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NUMERICAL APPROACHES FOR CALCULATING THE EFFECTIVE THERMO-MECHANICAL PROPERTIES OF THREE-PHASE COMPOSITES

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The aim of this article is to predict effective thermo-mechanical properties of three phase composites made up of coated unidirectional cylindrical fibers using homogenization techniques. The main focus is on square arrangements of cylindrical fibers in composite. The numerical approach is based on the micro-mechanical unit cell modeling technique using finite element method (FEM) with appropriate boundary conditions and it allows the extension to composites with arbitrary geometrical inclusion configurations, providing a powerful tool for fast calculation of their effective properties. The results obtained from the numerical technique are compared with those obtained by means of the analytical asymptotic homogenization method (AHM) for different fiber volume fractions. In order to analyze the interphase effect, the effective properties are compared with the results obtained from some theoretical approaches reported in the literature.

Keywords: *Three-phase composite; Thermo-mechanical effective properties; Homogenization; FEM*

1 Introduction

Thermo-elastic composites constitute an important class of materials with a wide variety of applications ranging from aerospace structures and electronic printed circuit boards to recreational and commercial equipment. Some of the most important and useful properties of these composites are lightweight, high strength and stiffness, excellent frictional properties, good resistance to fatigue and retention of these properties at high temperatures. The combination of these properties has placed thermo-elastic composites at first rank among materials used for heat shields, leading edges, re-entry tips, rocket nozzles and brakes for military and advanced civilian aircrafts. The effective thermo-mechanical properties of the composite depend upon properties of the constituents and the fiber volume fraction.

Many authors have developed techniques to study the elastic behavior of fibrous composites. They take into account the existence of an intermediate layer between the matrix and the fiber. These thin layers are called interphases between fiber and matrix. These interphases are formed due to, for example, chemical reaction between the matrix and fiber materials or the use of protective coatings on the fiber during manufacturing. Although small in thickness, interphases can significantly affect the overall mechanical properties of the fiber-reinforced composites.

Several authors have developed techniques to study the elastic behavior of multiphase fibrous composites. Hill [1] provides widely established benchmarks for validating the predicted effective properties of multiphase fiber reinforced composites with arbitrary phase geometry. The stress field in a coated continuous fiber composite subjected to thermo-mechanical loading has been considered by Mikata et al. [2].

Two models to approximate the thermo-elastic response of a composite body reinforced by coated fibers oriented in various directions were developed in Pagano et al. [3]. The fundamental unit cell is a three-phase concentric circular cylinder under prescribed displacement components and surface tractions. The analysis leads to estimating how a coating applied to the fiber influences the effective thermo-elastic properties of fiber reinforced composites.

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Lagache et al. [4] determined numerically the effect of a mesophase using a finite element formulation in order to solve the local problems derived from the homogenization method. They propose analytical and semi-analytical models for determining the thermal behavior of composites.

Guinovart-Diaz et al. [5] developed analytical formulae for prediction of elastic and thermo-elastic effective material constants based on the asymptotic homogenization method (AHM). In our own work a comprehensive numerical homogenization tool using a finite element approach was developed to investigate more complex composite structures (Berger et al. [6], Kari et al. [7]).

However, in many cases of interest the perfect interphase is not an adequate model, and it is necessary to include in unit cell modeling one or more interphases separating the reinforcement inclusion phase from the host matrix phase.

In the present study, the above previous experiences of the authors for two-phase composites are extended, considering now a third phase between the fiber and matrix. In this work, effective thermo-mechanical properties of three-phase composites for different volume fractions of reinforced fiber material are predicted using micro-mechanical unit cell modeling. The unit cell is analyzed using finite element method and appropriate periodic boundary conditions for different loading conditions. In this model the perfect adhesion between the phases and the matrix is considered.

2 Unit Cell and Finite Element Procedure

The macrostructure can be seen as a periodic array of repeated unit cells. Also for particulate reinforced composites, a repeated unit cell can still be constructed after assuming a uniform distribution and the same geometry for the reinforcing phase. In the present work, micro-mechanical analysis method is applied to periodic unit cell (Fig. 1).

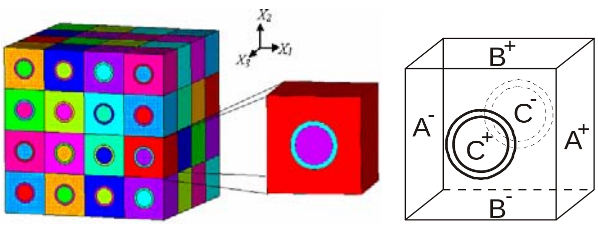

Figure 1: Periodic unit cell and surface notation

The micro-mechanical method provides the effective thermo-mechanical properties of three phase composites from the known properties of their constituents (fiber, matrix and interphase) for different volume fractions using a unit cell model. Here the unit cells are discretized and analyzed using finite element method to predict the effective thermo-mechanical properties of unidirectional periodic coated (interphase) cylindrical fiber composites for different volume fractions.

This constitutive law can be determined based on the detailed fields in the selected unit cell through an "averaging" procedure. Specifically, if the exact micro fields σ_{ij} and ε_{ij} in the unit cell are known under the applied load, the averaged stresses and strains over the unit cell are given by

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_{V_e} \sigma_{ij} dV_e, \quad \bar{\varepsilon}_{ij} = \frac{1}{V}\int_{V_e} \varepsilon_{ij} dV_e \tag{1}$$

where V is the volume of the unit cell and V_e is the element volume. The averages are then treated as the effective stress and strain fields in the homogenized unit cell. The relations between $\bar{\sigma}_{ij}$ and $\bar{\varepsilon}_{ij}$ can be determined by the "effective" constitutive law. For transversaly isotropic symmetry it can be expressed in matrix form as (longitudinal and transverse directions correspond with the coordinate system in Fig. 1)

$$\begin{bmatrix} \bar{\sigma}_{11} \\ \bar{\sigma}_{22} \\ \bar{\sigma}_{33} \\ \bar{\sigma}_{23} \\ \bar{\sigma}_{13} \\ \bar{\sigma}_{12} \end{bmatrix} = \begin{bmatrix} \bar{C}_{11} & \bar{C}_{12} & \bar{C}_{13} & 0 & 0 & 0 \\ & \bar{C}_{11} & \bar{C}_{13} & 0 & 0 & 0 \\ & & \bar{C}_{33} & 0 & 0 & 0 \\ & & & \bar{C}_{44} & 0 & 0 \\ & symm. & & & \bar{C}_{44} & 0 \\ & & & & & \bar{C}_{66} \end{bmatrix} \begin{bmatrix} \bar{\varepsilon}_{11} - \bar{\alpha}_{11}\Delta T \\ \bar{\varepsilon}_{22} - \bar{\alpha}_{11}\Delta T \\ \bar{\varepsilon}_{33} - \bar{\alpha}_{33}\Delta T \\ \bar{\varepsilon}_{23} \\ \bar{\varepsilon}_{31} \\ \bar{\varepsilon}_{12} \end{bmatrix}. \tag{2}$$

For instance, to predict the unknown effective elastic coefficients $\bar{C}_{ij}$ of the first column of stiffness matrix we impose the boundary conditions in such away that the macroscopic strain $\bar{\varepsilon}_{11}$ is not equal to zero and all other strains and ΔT are zero. The remaining coefficients can be determined in a similar way. Once all the independent constants of stiffness matrix are known, coefficients of thermal expansion $\bar{\alpha}_{kl}$ can be obtained by solving the constitutive equation with all $\bar{\varepsilon}_{kl}$ equal to zero and nonzero ΔT (by providing temperature difference to the unit cell as a body force and fix all the faces in all directions). Due to temperature difference there may be stresses developed inside the unit cell. From averaging relations in Eq. (1) stresses $\bar{\sigma}_{ij}$ are calculated. Once we know stresses $\bar{\sigma}_{ij}$ and stiffness coefficients $\bar{C}_{ij}$ and temperature difference ΔT , we can solve for the effective coefficients of thermal expansion $\bar{\alpha}_{kl}$.

All the finite element calculations were done with commercial finite element program ANSYS within the framework of the small displacements theory, and the materials are assumed to behave as linear elastic and isotropic solids. The finite element mesh is created using three dimensional multi-field 20-node hexagonal elements. To ensure equal mesh configurations on opposite surfaces for applying periodic boundary conditions three surfaces are first meshed with plane elements. Then the plane mesh configurations are copied to the opposite surfaces and the three dimensional mesh is generated based on the pre-meshed surfaces. With these identical nodal configurations on opposite surfaces the periodic boundary conditions can be applied as constraint equations between the appropriate nodal pairs.

In the next paragraphs the numerical homogenization procedure is explained in detail for calculation of selected material constants with the help of notations in Fig. 1.

For the calculation of $\overline{C}_{11}$ and $\overline{C}_{12}$, we impose the boundary conditions in such away that the macroscopic strain $\bar{\varepsilon}_{11}$ is not equal to zero and all other strains and ΔT are zero in Eq. (2). This can be achieved by applying appropriate constraint equations to the different surfaces of the unit cell. For instance, consider a cell with unit size ($x_j^{K+} - x_j^{K-} = 1$) and $\bar{\varepsilon}_{11} = 0.05$, then we have to apply the following constraint equations

$$
\begin{aligned}
&u_1^{A+} - u_1^{A-} = \bar{\varepsilon}_{11}(x_1^{A+} - x_1^{A-}) = 0.05 \\
&u_2^{B+} - u_2^{B-} = \bar{\varepsilon}_{22}(x_2^{B+} - x_2^{B-}) = 0 \text{ ; since } \bar{\varepsilon}_{22} = 0 \\
&u_3^{C+} - u_3^{C-} = \bar{\varepsilon}_{33}(x_3^{C+} - x_3^{C-}) = 0 \text{ ; since } \bar{\varepsilon}_{33} = 0
\end{aligned}
\tag{3}
$$

Here u_1, u_2 and u_3 are the displacements in x_1, x_2 and x_3 directions, respectively.

For the calculation of average stresses and strains $\bar{\sigma}_{11}$, $\bar{\sigma}_{22}$ and $\bar{\varepsilon}_{11}$ according to Eq. (1), the integral is replaced by a sum over averaged element values multiplied by the respective element volume. Using these averaged values the coefficients $\overline{C}_{11}$ and $\overline{C}_{12}$ can be calculated from the matrix Eq. (2). Due to zero strains and temperature fields except $\bar{\varepsilon}_{11}$, the first row becomes $\bar{\sigma}_{11} = \overline{C}_{11}\bar{\varepsilon}_{11}$. Then $\overline{C}_{11}$ can be calculated as the ratio of $\bar{\sigma}_{11}/\bar{\varepsilon}_{11}$. Similarly, $\overline{C}_{12}$ can be evaluated as the ratio of $\bar{\sigma}_{22}/\bar{\varepsilon}_{11}$ from the second row of matrix Eq. (2).

The other elastic coefficients can be calculated with the same procedure using appropriate constraint equations.

If we know all the independent stiffness constants in matrix Eq. (2), now in order to evaluate the effective coefficients of thermal expansion, we impose the boundary conditions in such a way that, all strain fields of strain vector in Eq. (2) are set to be zero and non-zero temperature field ΔT is applied by providing temperature difference to the unit cell as a body force and fix all the faces in all directions as follows here

$$
\begin{aligned}
&u_1^{A+} = u_1^{A-} = u_2^{A+} = u_2^{A-} = u_3^{A+} = u_3^{A-} = 0 \\
&u_1^{B+} = u_1^{B-} = u_2^{B+} = u_2^{B-} = u_3^{B+} = u_3^{B-} = 0 \\
&u_1^{C+} = u_1^{C-} = u_2^{C+} = u_2^{C-} = u_3^{C+} = u_3^{C-} = 0 \\
&\text{and } \Delta T = 1
\end{aligned}
\tag{4}
$$

Due to this temperature loading, stresses are induced inside the unit cell. From Eq. (1) we can evaluate the average stresses developed in all directions. Once we know the $\bar{\sigma}_{11}$, $\bar{\sigma}_{22}$ and $\bar{\sigma}_{33}$ with independent stiffness constants and temperature difference ΔT in Eq. (2), we obtain a system of three linear equations from which we can calculate all effective coefficients of thermal expansion.

3 Results and Discussion

At first the effective thermo-mechanical properties are evaluated for different fiber volume fractions ranging from 10% up to 70% using FEM and AHM approaches. AHM results are calculated with formulae reported in Guinovart-Diaz [5]. The material properties presented in Benveniste et al. [8] are used in the micro-mechanical unit cell modeling given in the Table 1.

Table 1: Material properties of composite constituents

Constituent	Young's Modulus (GPa)	Poisson's ratio	Thermal expansion coefficient (10^{-6})/K
Nickel matrix	214	0.3113	13.3
Tungsten fiber	345	0.2778	5.0
Carbon coating	34.48	0.2022	3.3

In all these calculations constant interphase volume fraction equal to 1.07% is considered, i.e., with increase of fiber volume fraction, the thickness of the interphase is reduced. The comparison of effective coefficients of thermal expansion α_a (fiber direction) and α_t (transverse fiber direction) between AHM and FEM is plotted in Fig. 2. The results show a good agreement between both methods. Similar good agreements were achieved for effective elastic constants.

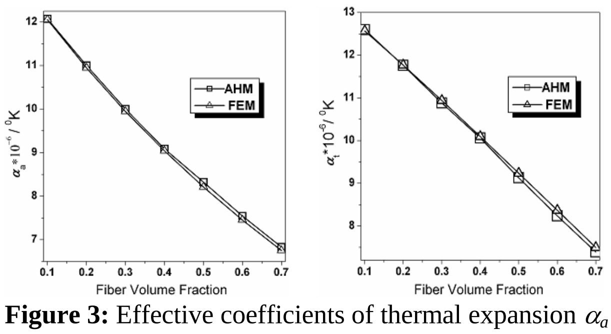

Figure 3: Effective coefficients of thermal expansion α_a and α_t comparison between FEM and AHM.

Then for further validation of the proposed method, the obtained results are compared with Guinovart-Diaz et al. [5], Pagano-Tandon [3] and Periodic Medium Homogenization (PMH) of Lagache et al. [4]. In these comparisons we use a composite material made of Nicalon fiber (volume fraction = 0.6) and barium magnesium aluminosilicate (BMAS) matrix with an isotropic interphase material (volume fraction = 0.08), which is the result of intermixing phenomena and migration of coupling agents inside the matrix as reported in Lagache et al. [4]. The material properties of the constituents are listed in Table 2.

Table 2: Material properties of BMAS/Nicalon composite with interphase

Constituent	Young's Modulus (GPa)	Shear Modulus (GPa)
BMAS matrix	106.0	43.0
Nicalon fiber	200.0	77.0
Interphase material	3.45	1.33

Here the effect of the thickness of coating material on the behavior of the Nicalon/BMAS composite system is investigated by considering two different volume fractions of interphase coating material: $V_2 = 0$ (no interface) and $V_2 = 0.08$. Table 3 shows that, with less than 8% of interphase volume fraction, the effective Young's modulus $\overline{E}_t$ and shear moduli $\overline{G}_a$, $\overline{G}_t$ (index *a* indicates fiber direction an *t* transvers fiber direction) of the composite decrease abruptly lower than 50% of the composite properties in comparison with no interphase. Also, we can observe a good agreement between the different approaches.

Table 3: Comparison between FEM, AHM and Pagano & Tandon [3] and PMH of Lagache et al. [4]

Model	$\overline{E}_a$ (GPa)	$\overline{E}_t$ (GPa)	$\overline{G}_a$ (GPa)	$\overline{G}_t$ (GPa)
FEM ($V_2 = 0$)	162.571	153.506	61.369	60.428
AHM ($V_2 = 0$)	162.578	153.508	61.363	60.431
Pagano ($V_2 = 0$)	162.530	152.840	60.615	60.357
FEM ($V_2 = 0.08$)	154.310	58.112	22.818	22.506
AHM ($V_2 = 0.08$)	154.307	58.105	22.823	22.512
Pagano $V_2 = 0.08$)	154.296	58.332	23.057	22.850
PMH ($V_2 = 0.08$)	154.131	58.438	22.909	22.668

4 Conclusions

A unit cell model is employed to predict the effective thermo-mechanical properties of three-phase coated unidirectional cylindrical fibers using homogenization techniques for different fiber volume fractions. The numerical approach is based on the finite element method. Longitudinal and transversal effective thermo-mechanical coefficients have been calculated with the finite element model and compared with analytical solutions based on the asymptotic homogenization method. The numerical results demonstrate that the developed FEM approach is very accurate and efficient for the analysis of unit cell models of fiber reinforced composites, with the presence of the interphases. The present work has laid down a foundation for further applications of micro-mechanical finite element analysis for problems, such as an investigation of stress field around the fiber in order to understand the onset and the development of inelastic behavior such as plastic deformation and possible damage. Furthermore the proved reliability of the introduced FEM approach opens new possibilities to investigate composites with arbitrary geometrical types of inclusions which cannot be covered by most other homogenization methods.

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References

[1] Hill, R., Theory of Mechanical Properties of Fiber Strengthened Materials, I Elastic Behavior, *J. Mech. Phys. Solids*, Vol. 12, p. 199, 1964.

[2] Mikata, Y. and Taya, M., Stress Field in and Around a Coated Short Fiber in an Infinite Matrix Subjected to Uniaxial and Biaxial Loadings, *ASME J. Appl. Mech.*, Vol. 52, p. 19, 1985.

[3] Pagano, N. J. and Tandon, G.P., Elastic Response of Multidirectional Coated-Fiber Composites, *Compos. Sci. Technol.*, Vol. 31, p. 273, 1988.

[4] Lagache, M. Agbossou, A. and Pastor, J., Role of Interphase on Elastic Behavior of Composite Materials: Theoretical and Experimental Analysis, *J. Comp. Mater.*, Vol. 28, p. 1141, 1994.

[5] Guinovart-Diaz, R., Rodriguez-Ramos, R., Bravo-Castillero, J., Sabina F.J. and Maugin, G.A., Closed-Form Thermo-Elastic moduli of a Periodic Three-Phase Fiber-Reinforced Composite. *J. Thermal Stresses*, Vol. 28, p. 1067, 2005.

[6] Berger, H., Kari, S., Gabbert, U., Rodriguez-Ramos, R., Guinovart, R., Otero J.A. and Bravo-Castillero, J., An Analytical and Numerical Approach for Calculating Effective Material Coefficients of Piezoelectric Fiber Composites, *Int. J. Solids Struct.*, Vol. 42, p. 5692, 2005.

[7] Kari, S., Berger, H., Rodriguez-Ramos, R., Gabbert, U. , Computational Evaluation of Effective Material Properties of Composites Reinforced by Randomly Distributed Spherical Particles. *Composite Structures*, Vol. 77, p. 2231, 2007.

[8] Benveniste, Y., Dvorak, G. J. and Chen, T., Stress Fields in Composites with Coated Inclusions, *Mech. Mater.*, Vol. 7, p. 305, 1989.