A study on the coefficients of thermal expansion of periodic unidirectional fiber reinforced composites

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Abstract. Composite materials have become an attractive alternative to traditional materials because of their advantages of high strength and stiffness combined with low density, excellent durability, and design flexibility. In many applications, the composites are subjected to temperature gradient that can produce critical thermal stress or strain fields. Then, the coefficients of thermal expansion of fiber reinforced composites are very important parameters for the design and analysis of composite structures. In this work, the effective coefficients of thermal expansion of periodic unidirectional fiber reinforced composites are studied using a micromechanical model based on the Levin's formula. The necessary effective elastic properties of the composites are evaluated through an analytical procedure based on the Eshelby equivalent inclusion method and expressed in terms of Fourier series. Numerical examples involving thermal expansion of traditional advanced composites are analyzed. The results provided by the model are compared with predictions obtained using finite element procedures and analytical simplified methods, as well as available experimental data. These comparisons demonstrate a very good performance of the presented micromechanical model.

Keywords: coefficients of thermal expansion, fiber reinforced composites, Levin's formula.

1 Introduction

Due to their unique characteristics, composite materials have become an attractive alternative to traditional materials because of their advantages of high strength and stiffness combined with low density, excellent durability, and design flexibility [1,2]. In many applications, the structural systems made with composite materials are subjected to high thermal gradients together with mechanical loadings. Then, for the design of such systems, the evaluation of the effective thermal expansion coefficients is an important task, as well as the effective elastic moduli. As it is well known, these effective properties are strongly dependent on the microstructural characteristics of the composite, such as geometry and distribution of the inhomogeneities, volume fractions of the constituent phases, and their coefficients of thermal expansion and elastic properties [3,4]. The heterogeneous nature of the microstructures of composites becomes the prediction of their effective behavior more elaborated than for the traditional homogeneous materials (metals and polymers, etc.) [4,5].

A large number of models for the prediction of the effective thermoelastic properties of composites have been proposed in the last six decades [6-9]. Such models, in general, are based on the micromechanics theory and present analytical or numerical formulations with varying degrees of complexity. Among the analytical thermoelastic models, those based on the mean-field theory, originated from the Eshelby equivalent inclusion problem [10]), have been very attractive and had an important role. In this category, it can be cited the models developed from the self-consistent [11,12], Mori-Tanaka [13,14], double-inclusion [15] and differential schemes [16,17]. The essential difference between such analytical approaches is basically in their strategies to consider the constituent interactions. These mean-field micromechanical models derived originally for elastic homogenization can be extended to evaluate the effective thermal conductivity [18] and thermal expansion coefficients [19,20] of composites. Levin [21] and Rosen and Hashin [22] derived expressions that allow determining the effective coefficients of thermal expansion of two-phase composites in function of coefficients of thermal expansion of the phases and effective elastic moduli.

The periodic composites constitute an important class of heterogeneous materials whose microstructure can be conceived as constructed by regularly replicated elementary block named repeating unit cell (RUC) [23,24]. A number of analytical and numerical models have also been proposed for homogenization of periodic composites. Usually, these models are based on the behavior of a repeating unit cell subjected to periodic boundary conditions and use numerical tools, such as finite-element method [3,9] and finite-volume theory[25-27]. Due to the periodicity of physical fluctuating fields generated in a material representative volume element (RVE) subjected to homogeneous boundary conditions, Fourier series have also been employed in the construction of analytical micromechanical models such periodic composites [15,28-31].

This paper presents a study on effective coefficients of thermal expansion of two-phase periodic composite materials using a model based on Levin's formula [21] with the effective elastic moduli evaluated through a micromechanical procedure expressed in terms of Fourier series and derived using the eigenstrain concept [10]. The results provided by the model are compared with predictions obtained using finite element procedures and analytical simplified methods, as well as available experimental data. These comparisons demonstrate a very good performance of the presented micromechanical model.

2 Effective thermal expansion coefficients: Levin's formula

Consider a statistically homogeneous N-phase composite material represented by a representative volume element (RVE) with volume V and boundary surface S (Fig.1). Suppose that the RVE is subjected to two different boundary conditions: 1) homogeneous stress $\boldsymbol{t}^0(\boldsymbol{x}) = \boldsymbol{\sigma}^0\boldsymbol{n}$, being $\boldsymbol{\sigma}^0$ a stress matrix whose elements are constant and $\boldsymbol{n}$ the outward unit vector normal to the surface S and 2) prescribed constant temperature $\theta(\boldsymbol{x}) = \theta^0$, for all $\boldsymbol{x} \in S$. Applying the virtual work theorem for the two systems subjected to the above boundary conditions,

$$\int_V \boldsymbol{\sigma}(\boldsymbol{x})^t \boldsymbol{\varepsilon}'(\boldsymbol{x}) dV = \int_S \boldsymbol{t}^0(\boldsymbol{x})^t \boldsymbol{u}'(\boldsymbol{x}) dS \tag{1}$$

where ($'$) is used to identify the field vectors (stress $\boldsymbol{\sigma}'$, strain $\boldsymbol{\varepsilon}'$and displacement $\boldsymbol{u}'$) of the RVE subjected to the temperature boundary condition. Making the integral decomposition into the sum of integrals over the phase volumes V_k and using the divergence theorem for the right side of eq. (1), results

$$\sum_{k=1}^{N} \int_{V_k} \boldsymbol{\sigma}(\boldsymbol{x})^t \boldsymbol{\varepsilon}'(\boldsymbol{x}) dV_k = \boldsymbol{\sigma}^{0t} \overline{\boldsymbol{\alpha}} \theta^0 V \tag{2}$$

where $\overline{\boldsymbol{\alpha}} = [\overline{\alpha}_{11}\ \overline{\alpha}_{22}\ \overline{\alpha}_{33}\ 2\overline{\alpha}_{23}\ 2\overline{\alpha}_{13}\ 2\overline{\alpha}_{12}]$ is the effective thermal expansion coefficient vector of the composite.

It is observed that the average stress $\overline{\boldsymbol{\sigma}}' = \boldsymbol{0}$ and $\overline{\boldsymbol{\varepsilon}}' = \overline{\boldsymbol{\alpha}}\theta^0$. Considering that the average stress vector in the kth phase can be written as $\overline{\boldsymbol{\sigma}}^{(k)} = \boldsymbol{B}^{(k)}\boldsymbol{\sigma}^0$, being $\boldsymbol{B}^{(k)}$ the phase stress concentration matrix [15], the following relation can be obtained from eq. (2):

$$\overline{\boldsymbol{\alpha}} = \sum_{k=1}^{N} c_k\, \boldsymbol{\alpha}^{(k)} \boldsymbol{B}^{(k)} \tag{3}$$

where $c_k = V_k/V$ indicates the volume fraction of the kth phase, which presents a volume V_k and coefficient of thermal expansion α_k. From micromechanics theory of elastic heterogeneous materials, the stress concentration matrix of the phase k can be related to its strain concentration matrix $\boldsymbol{A}^{(k)}$and stiffness matrix $\boldsymbol{C}^{(k)}$ by

$$\boldsymbol{B}^{(k)} = \boldsymbol{C}^{(k)} \boldsymbol{A}^{(k)} \overline{\boldsymbol{C}}^{-1} \tag{4}$$

being $\overline{\boldsymbol{C}}$ the effective stiffness matrix of the composite [15]. Substituting eq. (4) into eq. (3), the effective thermal expansion coefficient vector can be evaluated as

$$\overline{\boldsymbol{\alpha}} = \sum_{k=1}^{N} c_k\, \overline{\boldsymbol{C}}^{-1} \boldsymbol{A}^{(k)t} \boldsymbol{\Gamma}^{(k)} \tag{5}$$

where $\boldsymbol{\Gamma}^{(k)} = \boldsymbol{C}^{(k)}\boldsymbol{\alpha}^{(k)}$. Here, the matrix $\overline{\boldsymbol{C}}$ is computed through a model based on the eigenstrain concept and expressed in terms of Fourier series presented by the authors and outlined in the next section. Equation (5) represents the Levin's formula for evaluation of effective coefficients of thermal expansion [21].

3 Outline on the elastic homogenization model

Suppose a representative volume (RVE) of a two-phase periodic composite subjected to a strain homogeneous boundary condition $\boldsymbol{u}^0(\boldsymbol{x}) = \boldsymbol{\varepsilon}^0\boldsymbol{x}$ similar to that of Fig. 1. For this condition, the displacement field of a repeated unit cell (RUC) of the RVE is given by a two-scale representation in the form

$$\boldsymbol{u}(\boldsymbol{y}) = \boldsymbol{\varepsilon}^0\boldsymbol{x} + \widetilde{\boldsymbol{u}}(\boldsymbol{y}) \tag{6}$$

where $\boldsymbol{y}$ indicates the local coordinates of the RUC scale, the first term on the right side represents the macroscopic contribution and $\widetilde{\boldsymbol{u}}$ is the fluctuating displacement vector (Fig. 1). For the considered homogeneous boundary condition and material periodic microstructure, $\widetilde{\boldsymbol{u}}(\boldsymbol{y})$ is a periodic function over the RUC domain U. This periodicity allows writing the fluctuating displacement vector in Fourier series as [15]

$$\widetilde{\boldsymbol{u}}(\boldsymbol{y}) = \sum_{\xi}^{\pm\infty} \widehat{\boldsymbol{u}}(\boldsymbol{\xi}) \exp(i\boldsymbol{\xi}^t\boldsymbol{y}) \qquad \widehat{\boldsymbol{u}}(\boldsymbol{\xi}) = \frac{1}{U}\int_U \widetilde{\boldsymbol{u}}(\boldsymbol{y})\, exp(-i\boldsymbol{\xi}^t\boldsymbol{y})dU \tag{7}$$

with the components of the vector $\boldsymbol{\xi}$ defined by $\xi_r = \pi n_r/a_r$, $(r = 1,2,3)$, being $2a_r$ the RUC side dimensions and $n_r = 0, \pm 1, \pm 2, \dots \pm \infty$. Analogously, the fluctuating strain field $\tilde{\boldsymbol{\varepsilon}}(\boldsymbol{y})$ associated with $\widetilde{\boldsymbol{u}}(\boldsymbol{y})$ also can be expanded in Fourier series.

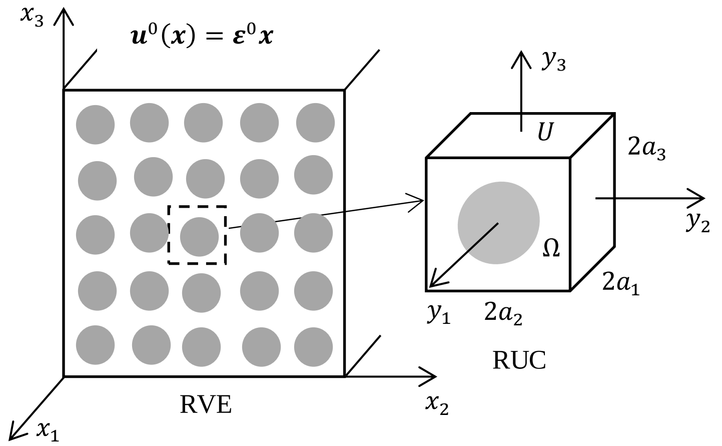


Figure 1. Representative volume element and repeating unit cell of a periodic composite.

Denoting by $\boldsymbol{C}_\Omega$ and $\boldsymbol{C}$ the stiffness matrices of the actual inclusion and matrix material, respectively, the consistency condition of the equivalent inclusion method [10] is expressed in the form

$$\boldsymbol{\nabla} \cdot \boldsymbol{C}[\boldsymbol{\varepsilon}^0 + \tilde{\boldsymbol{\varepsilon}}(\boldsymbol{y}) - \boldsymbol{\varepsilon}^*(\boldsymbol{y})] = \boldsymbol{0} \tag{8}$$

where $\boldsymbol{\varepsilon}^*(\boldsymbol{y})$ is the periodic eigenstrain vector which represents the primary unknown of the homogenization problem. After considering the equilibrium conditions for the stress field inside the RUC, it is possible to show that [15]

$$\boldsymbol{\varepsilon}^0 = -(\boldsymbol{C}_\Omega - \boldsymbol{C})^{-1}\boldsymbol{C}\boldsymbol{\varepsilon}^*(\boldsymbol{y}) - \frac{1}{U}\sum_{\xi}^{\pm\infty} \boldsymbol{S}(\boldsymbol{\xi})\boldsymbol{C}\left[\int_\Omega \boldsymbol{\varepsilon}^*(\boldsymbol{y}') \exp(-i\boldsymbol{\xi}^t\boldsymbol{y}')d\Omega\right]\exp(i\boldsymbol{\xi}^t\boldsymbol{y}) \tag{9}$$

being $\boldsymbol{S}(\boldsymbol{\xi})$ a $(6\ x\ 6)$ matrix depending on the stiffness matrix $\boldsymbol{C}$ [31].. The homogenization model only requires the evaluation of the average value of $\boldsymbol{\varepsilon}^*(\boldsymbol{y})$ over the inclusion domain Ω more than its local values. Considering the mathematical complexity of the problem expressed by eq. (9), its solution is made by using approximate procedures. Here, the expression used to obtain the average eigenstrain vector $\bar{\boldsymbol{\varepsilon}}^*_\Omega$ is given by [31]

$$c_j\boldsymbol{\varepsilon}^0 = -c_j(\boldsymbol{C_\Omega} - \boldsymbol{C})^{-1}\boldsymbol{C}\bar{\boldsymbol{\varepsilon}}^*_{\Omega_j} - \frac{1}{U\Omega}\sum_{s=1}^{M}\sum_{\xi}^{\pm\infty}\boldsymbol{S}(\boldsymbol{\xi})\boldsymbol{C}\,g_s(-\boldsymbol{\xi})g_j(\boldsymbol{\xi})\bar{\boldsymbol{\varepsilon}}^*_{\Omega_s} \tag{10}$$

Equation (10) is solved by dividing the inclusion domain Ω into M subdomains or partitions Ω_s ($s = 1,2,\dots,M$) with volume fractions $c_s = \Omega_s/\Omega$ and assuming for each one of them the average value $\bar{\varepsilon}^*_{\Omega s}$.

The functions g_s and g_j appearing in eq. (10) represent the following integrals:

$$g_j(\boldsymbol{\xi}) = \int_{\Omega_j}\exp(i\boldsymbol{\xi}\cdot\boldsymbol{y})d\Omega_j \qquad g_s(-\boldsymbol{\xi}) = \int_{\Omega_s}\exp(-i\boldsymbol{\xi}\cdot\boldsymbol{y})d\Omega_s \tag{11}$$

The average eigenstrain vector over the total domain Ω can be expressed in terms of the average eigenstrain vectors of the partitions as

$$\bar{\boldsymbol{\varepsilon}}^*_{\boldsymbol{\Omega}} = \sum_{s=1}^{N} c_s\bar{\boldsymbol{\varepsilon}}^*_{\Omega_s} \tag{12}$$

which, using eq. (10), can be obtained in the compact form

$$\bar{\boldsymbol{\varepsilon}}^*_{\Omega} = \boldsymbol{\mathcal{F}}^t\boldsymbol{\mathcal{L}}^{-1}\boldsymbol{\mathcal{F}}\boldsymbol{\varepsilon}^0 \tag{13}$$

where

$$\boldsymbol{\mathcal{L}} = \begin{bmatrix} \boldsymbol{L}_{11} & \boldsymbol{L}_{12}\cdots\boldsymbol{L}_{1M} \\ \boldsymbol{L}_{21} & \boldsymbol{L}_{22}\cdots\boldsymbol{L}_{2M} \\ & \cdots\vdots \\ \boldsymbol{L}_{M1} & \boldsymbol{L}_{M2}\cdots\boldsymbol{L}_{MM} \end{bmatrix}_{(6M\times 6M)} \qquad \boldsymbol{\mathcal{F}} = [c_1\boldsymbol{I} \;\; c_2\boldsymbol{I} \;\cdots c_M\boldsymbol{I}]^t_{6\times 6M} \tag{14}$$

being $\boldsymbol{I}$ the 6×6 identity matrix and

$$\boldsymbol{L}_{js} = c_j(\boldsymbol{C_\Omega} - \boldsymbol{C})^{-1}\boldsymbol{C}\delta_{js} - \frac{1}{U\Omega}\sum_{\xi}^{\pm\infty}\boldsymbol{S}(\boldsymbol{\xi})\boldsymbol{C}g_s(-\boldsymbol{\xi})g_j(\boldsymbol{\xi}) \tag{15}$$

More details can be found in reference [31].

4 Effective coefficients of thermal expansion

Using the equivalent inclusion method together with eq. (13) the effective elastic stiffness matrix of the composite can be obtained as [31]

$$\overline{\boldsymbol{C}} = \boldsymbol{C}(\boldsymbol{I} - c_\Omega\boldsymbol{\mathcal{F}}^t\boldsymbol{\mathcal{L}}^{-1}\boldsymbol{\mathcal{F}}) \tag{16}$$

being $c_\Omega = \Omega/U$ the volume fraction of the inclusion in the repeating unit cell. Now, using eq. (5) for the case of two-phase composite ($N = 2$), the effective thermal expansion coefficients of the composite can be obtained by the expression

$$\overline{\boldsymbol{\alpha}} = c_\Omega\,\overline{\boldsymbol{C}}^{-1}\boldsymbol{A}^t_\Omega\boldsymbol{\Gamma}_\Omega + (1 - c_\Omega)\,\overline{\boldsymbol{C}}^{-1}\boldsymbol{A}^t\boldsymbol{\Gamma} \tag{17}$$

where $\boldsymbol{A}_\Omega$ and $\boldsymbol{A}$ are the strain concentration matrices of the inclusion and matrix, respectively, which are given by

$$\boldsymbol{A}_\Omega = \frac{1}{c_\Omega}(\boldsymbol{C_\Omega} - \boldsymbol{C})^{-1}(\overline{\boldsymbol{C}} - \boldsymbol{C}) \qquad \boldsymbol{A} = \frac{1}{(1 - c_\Omega)}(\boldsymbol{I} - c_\Omega\boldsymbol{A}_\Omega) \tag{18}$$

In eq. (17), $\boldsymbol{\Gamma}_\Omega = \boldsymbol{C_\Omega}\boldsymbol{\alpha}_\Omega$ and $\boldsymbol{\Gamma} = \boldsymbol{C}\boldsymbol{\alpha}$, being $\boldsymbol{\alpha}_\Omega$ and $\boldsymbol{\alpha}$ the vectors of thermal expansion coefficients of the inclusion and matrix, respectively.

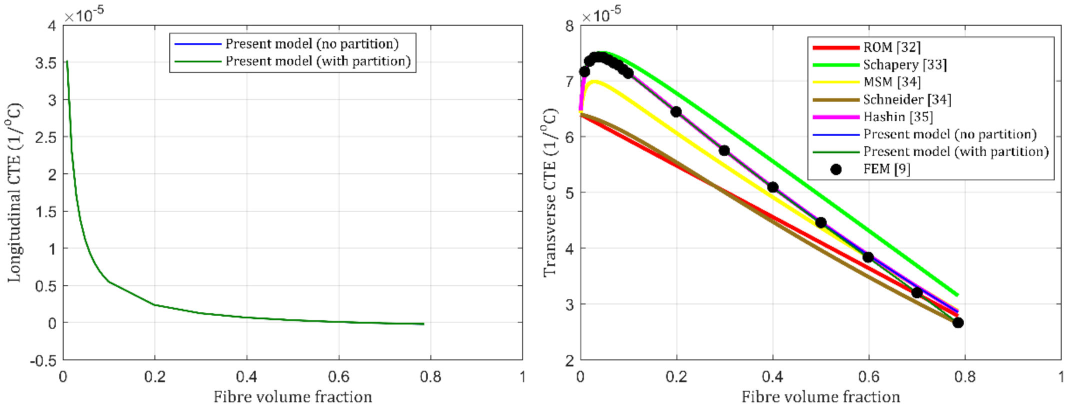
5 Numerical examples

5.1 Effective thermal expansion coefficients of a AS4/epoxy composite

This example treats of a composite constituted by an epoxy matrix reinforced with longitudinal long AS4 carbon fibers. The fibers are assumed as transversely isotropic and distributed in a square array. The properties of the phases are presented in Tab. 1 (see, Dong [9]). Here, the subscripts 1 and 2 represent the longitudinal and transverse directions, respectively. Figure 2 shows the results for the longitudinal and transverse effective coefficients of thermal expansion generated by the present model using $M = 1$ (without partition) and $M = 90$ in eq. (10). For comparison, results obtained by the finite-element method (FEM) [9] and several simplified analytical micromechanical models [32-35] are also shown in Fig. 2(b). As observed, the predictions of the present model are in excellent agreement with those obtained by the finite-element method and experimental test. Among all simplified analytical procedures, the Hashin model showed results with a very good approximation in relation to those generated by the present formulation and finite-element method.

Table 1. Properties of the epoxy matrix and AS4 carbon fiber [9]

	E_1 (GPa)	E_2 (GPa)	G_1 (GPa)	G_2 (GPa)	ν_1	ν_2	α_1 $(10^{-6}/^0C)$	α_2 $(10^{-6}/^0C)$
AS4	235	14	6.917	5	0.2	0.4	-0.40	18
Epoxy	2.581				0.265		64	



(a) (b)

Figure 2. Effective thermal expansion coefficients of the AS4/epoxy composites: (a) longitudinal direction and (b) transverse direction.

5.2 Effective thermal expansion coefficients of a T300/epoxy composite

In this example, the model is employed to evaluate the longitudinal and transverse effective coefficients of thermal expansion (CTE) of a periodic composite with an epoxy matrix reinforced by unidirectional T300 carbon fiber. The thermoelastic properties of the constituent materials are shown in Tab. 2. The transversely isotropic fibers are assumed as having a square packing arrangement inside the isotropic epoxy matrix.

Table 2. Thermoelastic properties of the epoxy matrix and T300 fiber

	E_1 (GPa)	E_2 (GPa)	G_1 (GPa)	G_2 (GPa)	ν_1	ν_2	α_1 $(10^{-6}/^0C)$	α_2 $(10^{-6}/^0C)$
T300	233.13	23.11	8.97	8.28	0.2	0.4	-0.54	10.08
Epoxy	4.35		1.59		0.37		43.92	

Figure 3 shows the results obtained for the longitudinal and transverse coefficients of thermal expansion compared with finite-element method (FEM) predictions [3], analytical solutions [32-35], and experimental data [36]. The finite-element solutions have been obtained using refined unit cell discretizations with ten-node tetrahedral coupled field solid elements available in a commercial finite-element program, as described in [3]. Figure 3 illustrates also that the results provided by the micromechanical model are in excellent agreement with the mentioned finite-element solutions and present a very small deviation with respect to the experimental data for the effective transverse coefficient of thermal expansion. Again, as can be seen in Fig.3(b), the predictions of the Hashin model are in good agreement with the results of the present formulation, as well as with those corresponding to the finite-element solution.

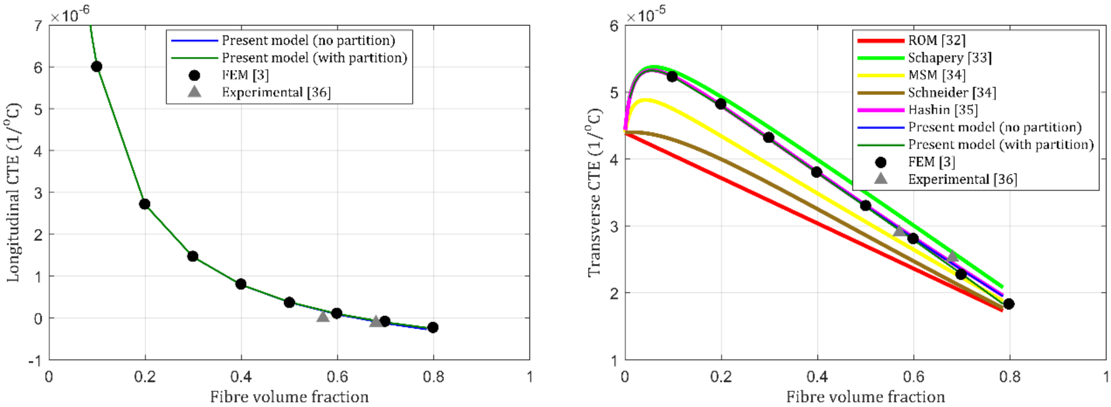


Figure 3. Effective thermal expansion coefficients for the T300/Epoxy composite: (a) longitudinal direction and (b) transverse direction.

6 Conclusions

In this work a model based on Levin's formula has been presented to evaluate the effective coefficients of thermal expansion of two-phase elastic periodic composites. For the computation of the effective stiffness of the material, it is employed a procedure derived using the eigenstrain concept and expressed in term of Fourier series. The model is applied to obtain the transverse effective thermal expansion coefficients of polymer composites reinforced with unidirectional transversely isotropic carbon fiber. The results provided by the present model have been compared with predictions obtained by analytical and finite-element micromechanical procedures, as well as experimental data. These comparisons show a very good performance of the presented model, especially in relation to the finite-element solutions.

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