Micromechanics-BE solution for properties of piezoelectric materials with defects

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Abstract

A micromechanics boundary element (BE) algorithm is developed to predict the overall properties of a piezoelectric material with defects such as cracks or holes. The algorithm is based on micromechanics models and boundary element formulation for piezoelectric materials with cracks or holes. In particular, the self-consistent and Mori–Tanaka methods are considered. A representative volume model for materials with defects is employed and introduced into a BE formulation to provide an effective means for estimating overall material constants of the defected materials. The micromechanics method produces formulas for overall material constants as functions of the concentration matrix $A_2$, and $A_2$ is in turn related to the boundary displacement. The boundary element simulation presents numerical solutions of boundary displacement and electric potential for crack or hole problems. In the micromechanics-BE model, the volume (or area) average stress and strain is calculated by the boundary tractions and displacements of the RVE. Thus BEM is suitable for performing calculations on average stress and strain fields of such defected materials. An iterative scheme is introduced for the self-consistent-BE method. Numerical results for a piezoelectric plate with elliptic holes are presented to illustrate the application of the proposed micromechanics BE formulation.

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1. Introduction

The problem of reduction in stiffness of engineering materials due to the development or presence of multiple defects such as cracks or voids is of scientific significance and engineering importance and has been the subject of many investigations. By relating this stiffness reduction to the state of microcracking or microvoiding, it may be possible to assess the integrity of a structure and the mechanism of failure in materials [1–4]. Over the past decades, several approaches have been proposed to estimate the stiffness reduction of a cracked or voided solid. 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 well-known stress and strain concentration factors obtained through the solution of a single crack or hole embedded in an infinite medium. However, for a complex problem where complexity lies in the aspects of geometry and mechanical deformation, a combination of these approaches with numerical methods such as finite element (FE) and BE methods presents a powerful computational tool for estimating effective material properties. It should be mentioned that the main disadvantage of the FE method 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 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 are calculated through the boundary displacement and electric potential of the solid only. Therefore, the BE approach is very suitable for performing this type of calculation. In this paper, a micromechanics BE algorithm is
proposed for analysing the overall properties of piezoelectric material with cracks or voids of various shapes. The algorithm is based on two typical micromechanics models (self-consistent and Mori–Tanaka methods) and BE formulation. An iterative scheme is combined with the self-consistent BE method. Numerical results of effective material constants are obtained by the proposed formulation for a voided piezoelectric plate, and comparison is made with results obtained from a theoretical model [9].

2. Micromechanics models

In our analysis, the defective piezoelectric material is considered to be an infinite piezoelectric solid containing randomly distributed defects which may be cracks or holes. To obtain the effective properties of such materials, a representative volume (or area for 2D case) element (RVE) \( \Omega \) is chosen so as to be statistically representative of the infinite piezoelectric solid. In particular, the characteristic size of heterogeneities is supposed to be small with respect to the dimension of the RVE, which in turn is large compared to the scales of microstructural, but is still small compared to the entire body. Thus, micromechanics theories of the defective piezoelectric solid may be established based on some fundamental results in the theory of two-phase elastic media. In the case of two-phase materials, the volume average of a physical variable \( F \) is defined by

\[
F = v_1F_1 + v_2F_2
\]

where subscripts ‘1’ and ‘2’ denote the matrix and inclusion phases, respectively, \( v_1 \) and \( v_2 \) their volume (or area) fractions, and overbar denotes the volume (or area) average over a RVE, i.e.

\[
\langle \bullet \rangle = \frac{1}{\Omega} \int_{\Omega} \bullet \, d\Omega
\]

(2)

The overall elastic, piezoelectric, and dielectric constants of the piezoelectric solid, \( C^*, \varepsilon^*, \) and \( \kappa^* \) are defined by

\[
\varepsilon = C^* \varepsilon^* - (\varepsilon^*)^T \mathbf{E}, \quad \mathbf{D} = \varepsilon^* \varepsilon^* + \kappa^* \mathbf{E}
\]

(3)

where \( \varepsilon, \varepsilon^*, \mathbf{D}, \) and \( \mathbf{E} \) are, respectively, stress, strain, electric displacement and electric field tensor, and the superscript \( T \) stands for the transpose operation of a matrix.

Using definition (3) the following two types of boundary condition can be used to evaluate overall material properties:

(a) Uniform traction, \( \sigma^0 \), and electric displacement, \( \mathbf{D}^0 \), on boundary \( \Gamma \) of the RVE:

\[
\sigma = \sigma^0, \quad \mathbf{D} = \mathbf{D}^0
\]

(4)

(b) Uniform strain, \( \varepsilon^0 \), and electric field, \( \mathbf{E}^0 \), on boundary \( \Gamma \) of the RVE:

\[
\varepsilon = \varepsilon^0, \quad \mathbf{E} = \mathbf{E}^0
\]

(5)

Since the material behaviour is linear, the principle of superposition is used to decompose the load \( \langle \sigma^0, \mathbf{E}^0 \rangle \) into two elementary loadings \( \langle \sigma^0, \mathbf{E}^0 \rangle = 0 \) and \( \langle \varepsilon^0, \mathbf{E}^0 \rangle \). For the loading case \( \langle \varepsilon^0, \mathbf{E}^0 \rangle \), Eq. (3) becomes

\[
\sigma = C^* \varepsilon^0, \quad \mathbf{D} = \varepsilon^* \varepsilon^0
\]

(6)

Using relations (1) and (6), we have

\[
C^* = C_1 + (C_2 - C_1)A_2 v_2
\]

(7a)

\[
\varepsilon^* = \varepsilon_1 + (\varepsilon_2 - \varepsilon_1)A_2 v_2
\]

(7b)

where the concentration tensor \( A_2 \) is defined by the linear relation

\[
\varepsilon_2 = A_2 \varepsilon^0
\]

(8)

Following the average strain theorem [9], the strain tensor, \( \varepsilon_2 \), can be expressed as

\[
(\varepsilon_2)_{ij} = \frac{1}{2\Omega_2} \int_{I_2} (u_{i}n_j + u_jn_i) \, dS
\]

(9)

where \( \Omega_2 \) and \( I_2 \) are the total volume and boundary of phase 2, \( u_i \) is the \( i \)th component displacement vector, and \( n_i \) the \( i \)th component of unit outward vector normal to the boundary. When inclusions become cracks, Eq. (9) cannot be directly used to calculate the average strain. This problem can be bypassed by considering cracks to be very flat voids of vanishing height and thus also of vanishing volume. Multiplying both sides of Eq. (9) by \( v_2 \) and considering the limit of flattening out into cracks, i.e. \( v_2 = \Omega_2/\Omega \to 0 \), one obtains

\[
\lim_{v_2 \to 0} (\varepsilon_2)_{ij} = \frac{v_2}{2\Omega_2} \int_{L} (\Delta u_{i}n_j + \Delta u_jn_i) \, dS
\]

(10)

where \( \Delta u_i \) is the jump of displacement across the crack faces, \( L = l_1 \cup l_2 \cup \cdots \cup l_N, l_i \) is the length of \( i \)th crack, \( N \) the number of cracks within the RVE under consideration. For convenience, we define

\[
P = \lim_{v_2 \to 0} (A_2 v_2)
\]

(11)

where \( P \) can be calculated by the relation:

\[
(P \varepsilon^0)_{ij} = \lim_{v_2 \to 0} (\varepsilon_2)_{ij} = \frac{1}{2\Omega} \int_{L} (\Delta u_{i}n_j + \Delta u_jn_i) \, dS
\]

(12)

Substituting Eq. (11) into Eq. (7) and considering \( C_2 \to 0 \) and \( \varepsilon_2 \to 0 \) when inclusions become cracks, yields

\[
C^* = C_1 (I - P), \quad \varepsilon^* = \varepsilon_1 (I - P)
\]

(13)
On the other hand, for the loading case \( e^0 = 0, E^0 \), Eq. (3) leads to
\[
\sigma = -(e^*)^T E^0, \quad D = k^e E^0
\] (14)

Similar to the treatment in Eq. (7), we have
\[
e^* = e_1 + B_1(e_2 - e_1)v_2 \
\kappa^* = \kappa_1 + (\kappa_2 - \kappa_1)B_2v_2
\] (15a, 15b)

where the tensor \( B_2 \) is defined by
\[
E_2 = B_2 E_0
\] (16)

By comparing Eqs. (7b) and (15a), it is evident that
\[
(e_2 - e_1)A_2 = B_2(e_2 - e_1)
\] (17)

Therefore, the effective constitutive law (3) is completely defined once the concentration factor \( A_2 \) has been determined.

The estimation of integral equation (9) or (10) and thus \( A_2 \) (or \( P \)) is the key to predicting the effective electroelastic moduli \( C^e, e^*, \) and \( \kappa^* \). Calculation of integral equation (9) or (10) through the use of the BE method is the subject of the following section.

3. Boundary element formulation

Let us consider a linear piezoelectric RVE (Fig. 1) occupying the region \( \Omega \) with boundary \( \Gamma \). Further, let \( \Omega_1 \) be the region of the matrix and \( \Omega_2 \) the region occupied by the inhomogeneities. The BE formulation for such an RVE is in a different form for different inhomogeneities (Fig. 1). These formulations are described below.

(a) Cracks. The BE formulation presented in Refs. [11–13] is employed in our analysis. For illustration, consider a finite region \( \Omega \) bounded by \( \Gamma = \Gamma_1 + \Gamma_2 \), as shown in Fig. 2. The governing equation and the boundary conditions of the electroelastic problem to be considered are described as follows:
\[
\Pi_{ij} j = 0 \quad \text{in} \ \Omega, \quad \text{on} \ \Gamma_1 + \Gamma_2 \quad \text{on} \ \Gamma_1 + \Gamma_2
\] (18)

\[
t_{el} = \Pi_{ij} n_j = n_j^0 \quad \text{on} \ \Gamma_1
\] (19)

(b) Holes. For a linear piezoelectric solid, the BE formulation takes the form [14]
\[
C(\xi) U_{ij}(\xi) = \int_{S+I} \left[ T_{ij}(x, \xi) u_j(x) - T_{ij}(x, \xi) U_{ij}(x) \right] dS(x)
\] (26)

where \( U_{ij} \) and \( T_{ij} \) are fundamental solutions of EDEP and SED which have been defined in Ref. [14].
To obtain a weak solution of Eq. (26), as in the conventional BE method (BEM), the boundary \( S + \Gamma \) (Fig. 1) 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, constant element is used in our analysis) and collecting the unknown terms to the left-hand side and the known terms to the right-hand side, the boundary integral equation (26) becomes a set of linear algebraic equations:

\[
AY = P
\]

(27)

where \( Y \) and \( P \) are the total unknown and known vectors, respectively, and \( A \) is the known coefficient matrix.

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

4.1. Self-consistent BEM approach

As stated in Refs. [4,9], in the self-consistent method, for each crack (or hole), the effect of crack (or hole) interaction is taken into account approximately by embedding each crack (or hole) in the effective medium whose properties are unknown. In this case, the material constants appearing in each crack (or hole), the effect of crack (or hole) interaction is required with the Mori–Tanaka BE method. Therefore, no iteration is needed in our analysis. Consequently, a set of initial trial values of the effective properties is needed and an iteration algorithm is required. The algorithm is described in detail below.

(a) Assume initial values of material constants \( C_{\text{eff}}^0 \), \( e_{\text{eff}}^0 \), and \( k_{\text{eff}}^0 \) (\( C^0 = C_{\text{eff}}^0 = e_{\text{eff}}^0 = k_{\text{eff}}^0 \) are used as initial value in our analysis).

(b) Solve Eqs. (24) and (25) for \( b_{\text{me}0} \) (or Eq. (26) for \( U_i \)) using the values of \( C_{\text{eff}}^0 \), \( e_{\text{eff}}^0 \), and \( k_{\text{eff}}^0 \), where the subscript \( i \) stands for the variable associated with the \( i \)th iterative cycle.

(c) Calculate \( A_{i0} \) in Eq. (8) (or \( P \) in Eq. (11)) by way of Eq. (9) (or Eq. (12)) using the current values of \( b_{\text{me}0} \) (or \( U_i \)), and then determine \( C_{\text{eff}}^0 \), \( e_{\text{eff}}^0 \), and \( k_{\text{eff}}^0 \) by way of Eqs. (7) and (15).

(d) If \( \| F_{i0} - F_{i-1} \| / \| F_{i0} \| \leq \varepsilon \), where \( \varepsilon \) is a convergent tolerance, terminate the iteration; \( F \) may be \( C \), \( e \) or \( k \), otherwise take \( C_{\text{eff}}^0 \), \( e_{\text{eff}}^0 \), and \( k_{\text{eff}}^0 \) as the initial values and go to Step (b).

4.2. Mori–Tanaka-BEM approach

The key assumption in the Mori–Tanaka theory [15] is that the concentration matrix \( A_{\text{eff}}^\text{MT} \) (here, we use \( A_2^\text{MT} \), rather than \( A_2 \), simply to distinguish it from \( A_2 \) in Section 4.1, and \( P^\text{MT} \) for crack problems with the Mori–Tanaka approach) is given by the solution for a single void (or crack) embedded in an intact solid subject to an applied strain field equal to the as yet unknown average field in the solid, which means that the introduction of defects in the solid results in a value of \( \varepsilon_2 \) given by

\[
\varepsilon_2 = A_{\text{eff}}^{\text{DIL}} \varepsilon_1
\]

(28)

where \( A_{\text{eff}}^{\text{DIL}} \) is the concentration matrix related to the dilute model. As such, it is easy to prove that [4,9]

\[
A_2^\text{MT} = A_{\text{eff}}^{\text{DIL}} (\nu_1 I + \nu_2 A_{\text{eff}}^{\text{DIL}})^{-1}
\]

(29)

for hole problems, and

\[
P^\text{MT} = P^{\text{DIL}} (I + P^{\text{DIL}})^{-1}
\]

(30)

for crack problems, where \( I \) is unit matrix. It can be seen from Eqs. (29) and (30) that the Mori–Tanaka approach provides explicit expressions for effective constants of defective piezoelectric solids. Therefore, no iteration is required with the Mori–Tanaka BE method.

5. Numerical example

As an illustration, the proposed micromechanics BEM is applied to the numerical example below. In the calculation, the convergent tolerance \( \varepsilon \) is set to be 0.0001.

Consider a voided BaTiO 3 [9], the properties of which are given as follows:

\[
\begin{align*}
\sigma_1^0 &= 150 \text{ GPa}, & \sigma_2^0 &= 44 \text{ GPa}, & \sigma_3^0 &= 4 \text{ GPa}, \\
\tau_{12}^0 &= 28 \text{ GPa}, & \tau_{13}^0 &= 12 \text{ GPa}, & \tau_{23}^0 &= 0 \text{ GPa}, \\
\kappa_0 &= 1260 \text{ GPa}, & \kappa &= 8.85 \times 10^{-12} \text{ C}^2/\text{N m}^2.
\end{align*}
\]

Figs. 3 and 4 show the plot of \( c_1^0 / c_{11}^0 \) as a function of the area fraction of holes \( \nu_2 \) for the voided piezoelectric ceramic, obtained by the self-consistent BEM, the Mori–Tanaka BEM, and the theoretical model of Ref. [9]. For simplicity, the elliptic hole is used in our analysis. The ratio of major and minor axes \((a/b)\) is assumed to be \( a/b = 2 \).
It is clearly observed from Figs. 3 and 4 that both the self-consistent BEM and the Mori–Tanaka BEM can provide almost the same results as those obtained from the corresponding theoretical model [9], the maximum discrepancy between them being less than 3%. It is also evident from Fig. 5 that the self-consistent BEM underestimates the $c_{11}/c_{01}$ relative to the Mori–Tanaka BEM. This phenomenon is similar to that observed in Ref. [9].

6. Conclusion

A micromechanics BE algorithm including the self-consistent BEM and the Mori–Tanaka BEM has been developed for estimating the effective properties of piezoelectric materials with cracks or voids. The study shows that among $C^e$, $e^e$, and $k^e$, only $C^e$ is independent, which means that once $C^e$ is determined, $e^e$ and $k^e$ can be predicted from $C^e$. The performance of both the self-contained BEM and the Mori–Tanaka BEM in calculating the effective electroelastic moduli has been examined. The numerical results indicate that both the self-contained BEM and the Mori–Tanaka BEM can provide almost the same results as those obtained from the corresponding theoretical model and the maximum discrepancy between them is less than 3%. This is acceptable from an engineering point of view.

Appendix A. The derivation of Eqs. (24) and (25) [11–13]

The BE Eqs. (24) and (25) can be derived by way of a potential energy method. The generalized potential energy used for this purpose is given by [11–13]

$$P(b) = \frac{1}{2} \int_{L} \varphi(b) \cdot b \, ds - \int_{\Gamma} \mathbf{F} \cdot \mathbf{b} \, ds$$

(A1)

where $\varphi(b)$ defined by the relation, $\Pi_{e} = \varphi_{e}$, is a vector of SED function in terms of $\mathbf{b} = [b_1, b_2, b_3, b_4]^T$. As in conventional BEM, the boundaries $\Gamma$ and $L$ (Fig. 2) are divided into $M_{\Gamma}$ and $M_{L}$ linear elements, for which the EDEP discontinuity may be approximated by the sum of elemental EDEP discontinuities

$$\mathbf{b}(s) = \sum_{m=1}^{M} \mathbf{b}_m F_m(s)$$

(A2)

where $\mathbf{b}_m$ is the EDEP discontinuity at node $m$, $M = M_{\Gamma} + M_{L} + N$, $N$ is the number of cracks, $s$ is a length coordinate ($s > 0$ in the element located at the right of the node $m$, $s < 0$ in the element located at the left of the node), $F_m(s)$ is a global shape function associated with the node $m$. $F_m(s)$ is zero-valued over the whole mesh except within two elements connected to the node $m$ (Fig. A1). Since $F_m(s)$ is assumed to be linear within each element, it has three possible forms

$$F_m(s) = (l_{m-1} + s)/l_{m-1}$$

(A3)

for a node located at the left end of a line (Fig. A1)

$$F_m(s) = (l_m - s)/l_m$$

(A4)

for a node located at the right end of a line.
for a node located at the right end of a line (Fig. A1)
\[ F_m(s) = \begin{cases} (l_m - s)l_{m-1}, & \text{if } s \in \text{element } l_{m-1}, \\ (l_m - l_{m-1})s, & \text{if } s \in \text{element } l_m \end{cases} \]
(A5)

for the remaining nodes, where \( l_m \) and \( l_{m-1} \) are lengths of the two elements connected to the \( m \)th node, \( l_m \) being to the right and \( l_{m-1} \) being to the left (Fig. A1), while
\[ s = \begin{cases} 0, & \text{at node } m, \\ s_m, & \text{at node } m + 1, \\ -l_{m-1}, & \text{at node } m - 1 \end{cases} \]
(A6)

With the approximation (A2), the EDEP and SED functions can be expressed in the form
\[ U(z) = \sum_{m=1}^{M} \text{Im}[\mathbf{A} \mathbf{D}_m(z) \mathbf{B}^T] \mathbf{b}_m, \]
(A7)
\[ \varphi(z) = \sum_{m=1}^{M} \text{Im}[\mathbf{B} \mathbf{D}_m(z) \mathbf{B}^T] \mathbf{b}_m \]

where \( \mathbf{A} \) and \( \mathbf{B} \) are two material eigenvector matrices which are well defined in the literature [11], and
\[ \mathbf{D}_m(z) = \frac{1}{\pi} \int_{l_{m-1}}^{l_m} \langle \text{Im}(z \alpha_m - s_z) \rangle l_{m-1} + s \, ds - \frac{1}{\pi} \int_{l_m}^{l_z} \langle \text{Im}(z \alpha_m - s_z) \rangle l_m - s \, ds \]
(A8)

where \( \langle (\cdot) \rangle_a = \text{diag}[(\cdot)_1, (\cdot)_2, (\cdot)_3, (\cdot)_4] \) is a diagonal matrix, \( \alpha = \text{diag}(\alpha) \), \( l_{m-1} \) and \( l_m \) are the coordinates at node \( m \), \( p_\alpha \) is an electroelastic eigenvalue of the material under consideration, \( \alpha_m \) is the angle between the element located at the right of node \( m \) and \( x_1 \)-axis, \( z_{m-1} \) and \( \alpha_{m-1} \) are defined similarly. In particular, the EDEP at node \( j \) is given by
\[ U(z_j) = \sum_{m=1}^{M} \text{Im}[\mathbf{A} \mathbf{D}_m(z_j) \mathbf{b}_m] \]
(A9)

The substitution of Eq. (A2) into Eq. (A1) yields
\[ P(b) = \sum_{j=1}^{M} \left[ \frac{1}{2} b_j^T \left( \sum_{j=1}^{M} K_j b_j \right) - g_j \right] \]
(A10)

where
\[ K_{ij} = \frac{1}{l_{j-1}} \int_{l_{j-1}}^{l_{j}} \text{Im}[D_i^T(d_{j} + z_{j}B)B^T] ds \\
- \frac{1}{l_{j}} \int_{l_{j}}^{l_{j+1}} \text{Im}[D_i^T(d_{j} + z_{j}B)B^T] ds, \]
(A11)
\[ g_j = \int_{l_{j-1}+1}^{l_{j}} \text{Im}[F_j(s) ds] \]
(A12)

The minimization of Eq. (A10) leads to a set of linear equations
\[ \sum_{j=1}^{M} K_{ij} b_j = g_j \]
(A13)

References