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AKAPIT

COMPUTER METHODS IN MATERIALS SCIENCE
Informatyka w Technologii Materiałów

Vol. 11, 2011, No. 1

COMPUTER MODELLING AND ANALYSIS OF EFFECTIVE PROPERTIES OF COMPOSITES

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Abstract

In this work, different formulations of the boundary element method (BEM) are presented for an analysis of composites containing rigid or deformable stiffeners and inclusions. The developed computer codes are used to compute effective material properties by considering a representative volume element (RVE) or a unit cell. The results computed by the proposed BEM are compared with available experimental, analytical or numerical results, shown in the literature.

Key words: boundary element method, composites, effective properties, homogenization, representative volume element, unit cell

1. INTRODUCTION

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

Several authors performed the static analysis of linear-elastic materials with inclusions, which modeled RVEs or unit cells of non-homogeneous materials, by using different formulations of the BEM. Eischen & Torquato (1993) analyzed 2-D unit cells containing inclusions forming the hexagonal array. The effective material properties for a number of inclusion-matrix elastic constants' ratios and volume fractions of inclusions were given. Yao et al. (2004) 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. Chen & Liu (2005) analysed composites reinforced by spherical particles or short fibers by the advanced BEM. Difficulties in dealing with nearly-singular integrals while modelling of composites with closely packed fillers were resolved by new and improved techniques. Qin (2004) considered the example of a piezoelectric square RVE with a circular rigid insulating fiber analyzed by the self-consistent – BEM and Mori-Tanaka – BEM approaches to determine the effective properties. Due to complexity of the piezoelectric constitutive equa-

ISSN 1641-8581

tions, a combination of the Mori-Tanaka method and the subregion BEM formulation was proposed (Davi & Milazzo, 2001).

In this work matrix equations of the boundary element method for composite containing rigid or deformable stiffeners and inclusions are shown. The developed methods are applied to compute effective properties using the unit cells or representative volume elements for nanocomposites, epoxy-glass composites and piezoelectric composites.

2. COMPUTER MODELLING OF COMPOSITES BY USING THE BOUNDARY ELEMENT METHOD

Composites can be modelled using different approaches of the boundary element method. Three cases are considered - composites containing: rigid stiffeners, deformable stiffeners and deformable inclusions (figure 1). Stiffeners are attached to the matrix and inclusions are embedded in the matrix. In the first case, shown in figure 1a, the rigid stiffener is perfectly bonded to the matrix. In the second case, the deformable stiffener is attached to the matrix (figure 1b). In the last case, shown in figure 1c, the boundary of the inclusion is connected with the internal boundaries of the matrix. The quantities related to the external boundaries and internal boundaries of the matrix, along which the stiffener (inclusion) are connected, are denoted by the index *"e"* and *"i"*, respectively. In order to simplify the notation, the name reinforcement will be used, which means both the stiffener and inclusion and quantities related to the reinforcement are denoted by *"r"*. It is assumed that the matrix and reinforcement are made of homogenous, isotropic and linear-elastic materials. Consider a body – the matrix or the inclusion, which has the boundary Γ and the domain Ω. The body is loaded by the boundary tractions t_j and the volume forces f_j. The relation between the loading and displacements u_j is expressed by the Somigliana identity (Brebbia & Dominguez, 1992)

$$c_{ij}(x')u_j(x') + \int_\Gamma T_{ij}(x',x)u_j(x)d\Gamma(x) = \int_\Gamma U_{ij}(x',x)t_j(x)d\Gamma(x) + \int_\Omega U_{ij}(x',X)f_j(X)d\Omega(X) \quad (1)$$

where x' is a collocation point, x is a boundary point, X is a point which belongs to the domain of the body, c_{ij} is a constant which depends on the position of the point x', U_{ij} i T_{ij} are fundamental solutions of elastostatics. The summation convention is used in the equation.

The external and internal boundaries of the matrix are divided into boundary elements. Displacements and tractions within each boundary element are interpolated using nodal values and shape functions. The boundary integral equations (1) are used for nodes along external and internal boundaries of the matrix. The interaction forces between the rigid or deformable stiffener and the matrix are treated as particular body forces f_j distributed only along the internal boundary. Therefore the formulations require only integration along the external and internal boundaries.

Along the interface between the matrix and the reinforcement the conditions of compatibility of displacements should be satisfied

$$\boldsymbol{u}_i = \boldsymbol{u}_r \quad (2)$$

where u_i are displacements of the matrix along the attachment of the reinforcement and u_r are displacements of the reinforcement.

Additionally equilibrium of tractions should be fulfilled

$$\boldsymbol{t}_i = -\boldsymbol{t}_r \quad (3)$$

where t_i are tractions acting on the matrix along the attachment and t_r are tractions acting on the reinforcement.

The proposed methods allow direct computing of unknown displacements and tractions along the external boundaries and along interfaces between the reinforcement and matrix.

The formulation of the methods will be demonstrated for a

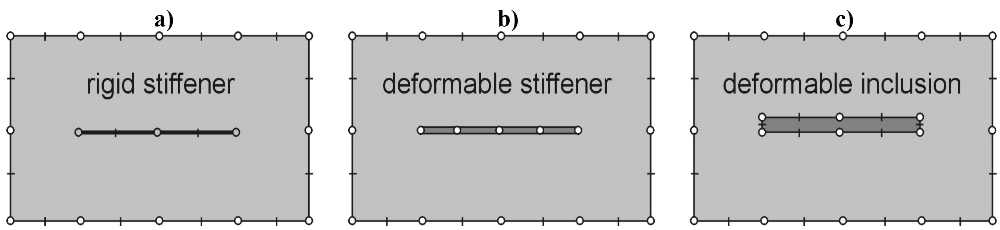

Fig. 1. *Boundary element modelling of composites containing: a) rigid stiffener, b) deformable stiffener, c) deformable inclusion.*

single reinforcement. Composites with multiple reinforcements can be modelled in a similar way.

2.1. Composites containing rigid stiffeners

The boundary integral equations (1) for nodes along the external and internal boundaries of the matrix can be written in the following matrix form

$$\begin{bmatrix} \boldsymbol{H}_{ee} & \boldsymbol{0} \\ \boldsymbol{H}_{ie} & \boldsymbol{I} \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_e \\ \boldsymbol{u}_i \end{bmatrix} = \begin{bmatrix} \boldsymbol{G}_{ee} & \boldsymbol{G}_{ei} \\ \boldsymbol{G}_{ie} & \boldsymbol{G}_{ii} \end{bmatrix} \begin{bmatrix} \boldsymbol{t}_e \\ \boldsymbol{t}_i \end{bmatrix} \tag{4}$$

where u_e, t_e and u_i, t_i are displacements and tractions of nodes along the external and internal boundaries of the matrix, respectively, submatrices H and G depend on integrals of fundamental solutions of elastostatics and shape functions, I is the unit matrix.

The displacements of nodes of rigid stiffener u_r can be defined by the parameters u_p (Fedeliński, 2006). The parameters u_p are displacements of an arbitrary selected point and angles of rotation of the rigid stiffener. The displacements of nodes of stiffener can be expressed by the following matrix equation

$$\boldsymbol{u}_r = \boldsymbol{D}\boldsymbol{u}_p \tag{5}$$

The elements of matrix D depend on the position of nodes.

Forces acting on the rigid stiffener should fulfill equilibrium equations. These equations can be written in the following form

$$\boldsymbol{E}\boldsymbol{t}_r = \boldsymbol{0} \tag{6}$$

where t_r are tractions acting on nodes of the stiffener. The elements of the matrix E depend on shape functions and position of nodes (Fedeliński, 2006).

Equations (4) and (5), supplied by equation (6) can be written as a single matrix equation

$$\begin{bmatrix} \boldsymbol{H}_{ee} & \boldsymbol{0} \\ \boldsymbol{H}_{ie} & \boldsymbol{D} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_e \\ \boldsymbol{u}_p \end{bmatrix} = \begin{bmatrix} \boldsymbol{G}_{ee} & -\boldsymbol{G}_{ei} \\ \boldsymbol{G}_{ie} & -\boldsymbol{G}_{ii} \\ \boldsymbol{0} & \boldsymbol{E} \end{bmatrix} \begin{bmatrix} \boldsymbol{t}_e \\ \boldsymbol{t}_r \end{bmatrix} \tag{7}$$

2.2. Composites containing deformable stiffeners

The equation for the matrix has the same form as equation (4). The deformable stiffener is modelled using beam finite elements. The matrix equation of equilibrium of the stiffener can be written in the form

$$\boldsymbol{K}\boldsymbol{u}_r = \boldsymbol{T}\boldsymbol{t}_r \tag{8}$$

where K is the stiffness matrix of the stiffener and T is the transformation matrix, which transforms tractions distributed along the stiffener into equivalent nodal concentrated forces (Fedeliński & Górski, 2006).

Equations (4) and (8) are coupled into a single matrix equation by taken into account conditions (2) and (3)

$$\begin{bmatrix} \boldsymbol{H}_{ee} & \boldsymbol{O} \\ \boldsymbol{H}_{ie} & \boldsymbol{I} \\ \boldsymbol{O} & \boldsymbol{K} \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_e \\ \boldsymbol{u}_r \end{bmatrix} = \begin{bmatrix} \boldsymbol{G}_{ee} & -\boldsymbol{G}_{ei} \\ \boldsymbol{G}_{ie} & -\boldsymbol{G}_{ii} \\ \boldsymbol{O} & \boldsymbol{T} \end{bmatrix} \begin{bmatrix} \boldsymbol{t}_e \\ \boldsymbol{t}_r \end{bmatrix} \tag{9}$$

2.3. Composites containing deformable inclusions

The boundary integral equations are used for nodes along the external and internal boundaries of the matrix. The equations can be written in the matrix form

$$\begin{bmatrix} \boldsymbol{H}_{ee} & \boldsymbol{H}_{ei} \\ \boldsymbol{H}_{ie} & \boldsymbol{H}_{ii} \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_e \\ \boldsymbol{u}_i \end{bmatrix} = \begin{bmatrix} \boldsymbol{G}_{ee} & \boldsymbol{G}_{ei} \\ \boldsymbol{G}_{ie} & \boldsymbol{G}_{ii} \end{bmatrix} \begin{bmatrix} \boldsymbol{t}_e \\ \boldsymbol{t}_i \end{bmatrix} \tag{10}$$

The matrix form of the boundary integral equations (1) for the inclusion is

$$\boldsymbol{H}_r\boldsymbol{u}_r = \boldsymbol{G}_r\boldsymbol{t}_r \tag{11}$$

Equations (10) and (11) can be written as a single equation by taken into account the conditions (2) and (3)

$$\begin{bmatrix} \boldsymbol{H}_{ee} & \boldsymbol{H}_{ei} \\ \boldsymbol{H}_{ie} & \boldsymbol{H}_{ii} + \boldsymbol{H}_r \end{bmatrix} \begin{bmatrix} \boldsymbol{u}_e \\ \boldsymbol{u}_r \end{bmatrix} = \begin{bmatrix} \boldsymbol{G}_{ee} & -\boldsymbol{G}_{ei} \\ \boldsymbol{G}_{ie} & -\boldsymbol{G}_{ii} + \boldsymbol{G}_r \end{bmatrix} \begin{bmatrix} \boldsymbol{t}_e \\ \boldsymbol{t}_r \end{bmatrix} \tag{12}$$

The present formulation can be extended to piezoelectric composites by using generalized quantities, i.e. generalized displacements and tractions including electrical degrees of freedom.

3. NUMERICAL EXAMPLES

The boundary element formulations shown in Section 2 are used to model different composites. A polymer/clay nanocomposite is modelled using deformable stiffeners and deformable inclusions, an epoxy-glass composite and a piezoelectric composite are modelled using deformable inclusions. Representative volume elements are applied to compute effective material properties of the polymer/clay nanocomposite and epoxy-glass composite, and the unit cell method is used for the piezoelectric composite.

3.1. Polymer/clay nanocomposite

The polymer/clay nanocomposite with aligned and randomly distributed intercalated particles is considered. The effective longitudinal Young modulus of the composite E_c is analyzed by two numerical methods: 1) the matrix and particles in the form of stacks of parallel clay sheets are analyzed by the BEM and FEM using plate and beam elements, respectively, and 2) the matrix and the homogenized isotropic effective particles (Sheng et al., 2004), are analyzed entirely by the BEM as plates. The materials of the matrix and particles are linear elastic and isotropic, in plane strain. The RVEs are rectangles of dimension $2a \times a$, and the side length a is changed in order to obtain different values of volume fraction of particles.

a)

b)

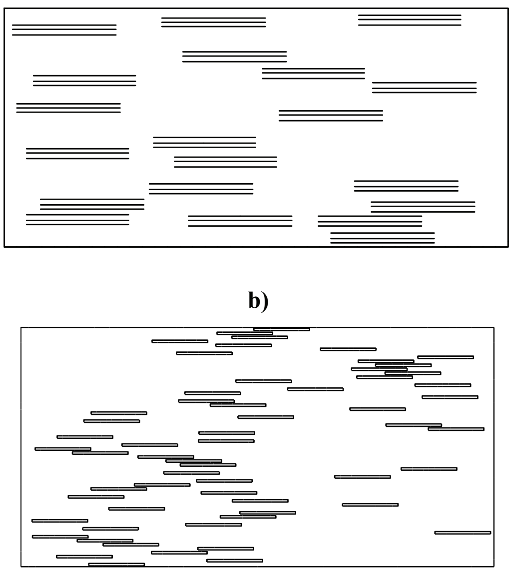

Fig. 2. Geometry of RVE with intercalated particles (W_c = 6%): a) stacks of silicate sheets, b) effective particles.

The traction and periodic conditions are imposed on the RVEs in the coupled BEM/FEM and BEM analysis, respectively. The number of silicate sheets in the coupled BEM/FEM analysis is 60 (20 stacks, 3 particles in a stack). The number of isotropic particles in the BEM analysis is 60. Typical RVEs in these two cases are shown in figures 2a and 2b, respectively. Remaining parameters of the models are: the length of nanoclays in a stack or the length of the effective particles is L = 200 nm, the aspect ratio L/t = 23 (where t is the thickness of the effective particle or stack), the inter-layer spacing $d_{(001)}$ = 4.1 nm, the silicate sheet thickness d_s=0.615 nm, E_p/E_m=21, E_m=4 GPa, E_s=385 GPa, where E_p, E_s and E_m are the Young moduli of the effective particle, silicate sheet and matrix, respectively, f_p/W_c=1.2, where f_p and W_c denote the volume fraction of the effective particles and the clay weight fraction, respectively.

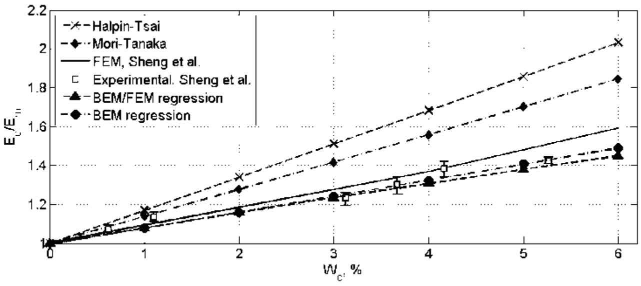

Fig. 3. Normalized effective Young's modulus obtained by different methods.

The numerical predictions of E_c normalized with respect to E_m obtained by the coupled BEM/FEM and BEM are presented in figure 3. The results are consistent with those presented by Sheng et al. (2004), i.e. experimental obtained by the tensile test and numerical by the FEM analysis. The stiffness predicted by the Halpin-Tsai and the Mori-Tanaka model in this case is significantly overestimated. The results show that the BEM or coupled BEM/FEM can be successfully applied to the evaluation of the effective Young modulus of polymer/clay nanocomposites with intercalated and aligned particles, modeled both as stacks of clay sheets or homogenized isotropic particles.

3.2. Epoxy-glass composite

In this example a model of a fibre-reinforced composite material is under consideration. The material consists of the epoxy resin matrix and aligned continuous glass fibres, of identical circular sections, which form the hexagonal array. The cross section of such composite is analyzed. Eight models with volume fraction of fibres f ranging from 5% to 40% are analysed. A typical model is shown in figure 4a. Each model is a square plate with the side length equal to 0.5 mm and containing 105 identical inclusions, which are the fibre sections. The model is in plane strain. The tensile traction force is t_2 = 50 MPa. The radii of the inclusions are adjusted so as to obtain required volume fractions of fibres. The Young moduli and Poisson ratios of the matrix and the fibres are: E_m = 3.6 GPa, ν_m = 0.35, E_f = 72 GPa and ν_f = 0.2 respectively.

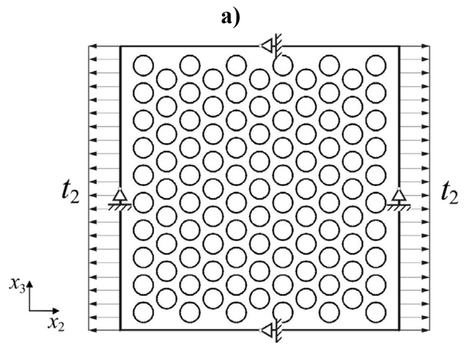

Fig. 4. RVE of the composite material: a) geometry and boundary conditions, b) deformed model.

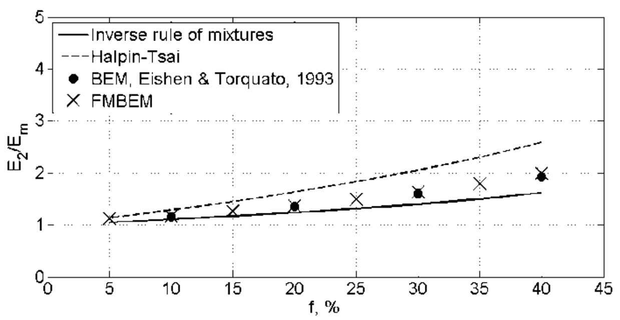

Fig. 5. Normalized effective transverse Young's modulus obtained by different methods.

Table 1. Material constants of piezoelectric composite.

Material	Elastic constants [GPa]				Piezoelectric moduli [C/m^2]			Dielectric permittivity [nF/m]	
	c_{11}	c_{13}	c_{33}	c_{55}	e_{51}	e_{31}	e_{33}	ε_{11}	ε_{33}
Matrix $BaTiO_3$	150.0	66.0	150.0	44.0	11.40	-4.35	17.50	9.86	11.15
Inclusion PZT5H	126.0	53.0	117.0	35.3	17.00	-6.50	23.30	15.10	13.00

Each inclusion is discretized by 18 boundary elements and each square side is discretized by 160 elements. The RVEs are analysed by the fast multipole BEM (Ptaszny & Fedeliński, 2010). A deformed model is shown in figure 4b. The transverse effective Young's modulus of the composite is computed and compared to other models, as it is shown in figure 5. The results were compared to Halpin-Tsai model, the rule of mixtures model and to the values given by Eischen & Torquato (1993), obtained by the analysis of unit cells using the conventional BEM. One can see that the results of the present FMBEM analysis agree very well with the ones computed by Eischen and Torquato. Both the series of numerical experiments gave values of the transverse Young modulus lower than the ones determined by the Halpin-Tsai model. The computed values are higher than the ones obtained by using the inverse rule of mixture. The rule is known to state the lower bound for the effective modulus.

3.3. Piezoelectric composite

The unit cell of the piezoelectric solid with a circular inclusion shown in figure 6 is analyzed. The overall properties of the piezoelectric composite are determined. The uniform strain and the uniform electric field boundary conditions are applied on the boundary of the unit cell (Qin, 2004). Two load cases are considered: 1) the uniform strain boundary conditions with zero electric field, and 2) the uniform electric field with no strains, are applied along the boundary. The first load case allows for determining the effective elastic constants and the effective piezoelectric moduli, while the second one for determining the effective piezoelectric moduli and the effective dielectric constants. To specify the generalized strain concentration tensor in the Mori-Tanaka theory, the relation between the generalized strain in the inclusion and in the matrix is determined by using the BEM numerical models.

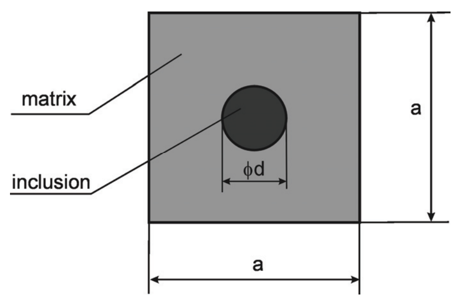

Fig. 6. The unit cell.

The materials are transversely isotropic and the x_3-axis is chosen as the poling direction and the plane x_1-x_3 is considered. The physical constants of composite are presented in table 1.

The effective piezoelectric moduli are calculated for different volume fractions of the inclusion and they are presented in figure 7. The effective piezoelectric moduli are normalized by the properties of matrix.

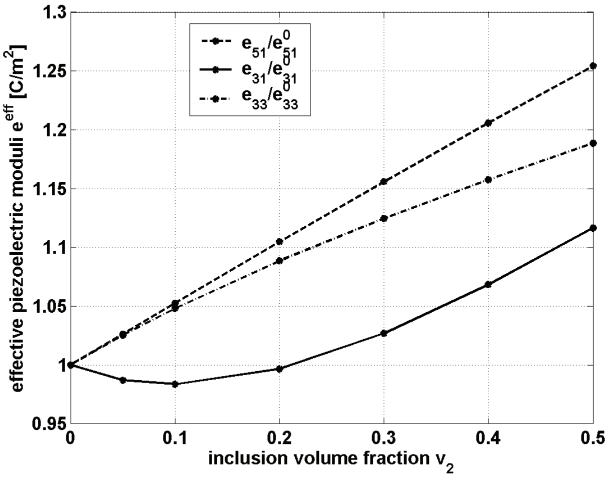

Fig. 7. *The effective piezoelectric moduli.*

4. CONCLUSIONS

Different boundary element techniques of modelling composites are applied to compute effective material properties of composites. The example of polymer/clay nanocomposite demonstrates that modelling nanoparticles as deformable stiffeners or their stacks as deformable inclusions gives similar effective Young's moduli of the nanocomposite. The effective Young's moduli for polymer/clay nanocomposite and epoxy-glass composite agree well with results obtained by experimental, analytical and other numerical results presented in the literature. The example of piezoelectric composite shows an application of the methods for new smart materials.

ACKNOWLEDGMENTS

The scientific research is financed by the Ministry of Science and Higher Education of Poland in years 2010-2012.

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MODELOWANIE KOMPUTEROWE I ANALIZA WŁASNOŚCI ZASTĘPCZYCH KOMPOZYTÓW

Streszczenie

W pracy przedstawiono różne sformułowania metody elementów brzegowych (MEB) w analizie kompozytów zawierających sztywne i odkształcalne elementy usztywniające lub wtrącenia. Opracowane programy komputerowe zastosowano do wyznaczenia zastępczych własności materiałowych poprzez analizę reprezentatywnego elementu objętościowego lub komórki elementarnej. Wyniki otrzymane proponowanymi sformułowaniami MEB porównano z wynikami doświadczalnymi, analitycznymi i numerycznymi, przedstawionymi w literaturze.

Received: October 13, 2010
Received in a revised form: October 19, 2010
Accepted: October 19, 2010