

ANALYSIS OF EFFECTIVE PROPERTIES OF PIEZOCOMPOSITES BY THE SUBREGION BEM-MORI-TANAKA APPROACH

SUMMARY

Recently, many approaches have been proposed to estimate the effective properties of composites. The most typical are: the self-consistent method and the Mori-Tanaka method. However, they are restricted to simple geometries of phases. Also for complex constitutive laws the analytical results are complicated. On the other hand, the combination of numerical methods and these approaches gives an efficient computational scheme for estimating effective properties of composite materials. In this paper the hybrid subregion boundary element method (BEM) and Mori-Tanaka approach is implemented to solve coupled field equations of linear piezocomposites in the unit cell approach and then to determine the effective properties. To obtain the BEM fundamental solutions, the Stroh formalism is used. The numerical examples demonstrate an effectiveness of the BEM-Mori-Tanaka approach.

Keywords: boundary element method, coupled fields, piezoelectric materials, homogenization, material properties

ANALIZA WŁASNOŚCI ZASTĘPCZYCH PIEZOKOMPOZYTÓW POŁĄCZONĄ METODĄ ELEMENTÓW BRZEGOWYCH I MORI-TANAKI

Do wyznaczania własności zastępczych kompozytów zostało opracowanych wiele metod. Do najbardziej znanych należą metody: samospójna (estymator wewnątrznie zgodny) oraz Mori-Tanaki. Są one jednak ograniczone do prostych geometrii faz kompozytu. Również dla złożonych związków konstytutywnych zależności analityczne są skomplikowane. Z drugiej strony, kombinacja metod numerycznych i wspomnianych metod mikromechaniki daje efektywne narzędzie obliczeniowe określania własności zastępczych materiałów kompozytowych. W niniejszej pracy opisano hybrydową metodę bazującą na połączeniu sformułowania metody elementów brzegowych dla podobszarów i metody Mori-Tanaki, którą zastosowano do rozwiązania równań pól sprzężonych liniowych piezokompozytów dla komórki elementarnej, aby wyznaczyć własności zastępcze. Do otrzymania rozwiązań fundamentalnych metody elementów brzegowych zastosowano formalizm Stroha. Przykłady numeryczne pokazują efektywność opracowanej metody.

Słowa kluczowe: metoda elementów brzegowych, pola sprzężone, materiały piezoelektryczne, homogenizacja, własności materiałowe

1. INTRODUCTION

The overall properties of composite materials are required during the design process of composites. The effective properties can be determined by applying analytical, empirical or numerical methods. Among most popular numerical methods of modelling composites are the finite element method (FEM) and the boundary element method (BEM). The BEM (Brebbia and Dominguez 1992) is particularly suitable for modeling composites because of its high accuracy and easy modification of geometry. Effective material properties can be computed numerically by considering a unit cell or a representative volume element of a composite (Nemat-Nasser and Hori 1999).

Several authors performed the static linear elastic analysis of materials with inclusions, which modelled RVEs or unit cells of non-homogeneous materials, by using different formulations of the BEM (Eischen and Torquato 1993). In (Yao *et al.* 2004) the authors applied the formulation for many identical inclusions to the evaluation of elastic constants of composites with direct bonding between inclusions and matrix, and also with interphases between inclusions and matrix. In (Qin 2004) the example of a piezoelectric square

RVE with a circular rigid insulating fiber was analyzed by the self-consistent – BEM and Mori-Tanaka – BEM approaches to determine the effective properties. In (Fedeliński *et al.* 2011), several BEM formulations for modeling and analysis of composites are also presented.

In this work the developed methods are applied to compute effective properties using the unit cell approach for piezoelectric composites. Due to complexity of the piezoelectric constitutive equations, a combination of the Mori-Tanaka method (Nemat-Nasser and Hori 1999) and the subregion BEM formulation was proposed (Davi and Milazzo 2001). In piezocomposites piezoelectrics are connected with other materials: conductors, dielectrics and also other piezoelectrics, hence special boundary conditions must be applied on the interfaces, between different materials. Models of non-piezoelectric materials are obtained by assuming particular material properties.

2. CONSTITUTIVE EQUATIONS

The piezoelectric materials are modeled as: homogenous, transversal isotropic, linear-elastic and linear – dielectric

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(Pan 1999). When the x_3 – axis is chosen as the poling direction and the plane x_1 – x_3 (x – z) is considered, the generalized constitutive equations for the generalized plane-strain state have the following form:

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{33} \\ \sigma_{13} \\ D_1 \\ D_3 \end{Bmatrix} = \begin{bmatrix} c_{11} & c_{13} & 0 & 0 & -e_{31} \\ c_{13} & c_{33} & 0 & 0 & -e_{33} \\ 0 & 0 & c_{44} & -e_{15} & 0 \\ 0 & 0 & e_{15} & \kappa_{11} & 0 \\ e_{31} & e_{33} & 0 & 0 & \kappa_{33} \end{bmatrix} \begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{33} \\ 2\varepsilon_{13} \\ E_1 \\ E_3 \end{Bmatrix} \quad (1)$$

or in matrix form:

$$\Sigma = CZ \quad (2)$$

where:

- $\sigma_{ij}, \varepsilon_{ij}$ – stress and strain tensor components;
- D_j, E_j – are electric displacement and electric field vector components;
- $c_{ij}, e_{ij}, \kappa_{ij}$ – the elasticity, piezoelectric moduli and dielectric tensor components, respectively;
- Σ and Z – the generalized stress and strain vectors, respectively;
- C – the generalized stiffness tensor.

The strain tensor ε_{ij} can be expressed by the displacement vector using the linear elasticity relation. Because the static electric field is irrotational the electric potential ϕ can be introduced:

$$E_j = -\phi_{,j} \quad (3)$$

Application of the equilibrium equation and the Gauss law allows to formulate the boundary-value problem of linear piezoelectricity, which can be expressed by using the displacement vector and the electric potential (Pan 1999).

3. MODELS OF MATERIALS

The probably most important analytical result of micromechanics has been found by Eshelby (Nemat-Nasser and Hori 1999). It is valid for an unbounded domain which contains an ellipsoidal inclusion. In the theory of elasticity, the relation between the constant eigenstrains in the inclusion and the total strains inside the inclusion is given by the fourth-order Eshelby tensor. The result by Eshelby holds for an arbitrary anisotropic material, but only in case of an isotropic material is a closed-form representation of the Eshelby tensor. Additionally, the elastic properties of an inclusion and the matrix are the same, otherwise the region is called an inhomogeneity and the concept of equivalent eigenstrain can be applied by using again the Eshelby's result (Nemat-Nasser and Hori 1999).

This approach can be extended to the piezoelectric case. The material is assumed to undergo an eigenstrain and eigenelectric field within the inclusion. When the eigenstrain and the eigenelectric field in the inclusion are uniform, the induced strain and electric field outside the inclusion can be expressed by so called the electroelastic Eshelby tensor (Mikata 2000). The presented assumptions allow to use the Mori-Tanaka approach.

In the present formulation, piezoelectric material is modeled as homogeneous, transversal isotropic, linear elastic and linear dielectric. For this material, the piezoelectric effect in the two-dimensional case depends on the nine material constants. These constants are: four elastic constants, three piezoelectric constants and two dielectric constants, as is shown in (1).

The linear dielectric, transversal isotropic and linear elastic material (for example the composite graphite/epoxy) may be described by the four elastic constants and two dielectric constants. In this case the piezoelectric effect does not occur, then the piezoelectric constants are equal to zero, then:

$$C = \begin{bmatrix} c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & \kappa_{11} & 0 \\ 0 & 0 & 0 & 0 & \kappa_{33} \end{bmatrix} \quad (4)$$

The isotropic, linear elastic and conducted material cannot be analyzed directly using the Stroh formalism (Pan 1999). The Stroh formulation requires the distinct eigenvalues, therefore only a quasi-isotropic material can be used. The difference between the solution based on a quasi-isotropic and pure isotropic model is negligible (Pan 1999). Another problem is a fact, that dielectric permittivity constants for the conductors are non-measurable. For a practical computations it can be assumed that the dielectric constants for the conducting material are equal to the vacuum dielectric constant κ_0 :

$$C = \begin{bmatrix} c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & \kappa_0 & 0 \\ 0 & 0 & 0 & 0 & \kappa_0 \end{bmatrix} \quad (5)$$

4. HOMOGENIZATION TECHNIQUE

In the case of two-phase piezocomposites, the volume average of the generalized strain tensor is given by:

$$\langle Z \rangle = v_1 \langle Z_1 \rangle + v_2 \langle Z_2 \rangle \quad (6)$$

where subscripts “1” and “2” denote the matrix and inclusion of the piezocomposite; v_i are volume fractions of phases; the volume average of the property F is calculated by using:

$$\langle \bullet \rangle = \frac{1}{\Omega} \int_{\Omega} F d\Omega \quad (7)$$

where Ω denotes the volume.

From the average generalized strain theorem (Nemat-Nasser and Hori 1999):

$$\begin{aligned} \langle \mathbf{Z} \rangle &= \mathbf{Z}^0 \\ \langle \boldsymbol{\Sigma} \rangle &= \mathbf{C}^* \mathbf{Z}^0 \end{aligned} \quad (8)$$

one can obtain the effective properties of the piezocomposite:

$$\mathbf{C}^* = \mathbf{C}_1 + v_2 (\mathbf{C}_2 - \mathbf{C}_1) \mathbf{A}_2 \quad (9)$$

where \mathbf{Z}^0 is the generalized uniform strain applied on the effective medium and tensor \mathbf{A}_2 is given by:

$$\langle \mathbf{Z}_2 \rangle = \mathbf{A}_2 \mathbf{Z}^0 \quad (10)$$

\mathbf{C}_1 and \mathbf{C}_2 denote the generalized stiffness tensor of the matrix and the inclusion, respectively. The average generalized strain of the inclusion is calculated by using the divergence theorem, for example the average strain ϵ_{11} of the inclusion takes a form:

$$\langle (\epsilon_{11})_2 \rangle = \frac{1}{\Omega_2} \int_{\Gamma_2} u_1 n_1 d\Gamma_2 \quad (11)$$

where:

- Ω_2 and Γ_2 – the volume and the boundary of the inclusion phase,
- u_1 – displacement in the x_1 – direction,
- n_1 – the unit normal vector component along the x_1 – axis.

In the present work the generalized displacements are calculated by using the BEM.

5. THE BEM-MORI-TANAKA METHOD FOR TWO-PHASE PIEZOELECTRIC COMPOSITE

The Mori-Tanaka method is one of the micromechanical approaches to estimating the concentration tensor (Nemat-Nasser and Hori 1999). The BEM-Mori-Tanaka method is a numerical procedure used to obtain the effective properties

of composites and it can deal with arbitrary shapes of inclusions. In this method, a typical inclusion is embedded in an infinite matrix subjected to a homogenous generalized strain boundary condition. The BEM is applied to calculate the dilute generalized strain concentration tensor \mathbf{A}_2^{DIL} , which is defined by the linear relations in the following form:

$$\langle \mathbf{Z}_2 \rangle = \mathbf{A}_2^{DIL} \langle \mathbf{Z}_1 \rangle \quad (12)$$

and then the effective properties \mathbf{C}^* of the piezocomposite can be found by using the following equation of the Mori-Tanaka approach:

$$\mathbf{C}^* = \mathbf{C}_1 + v_2 (\mathbf{C}_2 - \mathbf{C}_1) \mathbf{A}_2^{MT} \quad (13)$$

where v_2 is a volume fraction of the inclusion, \mathbf{A}_2^{MT} denotes the Mori-Tanaka concentration tensor (Qin 2004):

$$\mathbf{A}_2^{MT} = \mathbf{A}_2^{DIL} \left((1 - v_2) \mathbf{I} + v_2 \mathbf{A}_2^{DIL} \right)^{-1} \quad (14)$$

where \mathbf{I} denotes the identity matrix.

6. THE BEM FORMULATION

Let us assume that a piezoelectric solid occupies the simply connected domain Ω , which is an open and bounded subset of R^2 with boundary Γ of Lipschitz-type. The integral formulation of the boundary-value problem of linear piezoelectricity is simply the generalized Betti theorem (Brebbia and Dominguez 1992):

$$\begin{aligned} \forall \mathbf{u}, \mathbf{v} \in \left(H^1(\Omega) \right)^3: \quad & \int_{\Omega} (\mathbf{v} \mathbf{L}(\mathbf{u}) - \mathbf{u} \mathbf{L}(\mathbf{v})) d\Omega = \\ & = \int_{\Gamma} (\mathbf{v} \mathbf{P}(\mathbf{u}) - \mathbf{u} \mathbf{P}(\mathbf{v})) d\Gamma \end{aligned} \quad (15)$$

where:

- $\mathbf{L}(\cdot)$ – the elliptic operator of plane linear piezoelectricity;
- $\mathbf{P}(\cdot)$ – the traction operator;
- \mathbf{u}, \mathbf{v} – the generalized displacement vectors, which contain the displacement vector and the electric potential.

If \mathbf{v} is the fundamental solution of the operator $\mathbf{L}(\cdot)$ and the generalized body force vector is neglected, then one can obtain the following boundary integral equation of the present problem:

$$\mathbf{c} \mathbf{u} + \int_{\Gamma} \mathbf{u} \mathbf{P}(\mathbf{v}) d\Gamma = \int_{\Gamma} \mathbf{v} \mathbf{P}(\mathbf{u}) d\Gamma \quad (16)$$

where c is the coefficient which depends on the boundary regularity. Equations (15) can be solved approximately by using the BEM. Only the boundary Γ (which contains the inclusion boundary) is divided into boundary elements. The boundary generalized displacements and tractions are approximated using shape functions. The discretized equation is applied to all boundary nodes and the linear algebraic system of equations is obtained for unknown boundary quantities.

Since ceramic piezoelectric materials are anisotropic, the fundamental solutions are rather complicated, even for the transversal isotropic model of the material. To obtain the fundamental solutions, the Stroh formalism is used (Pan 1999). The Stroh formalism is a powerful and elegant analytic technique for the anisotropic elasticity, which is expanded to the linear piezoelectricity in this case.

7. THE SUBREGION BEM

Composites can be modelled using different approaches of the boundary element method. The BEM is a well-known procedure (Brebbia and Dominguez 1992, Davi and Milazzo 2001). This approach is based on the division of the primary region into several homogeneous subregions. For each subregion one can write equations of the BEM.

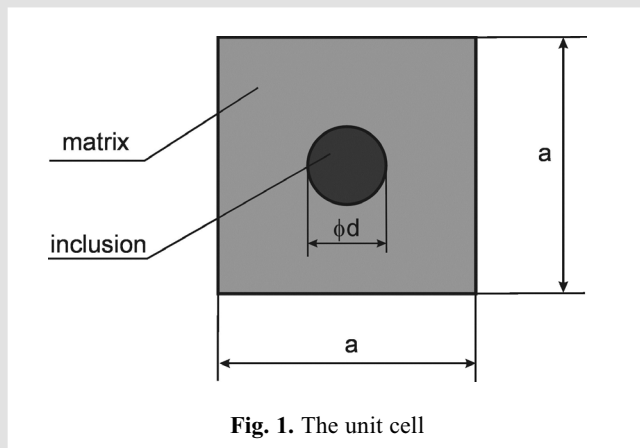


Fig. 1. The unit cell

Let the unit cell shown in Figure 1 be composed of two parts, which occupy the subdomains Ω_1 (the matrix, subscripts “1” and “3”) and Ω_2 (the inclusion, the subscript “4”) with boundaries Γ_1, Γ_2 . The boundary Γ_{12} denotes the common boundary (subscripts “3” and “4”).

The BEM equations for each subregion have a form:

$$\Omega_1 : \begin{bmatrix} \mathbf{H}_{11} & \mathbf{H}_{13} \\ \mathbf{H}_{31} & \mathbf{H}_{33} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1 \\ \mathbf{U}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{G}_{11} & \mathbf{G}_{13} \\ \mathbf{G}_{31} & \mathbf{G}_{33} \end{bmatrix} \begin{bmatrix} \mathbf{T}_1 \\ \mathbf{T}_3 \end{bmatrix} \quad (17)$$

$$\Omega_2 : \mathbf{H}_{44} \mathbf{U}_4 = \mathbf{G}_{44} \mathbf{T}_4$$

In equations (16) $\mathbf{H}_{ij}, \mathbf{G}_{ij}, \mathbf{U}_i$ and \mathbf{T}_i denote the parts of the \mathbf{H} and \mathbf{G} BEM matrices and parts of the vectors \mathbf{U} and \mathbf{T} , which contain the generalized displacements and tractions, respectively. Generalized quantities denote mechanical and electrical quantities, which are coupled due to the piezoelectric effect.

To obtain the final set of equations, the interface compatibility and equilibrium equations, must be implemented:

$$\begin{aligned} \mathbf{U}_3 &= \mathbf{U}_4 \\ \mathbf{T}_3 &= -\mathbf{T}_4 \end{aligned} \quad (18)$$

Equations (17) describe the perfect electromechanical bonding. Multiplying both sides of (16) by the inverse of \mathbf{G} and implementing (17) one can obtain the final system of equations for the generalized displacements:

$$\begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{13} \\ \mathbf{A}_{31} & \mathbf{A}_{33} + \mathbf{A}_{44} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1 \\ \mathbf{U}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{T}_1 \\ \mathbf{O}_3 \end{bmatrix} \quad (19)$$

where $\mathbf{A}_{ij} = (\mathbf{G}^{-1} \mathbf{H})_{ij}$; \mathbf{O}_3 is a null matrix of the appropriate dimensions.

The system of equations (19) can be rearranged using the prescribed boundary conditions.

When the connection between two piezoelectric or dielectric material is analyzed, the conditions (17) are still valid, but when the piezoelectric material is bonded with the other non-piezoelectric material, the electric boundary conditions on the interface may be discontinuous (Chue and Chen 2002, Sze *et al.* 2004). For a piezoelectric – conductor interface we have the equilibrium of the tractions and the continuity of the displacements. The additional condition is the ideal electric conductor condition. The ideal electric conductor condition is applied to the whole boundary Γ_2 – the constant electric potential solution follows from the Maxwell equations for the ideal conductor.

To determine overall properties of the piezoelectric composite the uniform generalized strain, namely the uniform strain and the uniform electric field boundary conditions can be applied on the boundary of the unit cell. As in (Qin 2004), two load subcases can be considered:

$$(\boldsymbol{\varepsilon}^0, \mathbf{E}^0 = 0), (\boldsymbol{\varepsilon}^0 = 0, \mathbf{E}^0) \quad (20)$$

The first load case allows to determine the effective elastic constants and the effective piezoelectric moduli, according to the constitutive equations (1); while the second one – the effective piezoelectric moduli and the effective dielectric constants. The homogenous boundary conditions are presented in Figure 2.

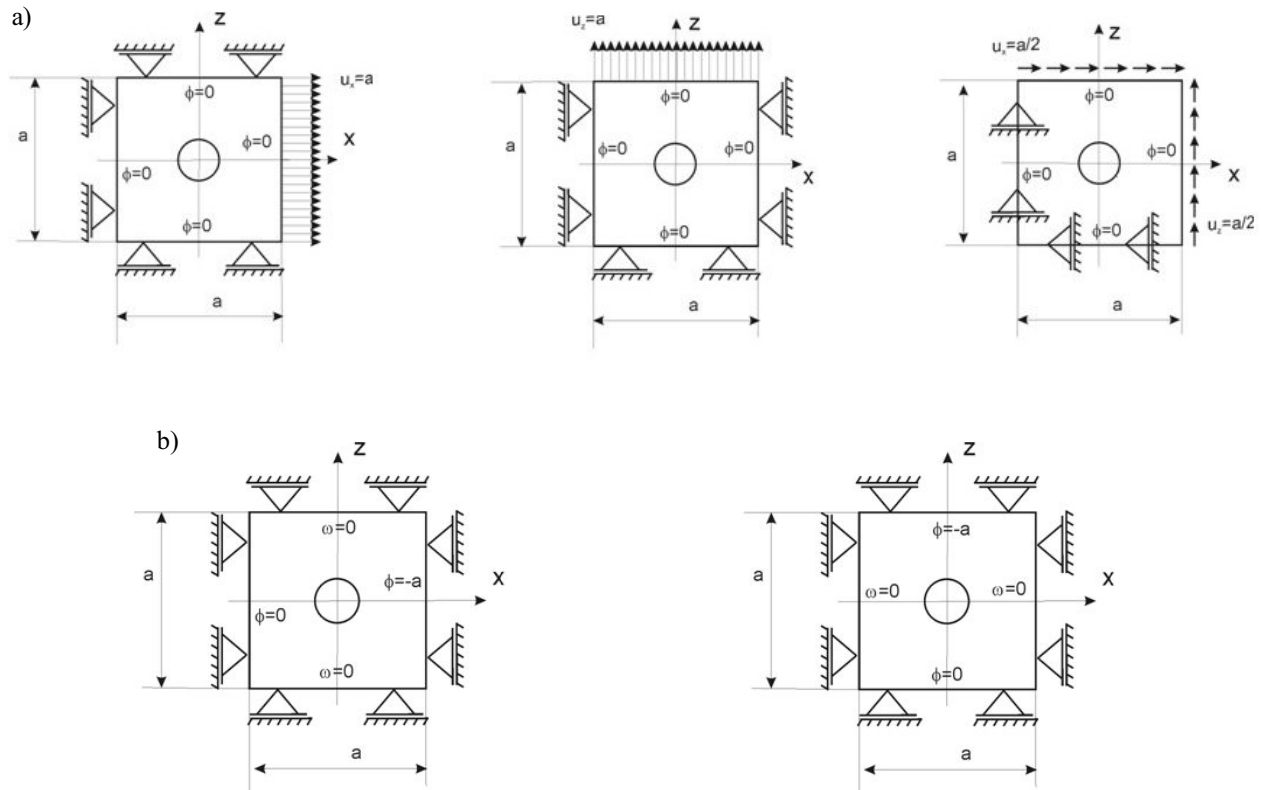


Fig. 2. The homogenous boundary conditions for the unit cell:
a) the first load case ($\epsilon^0, \mathbf{E}^0 = 0$); b) the second load case ($\epsilon^0 = 0, \mathbf{E}^0$)

8. NUMERICAL EXAMPLES

To verify the presented formulation, the benchmark numerical example was considered. The results for the voided piezoelectric are obtained and compared with data from (Wu 2002). In this case, the material properties are given in the Table 1. Also, the influence of the boundary element mesh size is taken into account.

Numerical results for the effective constant c_{33}^{eff} , e_{33}^{eff} and ϵ_{11}^{eff} are presented in Figures 3–5.

The presented results show good accuracy in comparison with results which are obtained by the analytical calculation (Wu 2002). The present BEM-Mori-Tanaka method predicts lower values than the results by the piezoelectric Eshelby tensor method (Mikata 2000, Wu 2002).

The most important physical constant, which describes the piezoelectric effect is the piezoelectric modulus. In the

next numerical example, the epoxy matrix with the piezoelectric inclusion is considered, as shown in Table 2 (Topolov and Bowen 2009). Results are obtained with the volume fraction of inclusions varied from 0 to 0.6. The effective properties are normalized by the properties of matrix. The total mesh size is equal to 52 boundary elements: 40 constant elements for the unit cell external boundary and 12 constant boundary element for the inclusion boundary.

Figure 6 shows the results of the composite effective piezoelectric moduli. As can be seen, e_{15} and e_{33} are increased when the inclusion fraction increases. A different behavior of the e_{31} has been found in responding to the change of the inclusion fraction. In this case, a non-monotonic volume fraction behavior of the effective property is observed (Topolov and Bowen 2009). In this case, it is possible to optimize the coupling effects of piezocomposites.

Table 1
Material constants of voided piezoelectric material

Material	Elastic constants [GPa]				Piezoelectric moduli [C/m ²]			Dielectric permittivity [nF/m]	
	c_{11}	c_{13}	c_{33}	c_{44}	e_{51}	e_{31}	e_{33}	ϵ_{11}	ϵ_{33}
Matrix BaTiO ₃	126.0	53.0	117.0	35.3	17.0	-6.5	23.3	15.1	13.0
Inclusion void	0	0	0	0	0	0	0	ϵ_0	ϵ_0

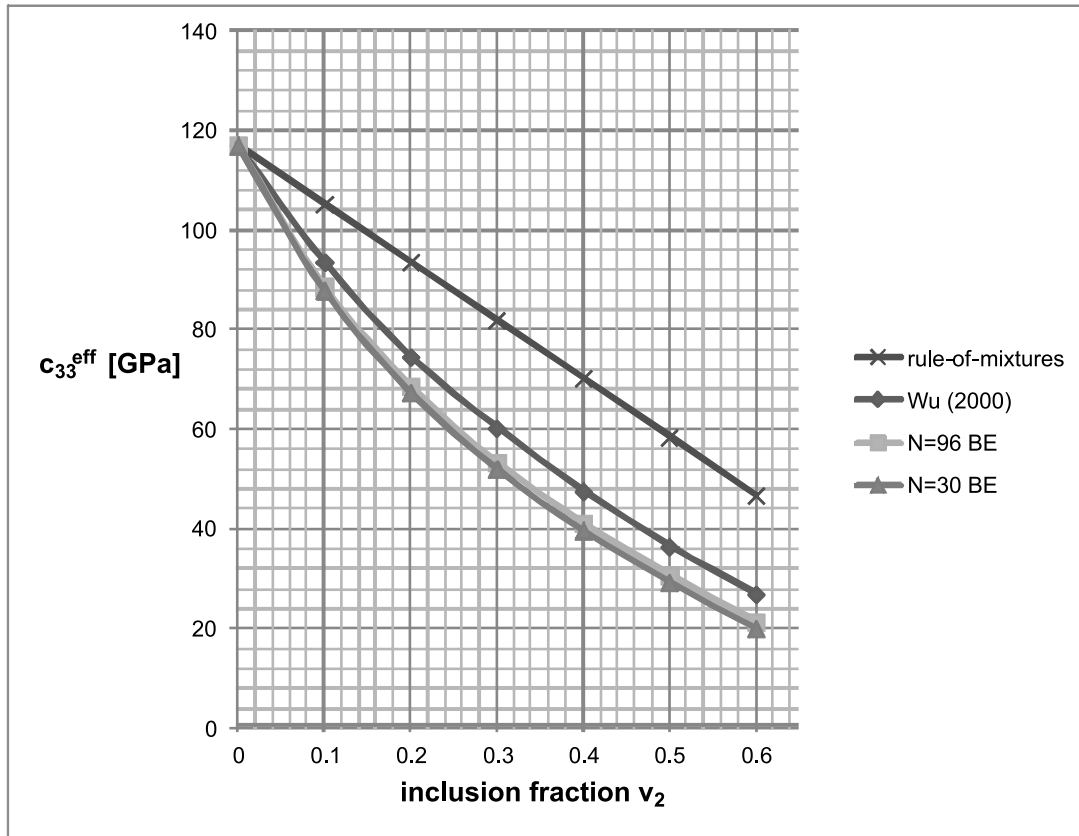


Fig. 3. The effective elastic constant c_{33}^{eff} for voided piezoelectric

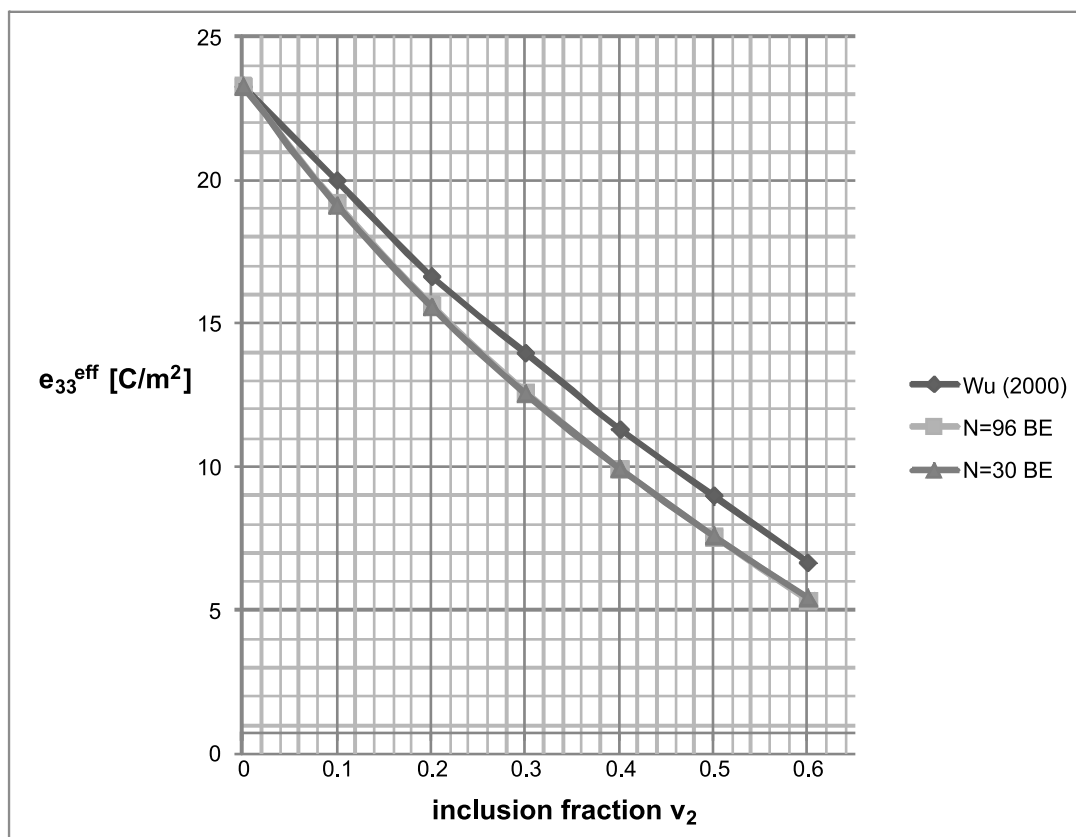


Fig. 4. The effective piezoelectric constant e_{33}^{eff} for voided piezoelectric

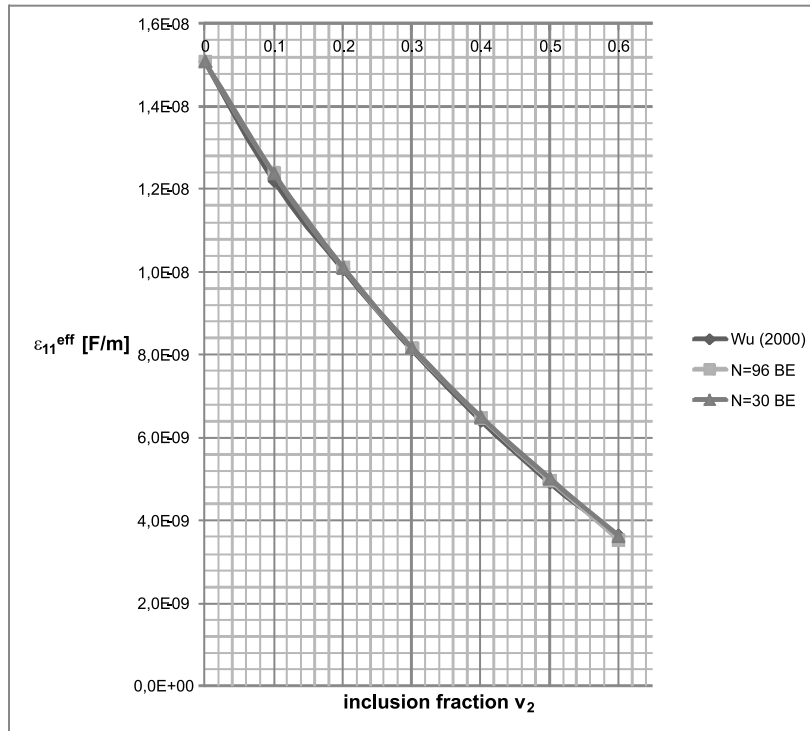


Fig. 5. The effective dielectric permittivity constant ϵ_{11}^{eff} for voided piezoelectric

Table 2
Material constants for epoxy/PZT7A composite

Material	Elastic constants [GPa]				Piezoelectric moduli [C/m ²]			Dielectric permittivity [nF/m]	
	c_{11}	c_{13}	c_{33}	c_{44}	e_{51}	e_{31}	e_{33}	ϵ_{11}	ϵ_{33}
Matrix Epoxy	8.0	4.4	8.0	1.8	0	0	0	0.037	0.037
Inclusion PZT7A	154.8	82.7	131.4	25.7	9.349	-2.121	9.522	4.065	2.079

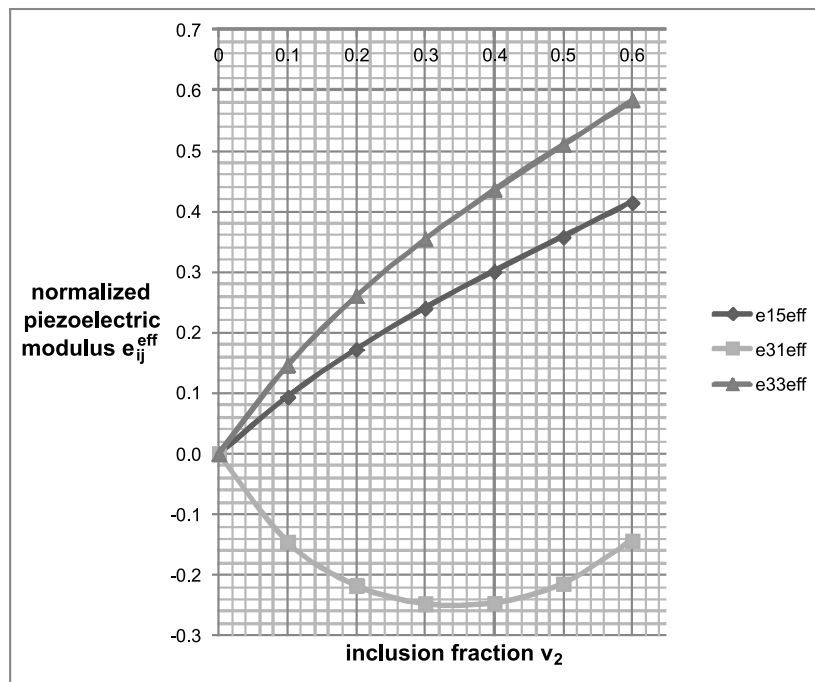


Fig. 6. The normalized piezoelectric moduli for epoxy/PZT7A composite

Similar to e_{15} and e_{33} , the normalized effective dielectric permittivity increases with the inclusion volume fraction, as shown in Figure 7.

Figure 8 shows the results of the normalized effective elastic constants; the c_{13} is significantly increased with the inclusion fraction, c_{11} and c_{33} increase in a similar way due to properties of the matrix, while the c_{44} increases less significantly than do other elastic constants.

9. SUMMARY

The BEM-Mori-Tanaka numerical scheme based on the Stroh formalism was developed. The BEM was used to solve an electroelastic boundary value problem within a unit cell of a piezocomposite and to determine the effective properties using the Mori-Tanaka approach. The subregion boundary element formulation is used to model different two-phase

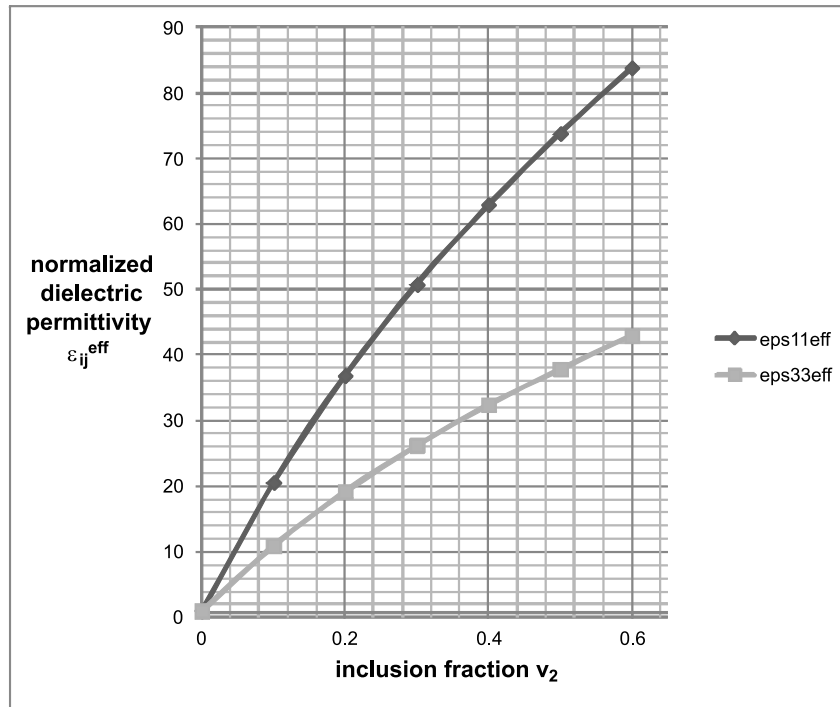


Fig. 7. The normalized dielectric permittivity for epoxy/PZT7A composite

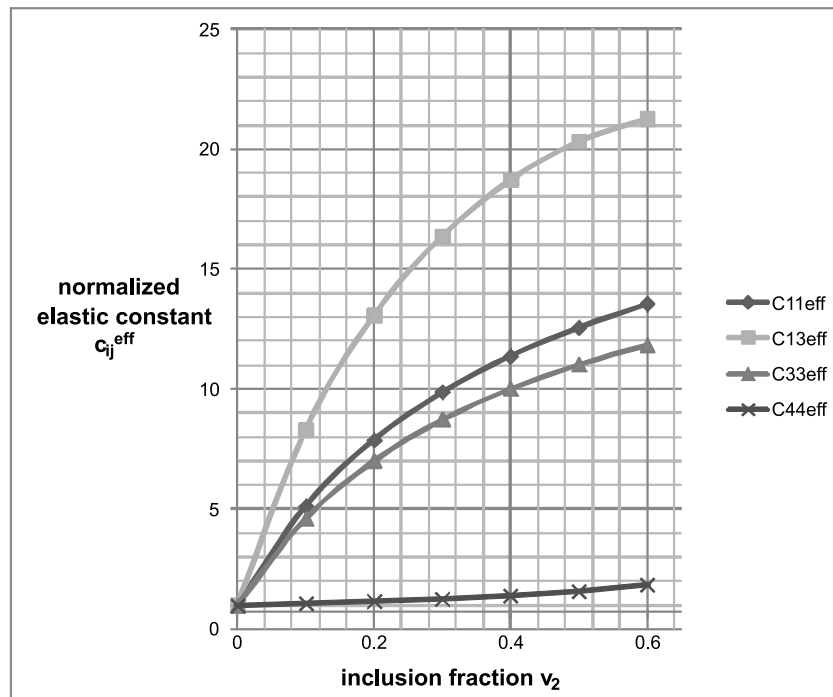


Fig. 8. The normalized elastic constant for epoxy/PZT7A composite

piezocomposites. The following deformable and quasi-rigid inclusions can be considered by using the presented formulation: piezoelectric, dielectric and conducting. The numerical examples demonstrate an efficiency of the BEM solutions.

The effective material constants for the voided BaTiO₃ and the epoxy/PZT7A composite were obtained. The most interesting results are the effective piezoelectric moduli of the epoxy/PZT7A composite. A different behavior of the e_{31} has been found in responding to the change of the inclusion fraction. In the case of the piezoelectric modulus e_{31} , a non-monotonic volume fraction behavior of the effective property is observed. In this case, it is possible to optimize the coupling effects of piezocomposites.

The BEM allows analyzing inhomogeneities of various shapes, the Stroh formalism allows to take into account the polarization direction and electric boundary conditions effect. The BEM requires only boundary fields calculation, hence the calculation of internal coupled fields can be neglected. The present formulation can be used for effective properties calculation of both anisotropic linear elastic and linear dielectric composites, but the Stroh formalism can be extended to piezomagnetism, thermopiezoelectricity, etc.

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