ANALYSIS OF THE INFLUENCE OF THE MICROSTRUCTURE CONFIGURATION ON THE EFFECTIVE CONDUCTIVITY OF FIBROUS COMPOSITE MATERIALS

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Abstract. *The computation of macroscopic thermal properties of composites is of fundamental and practical importance, given the widespread application of such multicomponent materials. Many factors are important to determine the effective thermal conductivity of a composite material body. The main physical parameters are the temperature-dependent thermal conductivities of the constituent phases and, possibly, an interfacial thermal resistance between the phases. Microstructural parameters are related to the geometry and the spatial and size distributions of the dispersed phase. They include the relative volume amounts of the phases and higher order moments. An important class of composite materials is that of fibrous composites. The geometrical arrangement of the fibers in the matrix will depend on the manufacturing process of the composite. Of course, different geometrical arrangements of the fibers lead to different microstructure configurations, which in turn affect the effective thermal conductivity of the material. In this paper a first analysis is conducted numerically, to verify the influence of the microstructure configuration on the effective conductivity of 3-D short-fiber composite bodies. For this purpose, previous continuous and discrete formulations and computational implementation are used. The continuous equations are obtained through application of homogenization theory to the variational form of the heat conduction boundary value problem for the multiscale composite medium. The variational form is well suited for subsequent numerical solution by the finite element method. An expression for the effective thermal conductivity of the composite is provided, such that it can be computed for each constructed microstructure configuration. Several sets of numerical results are then presented and analyzed.*

Keywords*: effective thermal conductivity, fibrous composites, microstructure configuration, heat conduction*

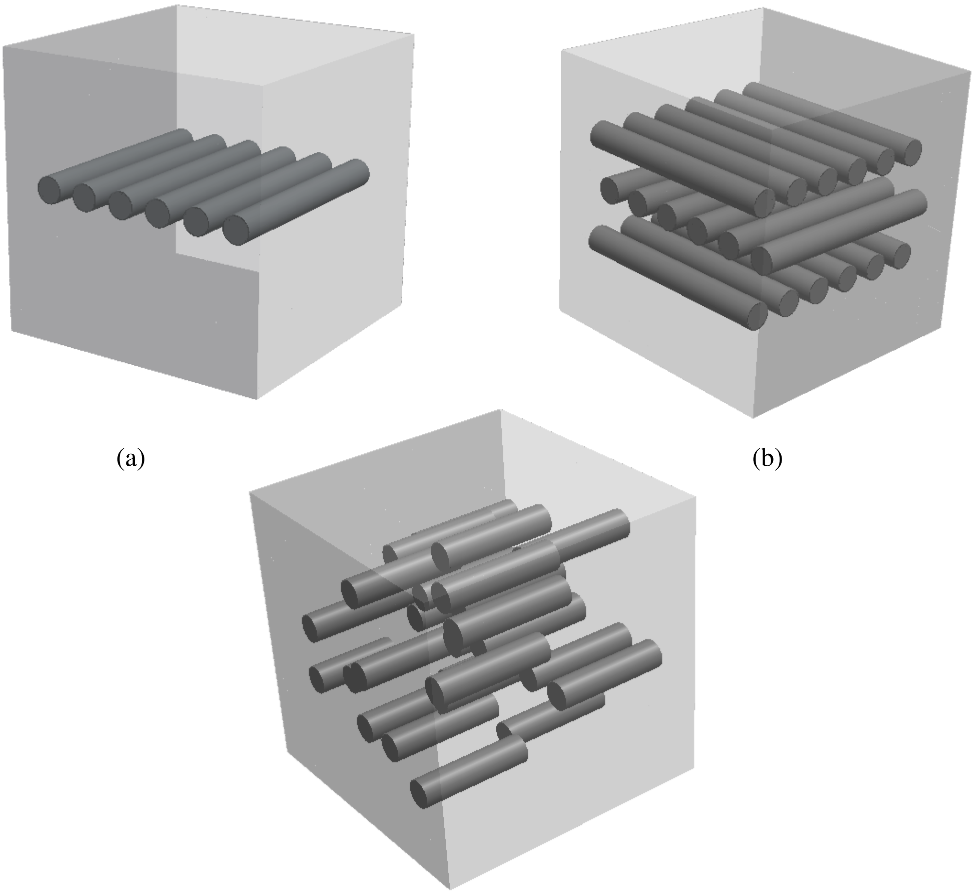
1. INTRODUCTION

Milton (2002) defines composites as materials with inhomogeneities on length scales that are much larger than the atomic scale, but which are essentially statistically homogeneous at macroscopic length scales. Therefore, one may use the equations of classical physics at the length scales of the inhomogeneities. Composites are useful because the synergistic combination of materials with different attributes permits a range of properties to be obtained (Tsai, 1992). The underlying problem of composites consists in the resolution of the pertinent classical physics principles at the microscopic level. In practice, however, a much simpler route is adopted: one decouples the original problem into the macromechanics problem formed by the macroscopic equations and the micromechanics problem formed by the microscopic cell problem; the latter establishes the relation between the properties of the constituents and those of the composite body. To effect the decoupling rigorously, homogenization theory (Bensoussan *et al.*, 1978; Auriault, 1983) is frequently employed.

Lately, an often manufactured type of composite used for heat transfer and other applications consists of solid short fibers dispersed in a solid matrix (Mirmira, 1999; Hine *et al.*, 2004). Short-fiber composites have low cost and are relatively easy to fabricate. For those thermal applications requiring strong directionality (i.e., anisotropy), short-fiber composites are suited, because the thermal conductivities in orthogonal directions may differ by more than one order of magnitude depending on the underlying microstructure. Common materials for fibers are carbon, glass and polymers, whereas common materials for matrices are thermosetting resins and thermoplastics (Hull, 1981).

1.1. Fundamentals and review of literature

The geometrical arrangement of the fibers in the matrix material will generally depend on the manufacturing process of the composite. Commonly when fabricating short-fiber composites, the matrix and fibers are mixed and pressed together, such that the fibers tend to align in planes perpendicular to the applied compression forces. Consequently, the fibers may become transversely aligned (lying on parallel planes but not parallel to each other in each plane) or even longitudinally aligned (lying on parallel planes and parallel to each other in each plane). Longitudinal alignment may be disrupted by possible small random deviations from the main direction of alignment. Other manufacturing routes may



(a) (b)

(c)

Figure 1. (a) Ordered one-layer composite with longitudinally-aligned short fibers. (b) Orthogonal two-layered microstructure. (c) Cell with multiple fibers at random locations.

distribute the fibers randomly throughout space, or may construct layered structures, in which fibers are oriented at different angles in each layer. Figure 1 illustrates various short-fiber composite microstructures.

Many parameters are important to determine the effective thermal conductivity of composite materials (Milton, 2002). In theory, only the temperature-dependent thermal conductivities, volume fractions, and spatial and size distributions of the constituent phases should be taken into account. However, in practice, other parameters may come into play. Because of manufacturing imperfections, the composite effective conductivity may also depend on an interfacial thermal resistance (or contact resistance) between the phases and also on a porosity (void) content in the matrix (Hasselman and Johnson, 1987; Mirmira, 1999; Hatta *et al.*, 2000; Garnier *et al.*, 2002).

Given the complexities involved in the study of heat conduction in short-fiber composites, flexible approaches that can accommodate geometrical (e.g., cell and fiber shapes) and physical (e.g., contact resistance) variations are needed, in order to predict properties and aid interpretation of experimental measurements. Reviews of analytical, computational and experimental investigations of heat conduction in composite materials are presented, respectively, by Furmanski (1997), Cruz (2001) and Mirmira (1999). Analytical (Han and Cosner, 1981; Furmanski, 1991) and phenomenological (Benveniste *et al.*, 1990; Dunn *et al.*, 1993) models developed to predict the effective thermal conductivity of short-fiber composites have limited accuracy and generally do not account for all the relevant physics and/or geometrical intricacies (e.g., the fibers are modeled as ellipsoids of revolution, rather than sharp-edged circular cylinders). An alternative to exact analytical treatments is statistical bound methods. The objective of these methods is to determine upper and lower bounds for the effective property of interest, based on a description of the medium's microstructure via correlation functions. Nomura and Chou (1980) developed bounds for the longitudinal and transverse effective thermal conductivities of longitudinally-aligned composites with isotropic ellipsoidal short fibers. Finally, computational approaches (Veyret *et al.*, 1993; Rolfes and Hammerschmidt, 1995), relative to analytical studies, are better suited to treat more complex geometries and phenomena. However, none of the approaches has been applied to short-fiber composites. Here, it is believed that finite-element based approaches should offer enough flexibility to handle more realistic models of actual composites microstructures and physics.

1.2. Scope of paper

In view of the preceding scenario, it is clear that an accurate determination of the effective thermal conductivity of short-fiber composites under controlled parametrical and microstructural specifications is of great practical interest. In this paper an earlier developed multiscale finite-element-based methodology (Matt and Cruz, 2001, 2002, 2006) is applied to solve the heat conduction problem in different cell microstructures for circular-cylindrical short-fiber composites. In the present investigation the focus is on the analysis of the influence of the three-dimensional cell microstructure configuration on the effective thermal conductivity of the composite material. Therefore, several other effects are not considered here, and should be taken into account in future follow-up studies. Specifically, the configurations considered are multiple particle parallelepipedonal cells, in which fiber volume fraction, fiber aspect ratio and fiber inter-spacing are controlled. The parallelepipedonal cells overcome the severe limitation on the range of fiber aspect ratios (Matt and Cruz, 2001). The fibers are considered isotropic and more conductive than the matrix. The interfacial thermal resistance and presence of voids in the matrix are disregarded. As a consequence, calculated values for the effective thermal conductivity are expected to overestimate measured values, provided a good, or candidate, microstructural configuration has been developed for the experimental composite specimens. In this case, the approach developed by Matt and Cruz (2008) to consider both contact resistance and voids in 3-D may then be employed to yield (expectedly) realistic results.

This paper is organized as follows. In the next section the continuous problem formulation is briefly presented. The method of homogenization is applied to the variational form of the appropriate multiscale heat conduction problem, to derive the periodic cell problem of interest, as well as an expression for the composite effective conductivity tensor. Subsequently, the numerical methods – three-dimensional mesh generation, isoparametric finite-element discretization and iterative solution – used to solve the cell problem are summarized. In the results section, the influence of the microstructure configuration on the effective conductivity is analyzed through the use of different sets of periodic cells, each with same fiber volume fraction, fiber and cell aspect ratios and matrix-to-fiber thermal conductivity ratio. When possible, the numerical findings are compared to some available experimental data. Finally, concluding remarks are stated.

2. CONTINUOUS PROBLEM FORMULATION

The continuous problem formulation introduced by Matt and Cruz (2001, 2002, 2006) is condensed here for completeness of the paper. Consider a composite medium whose three-dimensional representative volume element (RVE) or periodic cell is denoted by Ω_{pc}. The cell, illustrated in Fig. 2, may contain several short fibers of diameter D and length δ distributed in some fashion inside a parallelepipedonal matrix of height H and volume $\lambda^2 H$. The y_1, y_2 and y_3 axes form the Cartesian coordinate system attached to the cell. The fibers-to-cell volume ratio defines the concentration or fiber volume fraction c of the composite and the ratio δ/D defines the fiber aspect ratio ρ. The composite extends throughout a macroscale region $\Omega_c \cup \Omega_d$ of dimension L, over which an external temperature gradient $\Delta T/L$ is imposed; the geometric domains and the thermal conductivities of the continuous and dispersed phases are, respectively, denoted by Ω_c, k_c and Ω_d, k_d; $\alpha \equiv k_d/k_c$, $\alpha \geq 0$. It is assumed here that the two phases have a perfect thermal contact at the interface and are solid, homogeneous and isotropic. The parameter $\epsilon \equiv \lambda/L$, a ratio of two natural length scales of the composite medium problem, is further assumed to be much less than unity.

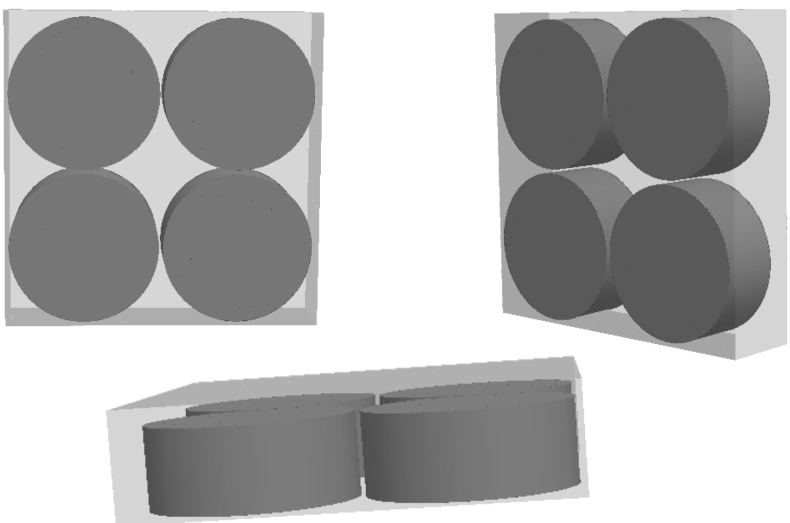


Figure 2. Illustration of the geometry of a periodic cell Ω_{pc}.

The multiscale periodic steady-state heat conduction problem in the composite medium is governed by:

$$-\frac{\partial}{\partial x_j}\left(k\frac{\partial T_\varepsilon}{\partial x_j}\right)=\dot{g} \quad \text{in} \quad \Omega_\mathrm{c}\cup\Omega_\mathrm{d}\,, \tag{1}$$

$$[T_\varepsilon]_{\partial\Omega_\mathrm{s}}=0\,, \tag{2}$$

$$\left[-k\frac{\partial T_\varepsilon}{\partial x_j}\right]_{\partial\Omega_\mathrm{s}} n_j=0\,, \tag{3}$$

$$T_\varepsilon=F(\mathbf{x}) \quad \text{on} \quad \partial(\Omega_\mathrm{c}\cup\Omega_\mathrm{d})\,, \qquad k,\,T_\varepsilon,\,\dot{g}=k_c,\,T^c,\,\dot{g}_c \;\text{ in }\; \Omega_\mathrm{c}\,, \quad k,\,T_\varepsilon,\,\dot{g}=k_d,\,T^d,\,\dot{g}_d \;\text{ in }\; \Omega_\mathrm{d}\,. \tag{4}$$

In Eqs. (1)-(4), summation over repeated indices is implied; $\mathbf{x}$ is the vector of macroscopic space coordinates; T is the temperature field; dotted g is the volume rate of heat generation; $\partial\Omega_\mathrm{s}$ is the union of all the interfaces between the matrix and the fibers; $\mathbf{n}$ is the unit vector locally normal to $\partial\Omega_\mathrm{s}$ and pointing into Ω_d; the bracket notation $[\phi]_{\partial\Omega}$ is used to indicate the discontinuity of the function ϕ at $\partial\Omega$; and, finally, $\partial(\Omega_\mathrm{c}\cup\Omega_\mathrm{d})$ in (4) is the union of the external boundaries of the body, where boundary conditions are imposed to generate the macroscopic temperature gradient $\Delta T/L$.

The application of homogenization theory (Bensoussan *et al.*, 1978; Auriault, 1983) to the variational form of the heat conduction problem (1)-(4) is presented by Matt and Cruz (2001). The idea of the method is to derive an equivalent macroscale, or homogenized, problem whose solution permits the calculation of engineering bulk quantities. The relevant input parameter in the homogenized problem is the effective thermal conductivity, the calculation of which requires the solution of an associated cell problem. The variational formulation naturally enforces the flux condition in Eq. (3) and casts the cell problem in a form suited for subsequent numerical solution by the finite-element method. The homogenization procedure starts with the introduction of the usual multiple-scale asymptotic expansion, in which T_ϵ is written as a function of the slowly-varying coordinate $\mathbf{x}$ and the rapidly-varying coordinate $\mathbf{y} \equiv \mathbf{x}/\epsilon$. After some manipulation and collection of terms of equal powers of ϵ, the following equations are derived:

$$\frac{\partial T_0}{\partial y_j}=0 \quad \text{or} \quad T_0=T_0^c=T_0^d=T_0(\mathbf{x})\,, \tag{5}$$

$$\int_{\Omega_\mathrm{c}\cup\Omega_\mathrm{d}} k\left(\frac{\partial T_0}{\partial x_j}+\frac{\partial T_1}{\partial y_j}\right)\left(\frac{\partial v_0}{\partial x_j}\right)d\mathbf{x}=\int_{\Omega_\mathrm{c}\cup\Omega_\mathrm{d}} v_0\dot{g}\;d\mathbf{x} \quad \forall v_0\in X(\Omega_\mathrm{c}\cup\Omega_\mathrm{d})\,, \tag{6}$$

$$\int_{\Omega_\mathrm{c}\cup\Omega_\mathrm{d}} k\left(\frac{\partial T_0}{\partial x_j}+\frac{\partial T_1}{\partial y_j}\right)\left(\frac{\partial v_1}{\partial y_j}\right)d\mathbf{x}=0 \quad \forall v_1\in X(\Omega_\mathrm{c}\cup\Omega_\mathrm{d})\,. \tag{7}$$

Equation (5) means that T_0 varies on the macroscale only. In Eqs. (6) and (7), the function space $X(\Omega_\mathrm{c}\cup\Omega_\mathrm{d})$ is defined as $X(\Omega_\mathrm{c}\cup\Omega_\mathrm{d}) = \{w \in H_0^1(\Omega_\mathrm{c}\cup\Omega_\mathrm{d}) \mid w_{|\Omega c} = w^c,\, w_{|\Omega d} = w^d\}$, where $H_0^1(\Omega_\mathrm{c}\cup\Omega_\mathrm{d})$ is the space of all functions which vanish on $\partial(\Omega_\mathrm{c}\cup\Omega_\mathrm{d})$, and for which both the function and derivative are square-integrable over $(\Omega_\mathrm{c}\cup\Omega_\mathrm{d})$. Equations (6)-(7) will then give rise to the cell and homogenized problems, as follows.

Now writing

$$T_1(\mathbf{x},\mathbf{y})=-\chi_p(\mathbf{y})\frac{L}{\Delta T}\frac{\partial T_0(\mathbf{x})}{\partial x_p}\,, \tag{8}$$

where χ_p is a periodic solution to (7) corresponding to a temperature gradient $\Delta T/L$ imposed in the x_p direction (summation over p, p = 1,2,3, is implied), substituting (8) into (7) and applying the periodicity property (Auriault, 1983; Matt and Cruz, 2001), one obtains

$$\int_{\Omega_\mathrm{pc,c}} k_c\frac{L}{\Delta T}\frac{\partial\chi_p^c}{\partial y_j}\frac{\partial v^c}{\partial y_j}d\mathbf{y}+\int_{\Omega_\mathrm{pc,d}} k_d\frac{L}{\Delta T}\frac{\partial\chi_p^d}{\partial y_j}\frac{\partial v^d}{\partial y_j}d\mathbf{y}=\int_{\Omega_\mathrm{pc,c}} k_c\frac{\partial v^c}{\partial y_p}d\mathbf{y}+\int_{\Omega_\mathrm{pc,d}} k_d\frac{\partial v^d}{\partial y_p}d\mathbf{y} \qquad \forall v\in Y(\Omega_\mathrm{pc})\,, \tag{9}$$

where $Y(\Omega_{pc}) = \{w \in H_\#^1(\Omega_{pc}) \mid w_{|\Omega pc,c} = w^c,\ w_{|\Omega pc,d} = w^d\}$, $H_\#^1(\Omega_{pc})$ is the space of all triply periodic functions (subscript #) in Ω_{pc} for which both the function and derivative are square-integrable. Equation (9) is the solvable cell problem of interest here: the left-hand side of (9) is the standard Laplacian operator and the right-hand side, although slightly non-standard, is easily computed for a chosen test function. For uniqueness, it is further required that χ_p integrates to zero over the cell Ω_{pc}.

The homogenized problem for the function $T_0(\mathbf{x})$ is derived to be (Matt and Cruz, 2001):

$$\forall v_0 \in X(\Omega_c \cup \Omega_d), \qquad \int_{\Omega_c \cup \Omega_d} k_{e,pq} \frac{\partial T_0}{\partial x_p} \frac{\partial v_0}{\partial x_q} d\mathbf{x} = \int_{\Omega_c \cup \Omega_d} \left(\frac{1}{|\Omega_{pc}|} \int_{\Omega_{pc}} v_0 \dot{g}\ d\mathbf{y} \right) d\mathbf{x}\,, \qquad (10)$$

where $|\Omega_{pc}|$ is the total volume of the cell. The quantity $k_{e,pq}$ in Eq. (10) is the tensorial effective thermal conductivity of the composite medium: once the solution to the cell problem (9) is obtained for χ_p, $p = 1,2,3$, one can calculate

$$k_{e,pq} \equiv \frac{1}{|\Omega_{pc}|} \left\{ \int_{\Omega_{pc,c}} k_c \left(\delta_{pq} - \frac{L}{\Delta T} \frac{\partial \chi_q^c}{\partial y_p} \right) d\mathbf{y} + \int_{\Omega_{pc,d}} k_d \left(\delta_{pq} - \frac{L}{\Delta T} \frac{\partial \chi_q^d}{\partial y_p} \right) d\mathbf{y} \right\}. \qquad (11)$$

For anisotropic short-fiber composites, it is necessary to solve the cell problem three times, for $p = 1$ (y_1-axis), $p = 2$ (y_2-axis) and $p=3$ (y_3-axis), to obtain the components of the tensorial effective conductivity.

3. NUMERICAL SOLUTION

Numerical solution of the cell problem (9) demands the execution of three tasks: geometry and mesh generation, finite element discretization and iterative solution of the resultant linear system of algebraic equations. Here, only the main aspects of the numerical solution of the desired conduction problem are presented.

Finite-element mesh generation consists in the subdivision of the physical domain of interest in a collection of non-overlapping conforming sub-domains, called the elements. The geometry and mesh generation procedures to construct unstructured quadratic tetrahedral meshes inside Ω_{pc} are described in detail by Matt and Cruz (2001, 2002, 2006), and exploit the resourceful third-party 2-D/3-D mesh generator NETGEN 4.0 (Schöberl, 1997, 2001). The periodic cell domain Ω_{pc} for the short-fiber composites contains N fibers, whose spatial positions and orientations are chosen to form microstructure configurations, that might approach those of real composites. In this study, the geometry and mesh generation procedures are simplified, and comprise three basic steps. In the first step, an ASCII data file is written with all domain and boundary conditions data. In the second step, a (sufficiently small) default mesh spacing is entered. NETGEN then reads the previously written data file and subsequently generates fine surface meshes on the faces of the cell (where periodicity is met) and on the surfaces of the fibers. In the third step, NETGEN constructs fine volume meshes in the various cell subdomains and automatically optimizes the meshes upon the user's request. The quality of meshes generated by this procedure is ascertained by the consistency of the numerical results (section 4). Figure 3 shows a pictorial tetrahedral mesh generated using the three-step procedure just described, for a cell with 16 short fibers and the concentration value of $c = 0.11$. As a final note, after the generation of the quadratic tetrahedra, one must identify the midside nodes on tetrahedra edges whose extremities lie on a fiber surface. These nodes must be moved to also lie on the fiber surface, in order to implement isoparametric quadratic discretization.

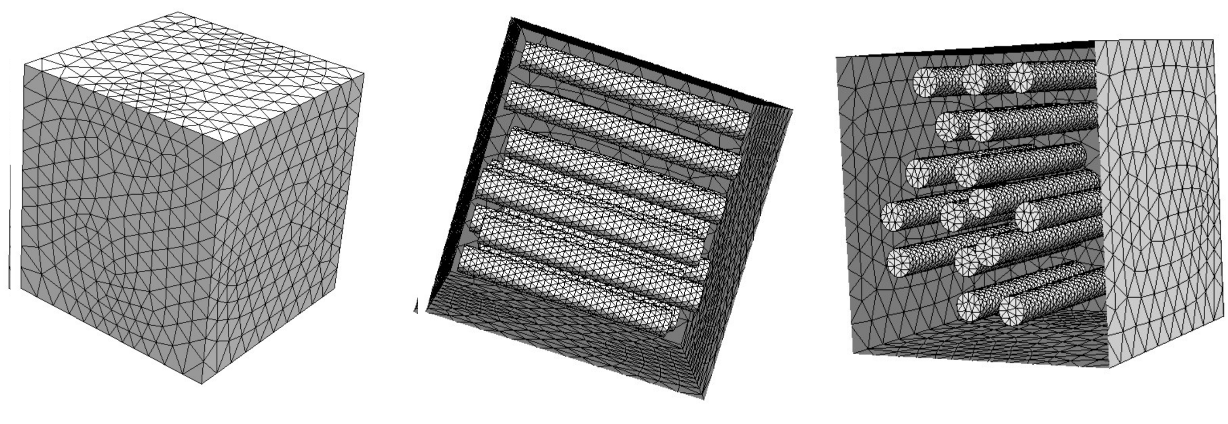


Figure 3. Tetrahedral mesh generated in a 3-D cell with 16 fibers and $c = 0.11$.

To carry out finite element discretization, Eq. (9) is first rewritten in the non-dimensional form

$$a(\chi^*, v) = l(v) \quad \forall v \in Y(\Omega_{pc}), \tag{12}$$

where the field variable of interest in the periodic cell is the temperature χ, $\chi \in Y(\Omega_{pc})$, $a(\chi,v)$ and $l(v)$ are, respectively, the usual bilinear form and the (non-dimensionalized) linear functional on the right-hand side of Eq. (9) (Matt and Cruz, 2001). In Eq. (12), $\chi^* = \chi_i^*$ when $p = i$, i = 1,2,3. The non-dimensional variables are defined as $\chi^* \equiv (\chi/\Delta T)(L/\lambda)$, $k^* \equiv k/k_c$, $\mathbf{y}^* \equiv \mathbf{y}/\lambda$. The Galerkin approximation (Hughes, 2000) to Eq. (12) is given by

$$a(\chi_h^*, v) = l(v) \quad \forall v \in Y_h(\Omega_{pc,h}), \tag{13}$$

where χ_h^* is the discrete approximation to χ^*, $Y_h(\Omega_{pc,h}) = \{w|_{T_K} \in P_2(T_K)\} \cap Y(\Omega_{pc,h})$, $P_2(T_K)$ is the space of all polynomials of degree 2 defined on the K^{th} tetrahedron T_K and $\Omega_{pc,h}$ is the numerical domain. Expressing χ_h^* and v in Eq. (13) in terms of the usual nodal Lagrangian interpolants and performing all the integrals by Gaussian quadrature with five points (Bathe, 1982), the following discrete linear system of equations is obtained,

$$\mathbf{A}\underline{\boldsymbol{\chi}}_h^* = \mathbf{F}, \tag{14}$$

where $\mathbf{A}$ is the global system matrix corresponding to the discrete (negative) Laplacian operator, $\underline{\boldsymbol{\chi}}_h^*$ is the vector of unknown global nodal values of the scalar field χ_h^* and $\mathbf{F}$ is the vector corresponding to the inhomogeneity $l(v)$, related to the (direction of the) imposed temperature gradient. The well-known conjugate gradient algorithm (Schewchuk, 1994) with no preconditioning is chosen for iterative solution of the discrete problem (14). The iteration proceeds until the square of the ratio of the Euclidean norm of the residual to the Euclidean norm of the initial residual is less than a user-specified tolerance, σ^2; in this work, $\sigma=10^{-4}$ has been used. The discrete equation for the numerically determined pq-component of the effective thermal conductivity tensor, made non-dimensional with respect to the matrix conductivity, is obtained by substituting χ_h^* for χ and the appropriate values of p and q in Eq. (11), so that

$$k_{e,pq}^N \equiv \frac{1}{|\Omega_{pc,h}|}\left\{ \int_{\Omega_{pc,h}} k^* \left(\delta_{pq} - \frac{\partial \chi_{h,q}^*}{\partial y_p^*} \right) d\mathbf{y}^* \right\}. \tag{15}$$

Henceforth, for the microstructures considered in the current study, the longitudinal and transverse effective thermal conductivities are denoted by the symbols $k_{e,L}$ (= $k_{e,11}^N$) and $k_{e,T}$ (= $k_{e,22}^N$ = $k_{e,33}^N$), respectively.

4. RESULTS

Numerical results for the effective conductivities of different microstructure configurations of composite materials are now presented. The main objectives in this section are, first, to investigate the effect of the microstructure configuration (varied, e.g., by changing the number of fibers) on the effective thermal conductivity and, second, to make a tentative comparison between the numerical results and some measured data provided by Mirmira *et al.* (2001). Those authors fabricated composites with short graphite fibers, named K22XX ($k_{d,\parallel}$ = 600 W/m·K), dispersed in a solid cyanate ester matrix (k_c = 0.3 W/m·K at 300 K) with three different fiber volume fractions– 0.55, 0.65 and 0.75–, and measured their effective thermal conductivities. The diameter of the graphite fibers is 10 μm, whereas their lengths lie within the range from 3 to 5 μm. Hence, in the computational runs performed here, the fiber-to-matrix conductivity ratio is set equal to 2000, and the three fiber volume fractions mentioned previously are considered. Furthermore, three fiber aspect ratios are analyzed, namely, 0.3, 0.4 and 0.5, in order to possibly reproduce values encountered in the composites fabricated by Mirmira and co-workers.

In the first set of results, the effects of changing fiber volume fraction and fiber aspect ratio on the effective thermal conductivities of a composite with one longitudinally-oriented fiber in the parallelepipedonal cell are indicated. Such one-fiber cell microstructure configuration is designated as Microstructure A (Fig. 1(a)). The numerical effective conductivities for Microstructure A along the longitudinal and transverse directions with respect to the fiber's alignment plane are presented in Tab. 1 for three values of the fiber aspect ratio, $\rho \in \{0.3, 0.4, 0.5\}$. The parallelepiped aspect ratio is defined as $\eta = H/\lambda$; it is worthwhile to mention that in each run for Microstructure A the value of η is set equal to that of ρ. For a fixed fiber volume fraction, the parallelepiped and fiber aspect ratios specify the distances between fibers in neighboring cells along the y_1-, y_2- and y_3-axes, thereby influencing the effective conductivities (Matt and Cruz, 2006). For instance, for Microstructure A with one particular value of η and ρ, as the fiber volume fraction increases, the distances between fibers in neighboring cells along the y_1- and y_2- (or y_3-) directions decrease (as more fiber material is added); therefore, because $k_d \gg k_c$, both the longitudinal and transverse effective conductivities increase as c increases, as can be verified in Tab. 1. On the other hand, for a fixed value of the fiber volume fraction c for Microstructure A, as the fiber aspect ratio decreases, both the longitudinal and transverse effective conductivities decrease. The latter behavior is explained by the fact that all the inter-fiber distances increase as η and ρ decrease at fixed c.

Table 1. Longitudinal and transverse numerical effective conductivity results for Microstructure A.

Fiber volume fraction, c	$\eta = \rho = 0.5$		$\eta = \rho = 0.4$		$\eta = \rho = 0.3$	
	$k_{e,L}$	$k_{e,T}$	$k_{e,L}$	$k_{e,T}$	$k_{e,L}$	$k_{e,T}$
0.55	6.826	4.712	6.499	4.640	6.390	4.628
0.65	12.89	7.051	12.68	7.044	12.48	7.040
0.75	51.47	16.21	51.39	16.12	50.04	16.05

In the second set of results, the effects of changing the microstructure configuration on the effective thermal conductivities are verified, when the number of longitudinally-aligned fibers with $\rho = 0.5$ in the parallelepipedonal cell is varied; the fiber volume fraction is $c \in \{0.55, 0.65, 0.75\}$. The microstructure configurations with 3 and 4 fibers are designated as Microstructure B and Microstructure C, respectively. Figures 4 and 5 show finite-element meshes inside the Microstructures B and C, respectively, for each of the three fiber volume fractions. The longitudinal and transverse effective conductivities for these microstructures are presented in Tab. 2.

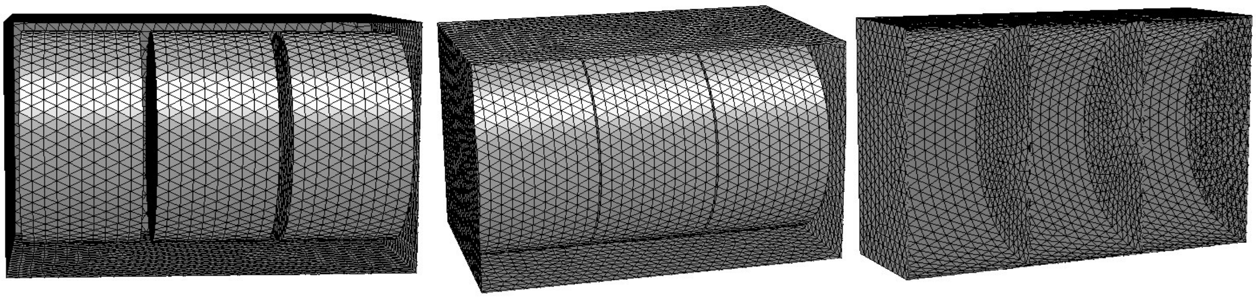


Figure 4. Tetrahedral meshes inside Microstructure B– 3 fibers with $\rho = 0.5$, $\eta = 1.5$– for $c = 0.55$ (left), $c = 0.65$ (middle) and $c = 0.75$ (right).

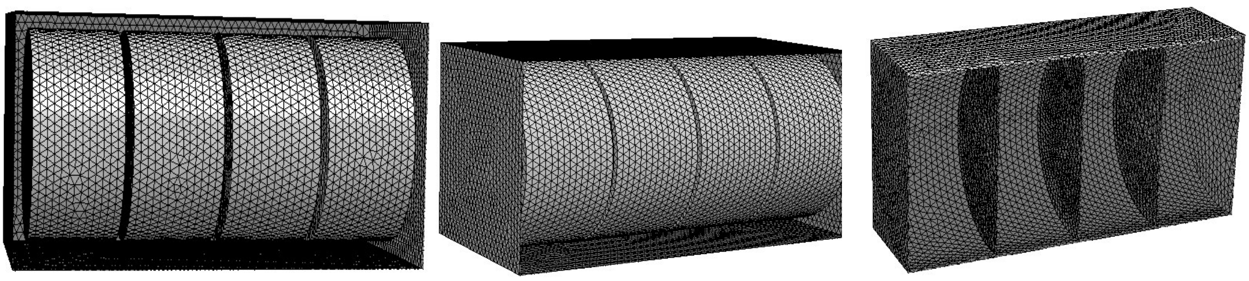


Figure 5. Tetrahedral meshes inside Microstructure C– 4 fibers with $\rho = 0.5$, $\eta = 2.0$– for $c = 0.55$ (left), $c = 0.65$ (middle) and $c = 0.75$ (right).

Table 2. Longitudinal and transverse numerical effective conductivity results for Microstructures B and C.

Fiber volume fraction, c	Microstructure B		Microstructure C	
	$k_{e,L}$	$k_{e,T}$	$k_{e,L}$	$k_{e,T}$
0.55	6.840	4.715	7.186	4.815
0.65	13.16	7.080	13.29	7.170
0.75	51.73	16.33	65.06	18.06

From the observation of Tab. 2 one may make the following comments. First, for both Microstructures B and C, as the fiber volume fraction increases, both the longitudinal and transverse effective conductivities also increase. Second, the largest effective conductivities are verified for Microstructure C with c = 0.75. Third, the effect of the number of fibers on the composite effective conductivities becomes more pronounced as the fiber volume fraction increases. Lastly, the number of fibers in the cell influences more significantly the longitudinal rather than the transverse effective conductivity.

Table 3 summarizes the numerical results obtained for the transverse effective thermal conductivities of all the microstructures considered in the current study. For purposes of comparison, in Tab. 3 some experimental data for the transverse effective conductivity measured by Mirmira *et al.* (2001) are also presented. From the analysis of Tab. 3 one verifies that the numerical predictions underestimate the measured data for the two lowest fiber volume fractions (c = 0.55 and c = 0.65), whereas for the highest value of c (0.75), the numerical calculations overestimate the measured conductivity. The discrepancies obtained between the numerical predictions and the measured data might be, in part, attributed to the geometrical deviations of the microstructure configurations constructed here with respect to the real microstructures. The current configurations, despite being fully three-dimensional and appropriate to investigate the effects of structural parameters of paramount importance on the composite effective conductivities (Matt and Cruz, 2006), do not consider fibers with different orientations and/or different aspect ratios inside the periodic cell. The continuous and numerical formulations employed here, however, can treat more complex cell configurations. Thus, such cells must be constructed in future investigations.

Table 3. Numerical results for the transverse effective conductivities of all the microstructures considered, and measured values provided by Mirmira *et al.* (2001).

Microstructure	c = 0.55		c = 0.65		c = 0.75	
	Numerical	Measured	Numerical	Measured	Numerical	Measured
A, ρ = 0.3	4.628	$12.8 \pm 0.4^*$	7.040	$11.4 \pm 0.4^*$	16.05	$10.0 \pm 0.3^*$
A, ρ = 0.4	4.640		7.044		16.12	
A, ρ = 0.5	4.712		7.051		16.21	
B	4.715		7.080		16.33	
C	4.815		7.170		18.06	

*The average overall uncertainty of the effective conductivity is reported by those authors to be approximately 3.2%.

5. CONCLUSIONS

In this study, a previously developed finite-element based procedure to compute the effective thermal conductivity of ordered or disordered short-fiber composite materials has been successfully applied to different microstructure configurations. It has been verified that, for the same values of the fiber volume fraction, ratio of phase conductivities and fiber aspect ratio, the composite effective conductivity varies as the configuration is changed. It has also been established that numerical and experimental results do deviate significantly. Thus, the investigation must be extended to consider more complex microstructure configurations, by including fibers with different orientations and aspect ratios in the periodic cell. Finally, to wrap up, it is recommended that experimental studies with short-fiber composites should be reported, as much as possible, with detailed quantitative information about the fabricated microstructures and the geometrical characteristics of the short fibers. It is believed that complementary numerical approaches will then help interpretation of experimental results.

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