ANALYTICAL AND NUMERICAL MODELING FOR 3D SMART ORTHOTROPIC GRID-REINFORCED COMPOSITE STRUCTURES

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Summary

A new comprehensive micromechanical modeling of a periodic smart composite structures reinforced with a 3D grid of orthotropic reinforcements and actuators is undertaken to fully determine effective piezoelectric and thermal expansion properties. Two different modeling techniques are presented; one is based on the asymptotic homogenization method (AHM) and the other is a numerical model based on the finite element analysis (FEA). The AHM transforms the original boundary value problem into a simpler one characterized by effective coefficients which are shown to depend only on geometric and material parameters of a periodicity cell. The developed models can be applied to various 3D smart grid-reinforced composite structures with generally orthotropic constituents.

Analytical formulae for the effective piezoelectric and thermal expansion coefficients are derived and a finite element analysis is subsequently developed and used to examine the aforementioned periodic grid-reinforced orthotropic structures. The electro-thermo-mechanical deformation responses from the finite element simulations are used to extract the homogenized piezoelectric and thermal expansion coefficients. The results of the FEA are compared to those pertaining to their AHM counterparts using a varying volume fractions and different poling directions. A very good agreement is shown between these two modeling techniques.

The prediction of the effective properties of 3D grid-reinforced smart composites is important for design and manufacturing of composite parts using such structures.

1. Introduction

Governing equations describing the behaviour of periodic or nearly periodic composite materials are given by a set of partial differential equations characterized by the presence of rapidly varying coefficients due to the presence of numerous embedded inclusions in close proximity to one another. To treat these equations analytically, one has to consider two sets of spatial variables, one for the microscopic (local) characteristics of the constituents and the other for the macroscopic (global) behaviour of the composite under investigation. The presence of the microscopic and macroscopic scales in the original problem frequently renders the pertinent partial differential equations extremely difficult to solve. One technique that permits us to accomplish the decoupling of the two scales is the AHM. The mathematical framework of the AHM can be found in [1-4]. This technique has been used to analyze periodic composite and smart structures, see e.g. the pioneering work of [5] on inhomogeneous plates. Other work can be found in heat conduction studies pertaining to thin elastic and periodic plates [6]. A wide variety of elasticity and thermoelasticity problems pertaining to composite materials and thin-walled composite structures reinforced shells and plates was examined in [7]. Expressions for the effective elastic, piezoelectric and hygrothermal expansion coefficients for general 3D periodic smart composite structures were derived in [8,9]. The authors in [10] have applied a general 3D micromechanical model for thin smart composite plates reinforced with a network of cylindrical reinforcements that may also exhibit piezoelectric behaviour. Asymptotic homogenization models for thin network-reinforced smart composite shells were developed in [11,12]. Other work can be found in [13] and [14].

Since work [15], a considerable number of micromechanically oriented numerical approaches based on the finite element method have been developed and extensively used in the analysis of the mechanical properties of composite materials with spatial repetition of a small microstructure. In [16] a
2D finite element approach for a microscopic region of a unidirectional composite using a generalized plane strain formulation which includes longitudinal shear loading has been developed. The method of cells [17] and its generalization [18] have proven to be successful micromechanical analysis tools for the prediction of the overall behaviour of various types of composites with known properties and geometrical arrangement of the individual constituents and give consistently accurate results for the elastic properties. A review of the work conducted using the two theories has been given by [19]. An alternative approach that retains the philosophy of Aboudi’s Method of Cells has been presented and the equations of equilibrium were applied to a representative volume element and in addition a unified method of homogenization of micromechanical effects was presented in [20]. The finite element method has been extensively used to examine unit cell problems and to determine the effective properties and damage mechanisms of composites. The applications considered include unidirectional laminates [21], cross-ply laminates [22], woven and braided textile composites and piezoelectric foams [23-25] and many others.

Pertaining to the various finite element models, the unit cells employed can be subjected to mechanical, thermal, electrical or other loading types. The introduction of the loading conditions to the representative unit cell is expressed, in general, in terms of macroscopic or averaged field quantities, such as stress or strain. The use of the unit cells of different shapes (square, hexagonal etc) for the analysis and modeling of unidirectional fiber reinforced composites was studied in [26,27] by considering the symmetries in the material and deriving appropriate periodic boundary conditions for the unit cell. The loads on the unit cell and its response in terms of macroscopic stresses or strains have been addressed in such a way that the effective properties of the material can be obtained from the micromechanical analysis of the unit cell in a standard manner. In [28] appropriate constraints on a representative volume element under various loadings have been determined from symmetry and periodicity conditions. The work of [29] involved piezoelectric composites and employed a rigorous finite element unit cell model to account for local fluctuations of the fields. A full set of material moduli, i.e. the macroscopic elastic, dielectric and piezoelectric coefficients were determined. The concept of ‘macroscopic degrees of freedom’ and the implementation of periodicity conditions for composites with periodic microstructure composed of linear or nonlinear constituents were discussed in [30]. The authors in [31] applied a numerical procedure for the computation of the overall macroscopic elasticity moduli of linear composite materials with periodic micro-structure. The underlying key approach is a finite element discretization of the boundary value problem for the fluctuation field on the micro-structure of the composite. A number of possible unit cell models can be developed according to the material microstructure. The authors of [32] have developed a 3D unit cell model for both unidirectional and cross-ply laminates. The proposed unified boundary conditions satisfy not only the boundary displacement periodicity but also the boundary traction periodicity of the representative volume element model. Recently, the study of [33] has integrated the asymptotic homogenization method into a finite element simulation to derive overall material properties for metal matrix composites reinforced with spherical ceramic particles. In [34] a technique to evaluate effective material properties related to unidirectional fiber reinforced composites having rhombic periodic microstructures and isotropic and transversely isotropic behaviour has been presented.

1.1. Piezothermoelastic Composite Structures

Piezoelectric materials have the property of converting electrical energy into mechanical energy and vice versa. This work considers piezoelectric material (PZT-5A) that responds linearly to changes in electric field, electric displacement, mechanical stress and strain and thermal effects. The coupling of electric fields and thermo-mechanical response in a smart composite is characterized by the coefficients of piezoelectric and thermal expansion.

1.2. Micromechanical Models of 3D Grid-reinforced Smart Composite Structure

The problem is represented by a unit-cell shown in Figs. 1 and 2 and the models are developed using (AHM) and (FEA) to determine the effective piezoelectric and thermal expansion coefficients. Each unit cell contains a number of 3D orthotropic inclusions in the form of structural reinforcements and actuators.

Following this introduction, the rest of the paper is organized as follows: The basic problem formulation and the general asymptotic homogenization model for 3D smart grid-reinforced composite structures is derived in Section 2. Section 3 discusses the development of the finite element model and Section
4 formulates and compares results of both, analytical and numerical approaches to illustrate the applicability of the derived models. Finally, Section 5 concludes the work.

2. Asymptotic Homogenization Method

The electromechanical deformation of the structure shown in Fig. 1 is expressed using the balance of linear momentum and Gauss’s law. In the absence of body forces and currents, the smart composite given in Fig. 1 should satisfy the following boundary problem:

\[
\sigma_{ij,\Omega} = 0 \quad \text{in } \Omega \quad (1a)
\]
\[
u_i'(x) = 0 \quad \text{on } \partial \Omega \quad \text{for } i, j = 1, 2, 3 \quad (1b)
\]
\[
D_{ij,\Omega} = 0 \quad \text{in } \Omega \quad (1c)
\]
\[
D_{ij}(x) = 0 \quad \text{on } \partial \Omega \quad \text{for } i, j = 1, 2, 3 \quad (1d)
\]

The behaviour of the piezothermoelastic composite is described by the following constitutive equations:

\[
\sigma_{ij} = C_{ijkl} e_{kl} - P_{ik} E_k - \Theta_{ij} \quad (2)
\]
\[
D_{ij} = P_{ik} e_{ik} + \kappa_{ij} E_i \quad (3)
\]

with a linearized strain-displacement relation assuming small displacement gradients,

\[
e_{ij} = \frac{1}{2} \left( u_{ij}^{(0)} + u_{ij}^{(1)} \right) \quad (4)
\]

where \( C_{ijkl} \) is a tensor of elastic coefficients, \( e_{ik} \) is a strain tensor which is a function of the displacement field \( u_i \), \( P_{ik} \) is a tensor of piezoelectric coefficients describing the effect of \( E_k \) is the electric field vector on the mechanical stress field \( \sigma_{ij} \), \( \Theta_{ij} \) is a thermal expansion tensor, \( T \) represents change in temperature with respect to a reference state, \( D_i \) is the electric displacement and \( \kappa_{ij} \) is the dielectric permittivity.

In Eqs. (1) – (4) as well as in the rest of the paper we use the following short-hand notation for the derivatives:

\[
\phi_{m,n} = \frac{\partial \phi_m}{\partial x_n} \quad (5)
\]

We note that as a consequence of the periodicity of the smart composite, the material coefficients (\( C_{ijkl}, P_{ik} \) and \( \Theta_{ij} \)) are periodic functions in microscopic or the so-called “fast” variables with a unit cell \( Y \) of characteristic small dimension \( \varepsilon \), whereas the dependent field variables (stresses, strains, electric displacement, electric field and temperature) are also dependent on \( \varepsilon \).

2.1. Governing Equations and the Unit Cell Problems

In this Section, only a brief overview of the steps involved in the development of the model are given in so far as it represents the starting point of the current work. The development of asymptotic homogenization model for the 3D grid-reinforced smart composite structures can be found in [35].

The first step is to define the so-called “fast” or microscopic variables according to:

\[
y_i = \frac{X_i}{\varepsilon}, \quad i = 1, 2, 3 \quad (6)
\]

As a consequence of introducing \( y_i \), the chain rule of differentiation mandates that the derivatives must be transformed according to [36]:

\[
\frac{\partial}{\partial x_i} \rightarrow \frac{\partial}{\partial x_i} + \frac{1}{\varepsilon} \frac{\partial}{\partial y_i} \quad (7)
\]

The basic asymptotic expansions in terms of \( \varepsilon \) for the displacement and electric fields as well as the derived asymptotic expansions for the stress and the electric displacement are next considered:

\[
u_i(x, y) = u_i^{(0)}(x, y) + \varepsilon u_i^{(1)}(x, y) + \varepsilon^2 u_i^{(2)}(x, y) + \ldots \quad (8)
\]
\[
E_i(x, y) = \varepsilon E_i^{(0)}(x, y) + \varepsilon^2 E_i^{(1)}(x, y) + \varepsilon^3 E_i^{(2)}(x, y) + \ldots \quad (9)
\]
\[
\sigma_{ij}(x, y) = \sigma_{ij}^{(0)}(x, y) + \varepsilon \sigma_{ij}^{(1)}(x, y) + \varepsilon^2 \sigma_{ij}^{(2)}(x, y) + \ldots \quad (10)
\]
\[
D_{ij}(x, y) = D_{ij}^{(0)}(x, y) + \varepsilon D_{ij}^{(1)}(x, y) + \varepsilon^2 D_{ij}^{(2)}(x, y) + \ldots \quad (11)
\]

Substitution of Eqs. (8, 9) into Eq. (2) results, on account of Eq. (6), in the following expressions for the asymptotic expansions of the mechanical stress,

\[
\sigma^{(0)}_{ij} = C_{ijkl} (u_{kl}^{(0)} + u_{kl}^{(1)}) - P_{ik} E_k^{(0)} - \Theta_{ij} T^{(0)} \quad (12a)
\]
\[
\sigma^{(1)}_{ij} = C_{ijkl} (u_{kl}^{(1)} + u_{kl}^{(2)}) - P_{ik} E_k^{(1)} - \Theta_{ij} T^{(1)} \quad (12b)
\]

Similarly substituting Eqs. (8, 9) into Eq. (3) gives the asymptotic expansions for the electric displacement field,

\[
D^{(0)}_{ij} = P_{ik} (u_{jk}^{(0)} + u_{jk}^{(1)}) + \kappa_{ij} E_i^{(0)} \quad (13a)
\]
\[
D^{(1)}_{ij} = P_{ik} (u_{jk}^{(1)} + u_{jk}^{(2)}) + \kappa_{ij} E_i^{(1)} \quad (13b)
\]

Combination of Eqs. (1a) and (12a) leads to the following expression:

\[
\frac{\partial}{\partial y_j} \left( C_{ijkl} u_{kl,j}^{(1)}(x, y) \right) = P_{ik,j} (y) E_k(x) + \Theta_{ij,j}(y) T(x) - C_{ijkl,j}(y) u_{kl,i}^{(0)}(x) \quad (14)
\]
The separation of variables on the right-hand-side of Eq. (14) prompts us to write down the solution for \( u^{(1)} \) as follows:

\[
u^{(1)}(x, y) = V_u(x) + E_h(x)N^k_h(y) + T(x)N^l(y) + u^{(1)}_{kh}(x)N^{kl}(y)
\]

where the auxiliary functions \( N^k_h \), \( N^k \) and \( N^l \) are periodic in \( y \) and satisfy:

\[
\left[ C_{ijmn}(y)N^{kl}_{m,ny}(y) \right]_{.,y} = - C_{ijkl,y}(y) \quad (16a)
\]

\[
\left[ C_{ijmn}(y)N^k_{m,ny}(y) \right]_{.,y} = + P_{ijk,y}(y) \quad (16b)
\]

\[
\left[ C_{ijmn}(y)N^l_{m,ny}(y) \right]_{.,y} = + \Theta_{ij,y}(y) \quad (16c)
\]

while the function \( V_u(x) \) is the homogenous solution of Eq. (15) and satisfies:

\[
\left[ C_{ijmn}(y)V_{m,ny}(y) \right]_{.,y} = 0 \quad (17)
\]

One observes that Eqs. (16a) – (16c) depend entirely on the fast variable \( y \) and are thus solved on the domain \( Y \) of the unit cell, remembering at the same time that \( C_{ijkl} \), \( P_{ijk} \), \( \Theta_{ij} \) and \( N^k \), \( N^k \), \( N^l \) are \( Y \)-periodic in \( y \). Consequently, Eqs. (16a) – (16c) are appropriately referred to as the unit-cell problems.

### 2.2. Effective Coefficients

The next important step in the model development is the homogenization procedure. This is carried out by first substituting Eq. (15) into Eq. (12a), and combining the result with Eq. (1b). The resulting expressions are then integrated over the domain \( Y \) of the unit cell, remembering that all \( x \) parameters as a parameter as far as integration with respect to \( y \) is concerned. This leads to (after canceling out terms that vanish due to periodicity considerations):

\[
\tilde{C}_{ijkl} \frac{\partial^2 u^{(0)}(x)}{\partial x_i \partial x_j} - \tilde{P}_{ijk} \frac{\partial E_k(x)}{\partial x_j} - \tilde{\Theta}_{ij} \frac{\partial T(x)}{\partial x_j} = 0
\]

where the following definitions are introduced:

\[
\tilde{C}_{ijkl} = \frac{1}{|Y|} \int_Y \left( C_{ijkl}(y) + C_{ijmn}(y)N^{kl}_{m,ny}(y) \right) dv \quad (19a)
\]

\[
\tilde{P}_{ijk} = \frac{1}{|Y|} \int_Y \left( P_{ijk}(y) - C_{ijmn}(y)N^k_{m,ny}(y) \right) dv \quad (19b)
\]

\[
\tilde{\Theta}_{ij} = \frac{1}{|Y|} \int_Y \left( \Theta_{ij}(y) - C_{ijmn}(y)N^l_{m,ny}(y) \right) dv \quad (19c)
\]

It is noticed that the effective coefficients are free from the inhomogeneity complications that characterize their actual rapidly varying material counterparts \( (C_{ijkl}, P_{ijk} \) and \( \Theta_{ij} \)) and as such, are more amenable to analytical and numerical treatment.

In summary, the above derived expressions represent the governing equations of the homogenized model of a smart composite structure with periodically arranged reinforcements/actuators.

### 2.3. Smart 3D Grid-reinforced Composites

A general 3D smart orthotropic composite reinforced with \( N \) families of three mutually orthogonal reinforcements/actuators oriented along the three coordinate axes is considered, see Fig. 2.

It is assumed that the orthotropic reinforcements and actuators have significantly higher elasticity moduli than the matrix material, so we are justified in ignoring the contribution of the matrix phase in the analytical treatment. We first consider a simpler form of unit cell made of only a single reinforcement as shown in Fig. 3a. Having solved this, the effective piezoelectric and thermal expansion coefficients of structures with several families of reinforcements can be determined by the superposition of the solution for each of them found separately. One must recognize that an error will be incurred at the regions of intersection between the reinforcements and actuators. Nevertheless, our approximation will be quite accurate since these regions of intersection are very much localized and do not add significantly to the integral over the whole unit cell domain [37].

To determine the effective piezoelectric and thermal expansion coefficients for the simpler arrangement in Fig. 3a, the unit cell problem given in Eqs. (16b) and (16c) must be solved and Eqs. (19b) and (19c) must then be applied.

#### 2.3.1. Problem Formulation

The problem formulation for the smart composite structure shown in Fig. 1 begins with the introduction of the following piezoelectric and thermal expansion local functions:

\[
b^k_{ij} = P_{ijk}(y) - C_{ijmn}(y)N^k_{m,ny}(y) \quad (20a)
\]

\[
b^l_{ij} = \Theta_{ij}(y) - C_{ijmn}(y)N^l_{m,ny}(y) \quad (20b)
\]

We assume perfect bonding conditions at the interface between the reinforcement/actuator and the matrix. This assumption translates into the following interface conditions:
\[ N^k_s (r) = N^k_a (m) \Rightarrow b^k_j (r) n_j \mid_s = b^k_j (m) n_j \mid_s \] (21a)
\[ N^k_s (r) = N^k_a (m) \Rightarrow b^k_j (r) n_j \mid_s = b^k_j (m) n_j \mid_s \] (21b)

In Eqs. (21a) and (21b) the suffixes “s”, “a”, “m”, and “r” denote the “actuator/reinforcement”, “matrix”, and “reinforcement/matrix interface”, respectively; while \( n_j \) denote the components of the unit normal vector at the interface. As it was noted earlier, assume that \( C_{ijkl} (m) = 0 \) which implies that \( \Gamma^k_i = b^k_j (m) = b^k_j (y) = 0 \).

Therefore, the interface conditions becomes:
\[ b^k_j (r) n_j \mid_s = 0 \] (22a)
\[ b^k_j (r) n_j \mid_s = 0 \] (22b)

The unit cell problems that must be solved in combination with Eqs. (21a, b) are given by:
\[ b^k_j \mid_s = 0 \] (23a)
\[ b^k_j \mid_s = 0 \] (23b)

### 2.3.2. Coordinate Transformation

To solve the unit cell problems a coordinate transformation of the microscopic coordinate system \( \{ y_1, y_2, y_3 \} \) onto the new coordinate system \( \{ \eta_1, \eta_2, \eta_3 \} \) is performed, see Fig. 3b,
\[ \frac{\partial}{\partial y_j} = q_{ij} \frac{\partial}{\partial \eta_i} \] (24)

where \( q_{ij} \) are the components of the direction cosines characterizing the axes rotation. Subsequently, the problem becomes independent of \( (\eta_i) \) and the solution order is reduced by one.

### 2.3.3. Determination of the Effective Piezoelectric and Thermal Expansion Coefficients

#### 2.3.3.1. Effective Piezoelectric Coefficients

Referring to Fig. 3b, Eqs. (20a) and (22a) are written in terms of the \( \eta_i \) coordinates Eq. (24) to obtain:
\[ b^k_j \mid_s = P^{(k)}_{\eta} - C_{ijkl} q_{ij} N^k_{m,pn} (y) \] (25a)
\[ \left( b^k_j q_{ij} n_j^i (r) + b^k_j q_{ij} n_j^i (r) \right) \mid_s = 0 \] (25b)

Here \( n_j^i \) are the components of the unit normal vector in the new coordinate system.

Eqs. (25a) and (25b) can be solved by assuming a linear variation of the auxiliary functions \( N^k_i (y) \) with respect to \( \eta_2 \) and \( \eta_3 \), i.e.,
\[ N^k_i = \Gamma^k_i \eta_2 + \Gamma^k_i \eta_3, N^k_2 = \Gamma^k_2 \eta_2 + \Gamma^k_2 \eta_3, N^k_3 = \Gamma^k_3 \eta_2 + \Gamma^k_3 \eta_3 \] (26)

where \( \Gamma^k_i \) are constants to be determined from the boundary conditions. The local functions \( b^k_j \) can be expanded from Eq. (25a) on the basis of Eq. (26) as follows:
\[ b^k_{ij} = P^{(k)}_{ij} - \begin{cases} \Gamma^k_1 \{ C_{ijkl} q_{ij} + C_{ijkl} q_{ij} + C_{ijkl} q_{ij} \} \\ + \Gamma^k_2 \{ C_{ijkl} q_{ij} + C_{ijkl} q_{ij} + C_{ijkl} q_{ij} \} \\ + \Gamma^k_3 \{ C_{ijkl} q_{ij} + C_{ijkl} q_{ij} + C_{ijkl} q_{ij} \} \\ + \Gamma^k_4 \{ C_{ijkl} q_{ij} + C_{ijkl} q_{ij} + C_{ijkl} q_{ij} \} \\ + \Gamma^k_5 \{ C_{ijkl} q_{ij} + C_{ijkl} q_{ij} + C_{ijkl} q_{ij} \} \\ + \Gamma^k_6 \{ C_{ijkl} q_{ij} + C_{ijkl} q_{ij} + C_{ijkl} q_{ij} \} \end{cases} \] (27a)

The elastic, piezoelectric and thermal expansion coefficients in Eqs. (27a) and (27b) are referenced with respect to the \( \{ y_1, y_2, y_3 \} \) coordinate system. The relationships between these coefficients and their counterparts associated with the principal material coordinate system of the inclusion, \( C^{(P)}_{ijkl}, P^{(P)}_{ij}, \Theta^{(P)}_{ij} \) are expressed by means of familiar tensor transformation laws, namely,
\[ C_{ijkl} = q_{ij} q_{ij} q_{ij} C^{(P)}_{ijkl} \]
\[ P^{(P)}_{ij} = q_{ij} q_{ij} P^{(P)}_{ij} \]
\[ \Theta^{(P)}_{ij} = q_{ij} q_{ij} \Theta^{(P)}_{ij} \] (28)

where the superscript \( (P) \) denotes principal material coefficients and \( q_{ij} \) are the direction cosines between the principal material coordinate axes and the global \( y_1, y_2, y_3 \) axes.

From Eqs. (25b), (27a) and (27b) one obtains six linear algebraic equations for the solution of the constants \( \Gamma^k_i \) as follows:
\[ \sum_{m=1}^{20} D_m \Gamma_m^i + D_{i+1} = 0, \sum_{m=1}^{20} D_m \Gamma_m^j + D_{i+1} = 0 \]
\[ \sum_{m=21}^{31} D_m \Gamma_m^i + D_{i+1} = 0, \sum_{m=21}^{31} D_m \Gamma_m^j + D_{i+1} = 0 \]
\[ \sum_{m=32}^{41} D_m \Gamma_m^i + D_{i+1} = 0, \sum_{m=32}^{41} D_m \Gamma_m^j + D_{i+1} = 0 \]

Here \( D_m \) and \( D_i \), \( D_{i+1} \), \( D_{j+1} \), \( D_{2j} \), \( D_{3j} \) are constants which depend on the geometric parameters of the unit cell and the material properties of the reinforcement and actuators. Once the system of Eq. (29) is solved, the determined \( \Gamma_m^i \) coefficients are substituted back into Eqs. (27a) and (27b) to obtain the piezoelectric local functions \( b_{ij}^k \). In turn, these actuation local functions are used to calculate the effective piezoelectric coefficients of the smart 3D generally orthotropic grid-reinforced composite structure shown in Fig. 3.

\[ \bar{P}_{ij} = \frac{1}{|V|} \int_{V} b_{ij}^k \, dv \]  

(30)

Noting that the \( b_{ij}^k \) local functions are constant, denoting the length and cross-sectional area of the actuators/reinforcement (in coordinates \( y_1, y_2, y_3 \)) by \( L \) and \( A \) respectively, and the volume of the unit cell by \( V \), the effective piezoelectric coefficients become

\[ \bar{P}_{ij} = \frac{AL}{V} b_{ij}^n = \mu_f b_{ij}^n \]  

(31)

where \( \mu_f \) is the volume fraction of the actuators/reinforcements within the unit cell. The effective piezoelectric coefficients derived above pertain to grid-reinforced smart composite structures with a single family of actuator/reinforcement (or inclusions in general inclusions). For structures with multiple families of inclusions the effective actuation coefficients can be obtained by superimposition. For instance, pertaining to a 3D grid-reinforced smart structure with \( N \) families of actuators/reinforcements, the effective piezoelectric coefficients are given by

\[ \bar{P}_{ij} = \sum_{m=1}^{N} \mu_f^{(n)} b_{ij}^{(n)k} \]  

(32)

2.3.3.2. Effective Thermal Expansion Coefficients

Using the coordinate transformation defined in Eq. (24), Eqs. (20b) and (22b) can be written in terms of the \( \eta_i \) coordinates as follows:

\[ b_{ij} = \Theta_{ij}(\eta) - C_{ijn} q_{mn} N_{mn}(\eta) \]  

(33a)

\[ \left( b_{ij} q_{ij} n_i(r) + b_{ij} q_{ij} n_j(r) \right)_{\zeta} = 0 \]  

(33b)

Eqs. (33a) and (33b) can be solved by assuming a linear variation of the auxiliary functions \( N_m(\eta) \) with respect to \( \eta_2 \) and \( \eta_3 \), i.e.,

\[ N_i = \chi_i \eta_i, N_3 = \chi_3 \eta_i, N_6 = \chi_6 \eta_i \]  

(34a)

where \( \chi_i \) are constants to be determined from the boundary conditions. The local functions \( b_{ij} \) can be then expanded as follows:

\[ b_{ij} = \Theta_{ij} - \left[ \chi_1 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \right. \]
\[ + \chi_2 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \]
\[ + \chi_3 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \]
\[ + \chi_4 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \]
\[ + \chi_5 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \]
\[ \left. + \chi_6 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \right] \]

(35a)

\[ b_{ij} = \Theta_{ij} - \left[ \chi_1 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \right. \]
\[ + \chi_2 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \]
\[ + \chi_3 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \]
\[ + \chi_4 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \]
\[ + \chi_5 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \]
\[ \left. + \chi_6 \left( C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} + C_{\eta i \eta} q_{ij} \right) \right] \]

(35b)

From Eqs. (33b), (35a) and (35b) six linear algebraic equations for the solution of the constant \( \chi_i \) are obtained,

\[ \sum_{n=1}^{6} H_{\eta i} n_m + H_{ij} = 0, \sum_{n=8}^{13} H_{n} n_m + H_{ij} = 0 \]
\[ \sum_{n=15}^{20} H_{\eta i} n_m + H_{ij} = 0, \sum_{n=22}^{27} H_{n} n_m + H_{ij} = 0 \]
\[ \sum_{n=29}^{31} H_{\eta i} n_m + H_{ij} = 0, \sum_{n=32}^{41} H_{n} n_m + H_{ij} = 0 \]

(36)

where \( H_{n} \) and \( H_{ij} \), \( H_{n} \), \( H_{ij} \), \( H_{n} \), \( H_{ij} \), \( H_{n} \), \( H_{ij} \), \( H_{n} \), \( H_{ij} \) are constants which depend on the geometric parameters of the unit cell and the material properties of the reinforcement. Once the system of Eq. (36) is solved, the determined \( \chi_{ij} \) coefficients are substituted back into Eqs. (35a) and (35b) to obtain the thermal expansion local functions \( b_{ij} \). In turn, these thermal
expansion local functions are used to calculate the homogenized thermal expansion coefficients of the smart 3D generally orthotropic grid-reinforced composite structure shown in Fig. 3 as follows:

\[ \Theta_{ij} = \frac{1}{|V|} \int_V b_{ij} \, dv \]  

(37)

Noting that the \( b_{ij} \) local functions are constant, denoting the length and cross-sectional area of the actuators/reinforcement (in coordinates \( y_1, y_2, y_3 \)) by \( L \) and \( A \) respectively, and the volume of the unit cell by \( V \), the effective thermal expansion coefficients become

\[ \Theta_{ij} = \frac{\Delta L}{V} b_{ij} = \mu_f b_{ij} \]  

(38)

where \( \mu_f \) is the volume fraction of the actuators/reinforcements within the unit cell. The effective thermal expansion coefficients derived above pertain to grid-reinforced smart composite structures with a single family of actuator and reinforcement. For structures with multiple families of inclusions the homogenized thermal expansion coefficients can be obtained by superimposition. For instance, pertaining to a 3D grid-reinforced smart structure with \( N \) families of actuators/reinforcements the effective thermal expansion coefficients are:

\[ \Theta_{ij} = \sum_{n=1}^{N} \mu_f^{(n)} b_{ij}^{(n)} \]  

(39)

Before closing this Section, it would not be amiss to mention that if we assumed polynomials of a higher order rather than linear variation for the auxiliary functions \( N_m \), \( N_n \), with respect to \( \eta_2 \) and \( \eta_3 \), then after following the aforementioned procedure and comparing terms of equal powers of \( \eta_2 \) and \( \eta_3 \), all of the terms would vanish except the linear ones.

The resulting analytical expressions to be used in Eqs. (29) and (36) are too lengthy to be reproduced in this study, details can be found in [35]. However, typical homogenized piezoelectric and thermal expansion coefficients will be computed and plotted in Section 4.

3. Numerical Micromechanical Modeling using Finite Element Analysis (FEA)

A microscopic unit cell model is used that represents the heterogeneous microstructure with periodicity condition. The 3D smart grid-reinforced structure considered is periodic which permits the isolation of discrete unit cells for the analysis. The developed finite element model takes into account geometric and material parameters, microscopic aspect such as volume fraction and the linear electro-thermo-mechanical response of a perfectly bonded cylindrical reinforcement and actuator which are aligned and poled along the principle directions and embedded in an isotropic non-piezoelectric elastic matrix as given in Fig. 4.

Finite element software ANSYS® has been used for the analysis, and the 3D coupled-field twenty-node (Solid 226) linear piezoelectric brick element has been used to mesh the unit cell. The element has five degrees of freedom per node (3 translational, thermal and electric potential). A not solved (Mesh Facet) element was added to provide greater control over element sizes and to allow for volume meshing with or without mid-side nodes and most importantly to ensure equal meshing configurations on opposite boundary surfaces of the unit cell. This process has been automated using Parametric Design Language (APDL) to generate all required constraint equations [37].

3.1. Periodic Boundary Conditions and Unit Cell Model

The developed finite element analysis consists of three basic steps.

(i) The analysis begins with the determination and prescription of periodic boundary conditions to a representative unit cell. Hence, the unit cell shown in Fig. 5 is subjected to controlled electrical field and thermal loadings by constraining opposite surfaces of the unit cell to have equivalent electro-thermo-mechanical deformations and to ensure that there is no separation or overlap between the neighbouring unit cells.

Analogies between the adequately prescribed boundary conditions and displacement field for a periodically arranged structure can be expressed as follows [15]:

\[ u_i = \tilde{\epsilon}_i y_j + u^*_i, \quad u^*_i \text{ is periodic in } (y_1, y_2, y_3) \]  

(40)

where \( \tilde{\epsilon}_i \) indicates the macroscopic (global or averaged) strains of the unit cell, \( u^*_i \) is periodic function in \( (y_1, y_2, y_3) \), and \( y_j \) is the cartesian coordinate of a unit cell point. The term \( \tilde{\epsilon}_i y_j \) represents a linearly distributed displacement field while the term \( u^*_i \) accounts for the periodicity from one unit cell to another. The periodic term represents
a modification of the linear displacement field due to
the presence of the inhomogeneous inclusions.

The equations describing the displacement fields
on different boundary surfaces of the unit
(\( \phi', \phi \), \( \phi', \phi \)) with single inclusion
shown in Fig. 5 are summarized below:

\[
\begin{align*}
\varepsilon_{ij}^+ &= \varepsilon_{ij}^{\phi} + u_i^+; \\
\varepsilon_{ij}^- &= \varepsilon_{ij}^{\phi} - u_i^-; \\
\varepsilon_{ij}^\alpha &= \varepsilon_{ij}^{\phi} + u_i^\alpha; \\
\varepsilon_{ij}^\alpha &= \varepsilon_{ij}^{\phi} - u_i^\alpha.
\end{align*}
\]  

(41)

It should be noted that the periodicity function
\( u_i(\xi_1, \xi_2, \xi_3) \) is identical at the two opposite
boundaries. The boundary conditions (41) can be
applied in the finite element model in form of
constraint equations [37].

(ii) The non-homogenous electric fields and
electrical displacements obtained from the unit cell
analysis are reduced to homogenized or averaged
quantities through an averaging procedure. Once the
local (microscopic) stress, strain, electric potential
and electric displacements fields in the unit cell are
determined under the applied loading conditions, the
average stresses and strains and the equivalent
average electric fields and electric displacements can
be expressed as follows:

\[
\begin{align*}
\bar{\sigma}_g &= \frac{1}{V} \int \sigma_g dV \\
\bar{\varepsilon}_g &= \frac{1}{V} \int \varepsilon_g dV \\
\bar{E}_i &= \frac{1}{V} \int E_i dV \\
\bar{D}_i &= \frac{1}{V} \int D_i dV
\end{align*}
\]  

(42a)

(42b)

(43a)

(43b)

where \( V \) is the volume of the periodic unit cell

(iii) The corresponding effective piezoelectric
coefficients of the pertinent smart composite structure
can be predicted using the calculated average non-
zero value in the strain and electric field vector and
the calculated average values in the stress and
electrical displacement vector using the constitutive
Eq (44). As for the effective coefficient of thermal
expansion, an increase in temperature is applied to
the unit cell to provide thermal loading and due to the
temperature difference stresses are developed. The
constitutive relations in Eq. (45) are then solved to
determine the variation of the effective coefficients
of thermal expansion.

\[
\begin{bmatrix}
\bar{\sigma}_{ij} \\
\bar{\varepsilon}_{ij} \\
\bar{E}_i \\
\bar{D}_i
\end{bmatrix}
= \begin{bmatrix}
\bar{C}_{ij} \\
\bar{C}_{ij} \\
\bar{C}_{ij} \\
\bar{C}_{ij}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{ij}^{\phi} \\
\varepsilon_{ij}^{\phi} \\
E_i^{\phi} \\
D_i^{\phi}
\end{bmatrix}
+ \begin{bmatrix}
P_{ij} \\
P_{ij} \\
P_{ij} \\
P_{ij}
\end{bmatrix}
+ \begin{bmatrix}
\bar{P}_{ij} \\
\bar{P}_{ij} \\
\bar{P}_{ij} \\
\bar{P}_{ij}
\end{bmatrix}
+ \begin{bmatrix}
\bar{\varepsilon}_{ij} \\
\bar{\varepsilon}_{ij} \\
\bar{\varepsilon}_{ij} \\
\bar{\varepsilon}_{ij}
\end{bmatrix}

(44)

\[
\begin{bmatrix}
\bar{\sigma}_{ij} \\
\bar{\varepsilon}_{ij} \\
\bar{E}_i \\
\bar{D}_i
\end{bmatrix}
= \begin{bmatrix}
\bar{C}_{ij} \\
\bar{C}_{ij} \\
\bar{C}_{ij} \\
\bar{C}_{ij}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{ij}^{\phi} \\
\varepsilon_{ij}^{\phi} \\
E_i^{\phi} \\
D_i^{\phi}
\end{bmatrix}
+ \begin{bmatrix}
P_{ij} \\
P_{ij} \\
P_{ij} \\
P_{ij}
\end{bmatrix}
+ \begin{bmatrix}
\bar{P}_{ij} \\
\bar{P}_{ij} \\
\bar{P}_{ij} \\
\bar{P}_{ij}
\end{bmatrix}
+ \begin{bmatrix}
\bar{\varepsilon}_{ij} \\
\bar{\varepsilon}_{ij} \\
\bar{\varepsilon}_{ij} \\
\bar{\varepsilon}_{ij}
\end{bmatrix}

\]  

(45)

4. Examples on 3D Smart Grid-reinforced
Composite Structures

In this Section typical effective piezoelectric and
thermal expansion coefficients will be computed and
plotted. The representative effective coefficients are
determined and compared with respect to the unit cell
spatial arrangement and the volume fraction of the
reinforcements/actuators.

For illustration purposes, we will assume that the
actuators/reinforcements have material properties
given in Table 1 [38] and Table 2 [39]. The developed
numerical model applied to a periodic network of
orthotropic smart composite with cubic orientations
of reinforcement and actuators as shown in Fig. 6. A
perfect bonding at the fiber matrix interface was
assumed and various models of increasingly finer
discretization were developed to attain a satisfactory
convergence of mesh at the boundaries of the unit
cells and around the interface, particularly for models
for constituents with larger volume fractions.

4.1. Results and Discussion

The stress field and the electric displacement field
components that are developed in the unit cell as a
result of the applied strain, electric fields and change
in temperature on the unit cell are determined.

As an example of applying the matrix representation
given in Eq. (44) for coupled field response in the unit
cell, variation of effective piezoelectric coefficients
\( P_{33} \) and \( P_{31} \) can be given by:
\[ \hat{p}_{33} = -\frac{\sigma_{33}}{E_3} \]  
\[ \hat{p}_{31} = -\frac{\sigma_{11}}{E_3} \]  

Eq. (46) refers to the stress response in the same direction as that of the applied electric field \( (y_3) \) and Eq. (47) represents the stress response of the structure in the \( (y_3) \) direction when an external electric field is applied in the \( (y_3) \) direction.

An increase in temperature is applied to the unit cell to provide a temperature loading \( (\Delta T) \) and due to the temperature difference stresses are developed. The constitutive relations in Eq. (45) are then used to determine the variation of the effective coefficients of thermal expansion in the three global directions. For instance \( \Theta_{11} \) is expressed as follows:

\[ \Theta_{11} = C_{1111}\Theta_{11} + C_{1122}\Theta_{22} + C_{1133}\Theta_{33} \]  

4.1.1. Comparison of the Analytical (AHM) and Numerical (FEA) Results

The calculated effective coefficients are compared with results from the analytical model. Typical effective piezoelectric coefficients poled in the \( (y_3) \) direction and effective thermal expansion coefficients are plotted vs. volume fractions of the reinforcements/actuators as shown in Figs. 7 and 8 respectively. Notice that there is a good agreement between numerical results calculated using the FEA and analytical solutions obtained using the AHM with small discrepancies occur for higher fiber volume fractions of reinforcements/actuators and a satisfied error less than 5%.

5. Conclusion

A comprehensive micromechanical analysis of 3D periodic composite structures reinforced with smart grid of orthotropic reinforcement and actuator has been developed. The general orthotropy of the constituent materials is very important from a practical point of view and renders the mathematical problem at hand much more complex. The AHM decouples the microscopic characteristics of the composite from its macroscopic behaviour so that each problem can be handled separately. The solution of the microscopic problem leads to the determination of the effective coefficients of piezoelectric and thermal expansion which are universal in nature and can be used to study a wide variety of boundary value problems. The FEA has been also developed and used to examine the aforementioned smart structure. The electro-thermo-mechanical deformations from the finite element simulations have been used to calculate the effective piezoelectric and thermal moduli of the structures. The results are compared and a very good agreement is shown between the two models and this indicates that the developed finite element model can be further extended to study more complex unit cell geometries.

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Fig. 1: (a) 3D smart composite structure \( \Omega \), (b) representative unit cell \( \Gamma \).
Fig. 2: Smart 3D composite and unit cell.

Fig. 3. Unit cell in original coordinates, (b) rotated macroscopic coordinates.

Fig. 4. A two-phase composite.

Fig. 5. 3D unit cell for smart composite and notation of the unit cell boundary surfaces.

Fig. 6. Discretized meshing of the unit cell.

Fig. 7. Effective piezoelectric coefficients ($\tilde{P}_{333}$, $\tilde{P}_{311}$) vs. actuator volume fraction.

Fig. 8. Effective thermal expansion coefficients ($\tilde{\Theta}_{11}$) vs. actuator volume fraction.
Table 1. Properties of thermopiezoelectric material PZT-5A [38].

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{11}^{(p)} - C_{22}^{(p)}$ (MPa)</td>
<td>121000</td>
</tr>
<tr>
<td>$C_{33}^{(p)}$ (MPa)</td>
<td>111000</td>
</tr>
<tr>
<td>$C_{12}^{(p)}$ (MPa)</td>
<td>75400</td>
</tr>
<tr>
<td>$C_{13}^{(p)} - C_{23}^{(p)}$ (MPa)</td>
<td>75200</td>
</tr>
<tr>
<td>$C_{44}^{(p)}$ (MPa)</td>
<td>22600</td>
</tr>
<tr>
<td>$C_{55}^{(p)} - C_{66}^{(p)}$ (MPa)</td>
<td>21100</td>
</tr>
<tr>
<td>$P_{13}^{(p)} - P_{23}^{(p)}$ (C/mm²)</td>
<td>-5.45E-6</td>
</tr>
<tr>
<td>$P_{33}^{(p)}$ (C/mm²)</td>
<td>1.56E-5</td>
</tr>
<tr>
<td>$P_{42}^{(p)} - P_{51}^{(p)}$ (C/mm²)</td>
<td>2.46E-5</td>
</tr>
<tr>
<td>$\theta_{11}^{(p)} = \theta_{22}^{(p)}$ (1/°C)</td>
<td>-1.704E-10</td>
</tr>
<tr>
<td>$\theta_{33}^{(p)}$ (1/°C)</td>
<td>3.732E-10</td>
</tr>
</tbody>
</table>

Table 2. Material properties of isotropic epoxy matrix [39].

<table>
<thead>
<tr>
<th>Matrix Material Properties</th>
<th>$E$ (GPa)</th>
<th>$v_{12}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>36000</td>
<td>0.35</td>
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</table>

References


