=1,2)$ stand for the electric potential and surface charge at $\mathbf{x}$ due to an unit point force acting in the ith direction at $\boldsymbol{\xi}$, ϕ_3^* and ω_3^* denote the electric potential and surface charge at $\mathbf{x}$ due to an unit electric charge at $\boldsymbol{\xi}$. These fundamental solutions are well documented in the literature and can be found in [13].

To obtain a weak solution of Eq. (21) as in the conventional BEM, the boundary $S^{(\alpha)}$ is divided into a series of boundary elements. After performing discretization using various kinds of boundary element (e.g., constant element, linear element, higher-order element) and collecting the unknown terms to the left-hand side and the known terms to the right-hand side, as well as using continuity conditions at the interface S (Fig. 2), the boundary integral equation (21) becomes a set of linear algebraic equations:

$$\mathbf{AY} = \mathbf{P}, \tag{24}$$

where $\mathbf{Y}$ and $\mathbf{P}$ are the total unknown and known vectors, respectively, and $\mathbf{A}$ is a known coefficient matrix.

When the fiber in Fig. 1a becomes a hole, the boundary integral equation (21) still holds true if one takes $\alpha = 1$ only. In this case the interfacial continuity condition is replaced by the hole boundary condition: $T_j = 0$ along the boundary S (Fig. 1b).

4. Algorithms for self-consistent and Mori–Tanaka approaches

4.1. Self-consistent BEM approach

As stated in [4,9], in the self-consistent method, for each inclusion (or hole), the effect of inclusion (or hole) interaction is taken into account approximately by embedded each inclusion (or hole) in the effective medium whose properties are unknown. In this case, the material constants appeared in the boundary element formulation (21) are unknown. A set of initial trial values of the effective properties is, consequently, needed and an iteration algorithm is required. The algorithm is described in detail below:

(a) Assume initial values of material constants $\mathbf{C}^*_{(0)}$.
(b) Solve Eq. (16) for $\mathbf{U}_{(i)}$ using the values of $\mathbf{C}^*_{(i-1)}$, where the subscript "(i)" stands for the variable associated with the ith iterative cycle.
(c) Calculate $\mathbf{A}^{(2)}_{(i)}$ in Eq. (16) by way of Eq. (17) and using the current values of $\mathbf{U}_{(i)}$, and then determine $\mathbf{C}^*_{(i)}$, by way of Eq. (19).
(d) If $\varepsilon_{(i)} = \|\mathbf{C}^*_{(i)} - \mathbf{C}^*_{(i-1)}\| / \|\mathbf{C}^*_{(0)}\| \leqslant \varepsilon$, where ε is a convergent tolerance, terminate the iteration; otherwise take $\mathbf{C}^*_{(i)}$ as the initial value and go to step (b).

4.2. Mori–Tanaka-BEM approach

The key assumption in the Mori–Tanaka theory [8,11] is that the concentration matrix $\mathbf{A}^{(2)}_{\mathrm{MT}}$ (here we use $\mathbf{A}^{(2)}_{\mathrm{MT}}$, rather than $\mathbf{A}^{(2)}$, is just for distinction with $\mathbf{A}^{(2)}$ in Section 2) is given by the solution for a single inclusion (or void) embedded in an intact solid subject to an applied strain field equal to the as yet unknown average field in the composite, which means that the introduction of inclusions in the composite results in a value of $\overline{\mathbf{Z}}^{(2)}$ given by

$$\overline{\mathbf{Z}}^{(2)} = \mathbf{A}^{(2)}_{\mathrm{DIL}} \overline{\mathbf{Z}}^{(1)}, \tag{25}$$

where $\mathbf{A}^{(2)}_{\mathrm{DIL}}$ is the concentration matrix related to the dilute model, which can be calculated by way of Eqs. (16), (17) and (21). In this case, the material constants appeared in the boundary element formulation (21) are all known. As such, it is easy to prove that [4,11]

$$\mathbf{A}^{(2)}_{\mathrm{MT}} = \mathbf{A}^{(2)}_{\mathrm{DIL}} (v_1 \mathbf{I} + v_2 \mathbf{A}^{(2)}_{\mathrm{DIL}})^{-1}. \tag{26}$$

It can be seen from Eq. (26) that the Mori–Tanaka approach provides explicit expressions for effective constants of defective piezoelectric solid. Therefore, no iteration is required with Mori–Tanaka–BE method.

5. Numerical results

As a numerical illustration of the proposed approach, the example of a square RVE with a circular rigid insulating fiber was analyzed. The matrix used in the present example is chosen to be BaTiO3 and its material constants are as follows [9]:

$$c^0_{11} = 150 \text{ GPa}, \quad c^0_{12} = c^0_{13} = 66 \text{ GPa},$$
$$c^0_{33} = 146 \text{ GPa}, \quad c^0_{44} = 44 \text{ GPa},$$
$$e^0_{31} = -4.35 \text{ C/m}^2, \quad e^0_{33} = 17.5 \text{ C/m}^2,$$
$$e^0_{15} = 11.4 \text{ C/m}^2,$$

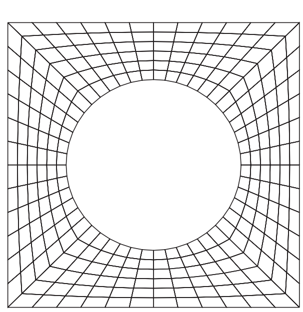

Fig. 2. The meshes used in FE and BE calculation.

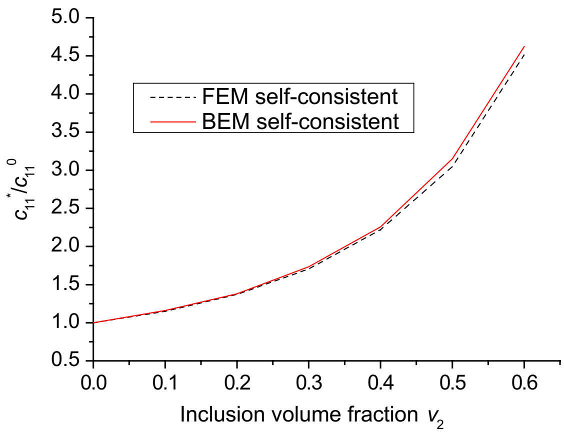

Fig. 3. Normalized modulus c_{11}^*/c_{11}^0 vs inclusion volume fraction v_2.

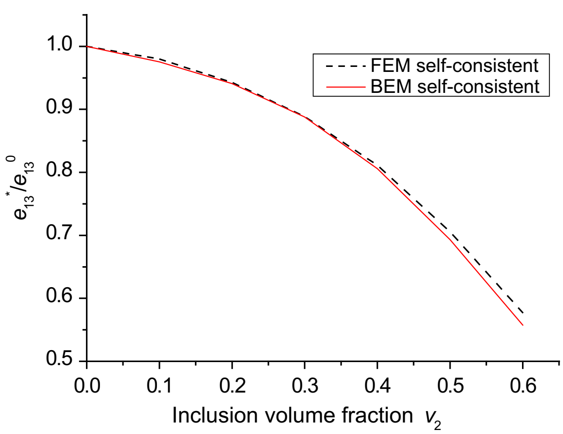

Fig. 4. Normalized modulus piezoelectric constant e_{13}^*/e_{13}^0 vs v_2.

$$\kappa_{11}^0 = 1115\kappa_0, \quad \kappa_{33}^0 = 1260\kappa_0,$$
$$\kappa_0 = 8.85 \times 10^{-12}\ \mathrm{C^2/N\,m^2}.$$

Some numerical results were obtained and comparison is made with those from the FE method. For simplicity, it is assumed that the rigid fiber has infinite length so that it can be treated as plane strain problem. When a specific uni-axial SEF state (generally unit SEF for simplicity) is applied in a unit cell, the average stresses are calculated by BEM or FEM. Then the plane-strain material coefficients of the composite can be obtained.

Both the BEM and FEM calculations are carried out for numerical comparison. In the finite element model, the 8-node quadratic element is employed. The BEM model uses the mesh on the boundary of the finite element model. The mesh used in the BEM and FEM calculation is shown in Fig. 2. It has 96 boundary elements and 192 nodes.

The results obtained from both the FEM and BEM are depicted in Figs. 3 and 4. Fig. 3 shows the normalized effective modulus c_{11}^*/c_{11}^0 as a function of the inclusion volume fraction v_2. It is found that the two methods provide almost the same results. The normalized effective piezoelectric constant e_{13}^*/e_{13}^0 vs inclusion volume fraction is shown in Fig. 4, where the results from BEM and FEM method are observed to agree within plotting accuracy. It is evident that for piezoelectric matrix reinforced by rigid inclusions, the normalized effective modulus c_{11}^*/c_{11}^0 increases along with the increase of inclusion volume fraction v_2, while the normalized effective piezoelectric constant e_{13}^*/e_{13}^0 decreases with the increase of inclusion volume fraction.

6. Conclusions

A BEM based homogenization model of a piezoelectric composite with inclusions or voids is presented for estimating overall material properties. The proposed formulation is capable of modeling two-phase composites with inhomogeneities such as holes or inclusions of various shapes. The study indicates that the boundary field values of a RVE are sufficient for calculation of the effective properties of the two-phase composites mentioned above. As a consequence, the calculation of internal fields can be omitted. The numerical example shows that the results from BEM are in agreement with those by FEM, but with less degree of freedom.

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