A PRELIMINARY NUMERICAL STUDY ON THE EFFECTIVE THERMAL CONDUCTIVITY OF COMPOSITES WITH TRANSVERSELY-ALIGNED SHORT FIBERS

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Abstract. *Composite materials are being continually developed for a wide range of engineering applications worldwide. An important class of composites consists of those with monodisperse solid short fibers of circular cylindrical shape dispersed in a solid matrix. Manufacturing processes for such composites usually press the components together, such that the fibers tend to align perpendicularly to the applied pressure. Consequently, the fibers may become transversely aligned (lying on parallel planes, but not parallel to each other in each plane). Few works in the literature focus on predicting bulk thermal properties of short-fiber composites. Many of the analytical, phenomenological and numerical approaches are restricted to much simplified microstructures, do not take into account the thermal interactions between neighboring particles, or yet are based on ad-hoc hypotheses. The purpose of the present work is to carry on a preliminary numerical study on the effective thermal conductivity of composites with transversely-aligned short fibers, based on first principles. The numerical approach used in this work stands out for its geometrical and physical flexibility, and is able to handle fairly complex microstructures. The steady heat conduction problem is solved in composites whose three-dimensional microstructures are modeled by periodic cells composed of either cubic or parallelepipedonal subcells. In the subcells, short circular cylindrical fibers are placed at their centers; the axes of the fibers lie in the same plane, but are not parallel to each other. The effective thermal conductivities of such composites are predicted as functions of the fiber volume fraction, ratio of phase conductivities and geometry of the microstructure, characterized by the aspect ratio and distribution of the fibers inside the matrix. At the present time, an interfacial thermal resistance between the phases is not considered, and neither is the presence of voids and cracks in the matrix.*

Keywords: *effective conductivity, fibrous composites, finite elements*

1. INTRODUCTION

Composite materials, often made with fibers or particles dispersed in a continuous matrix of another constituent, can attain a wide range of thermal properties, and are being continually developed for engineering applications worldwide. The determination of bulk thermal properties of composites, in terms of the microstructure and component properties, is thus a crucial effort. Flexible numerical approaches to the study of heat conduction in modern composites are needed in order to obtain more reliable and applicable results. Recent advances in computing capabilities have enabled increased quality of numerical simulations; in particular, finite-element methodologies are now able to handle three-dimensional geometries in a reasonable amount of time.

An important class of composites consists of those with monodisperse solid short fibers of circular cylindrical shape dispersed in a solid matrix. Manufacturing processes for such composites usually press the components together, such that the fibers tend to align perpendicularly to the applied pressure. Consequently, the fibers may become transversely aligned, i.e., lying on parallel planes, but not parallel to each other in each plane. Few works in the literature focus on predicting bulk thermal properties of short-fiber composites. Many of the analytical, phenomenological and numerical approaches are restricted to much simplified microstructures, do not take into account the thermal interactions between neighboring particles, or yet are based on ad-hoc hypotheses.

The purpose of the present work is to carry on a preliminary numerical study on the effective thermal conductivity of composites with transversely-aligned short fibers, based on first principles. The numerical approach used in this work stands out for its geometrical and physical flexibility, and is able to handle fairly complex microstructures. The following microstructural models are investigated: to represent the arrangement of fibers in the composite, periodic cells composed of either cubic or parallelepipedonal subcells are adopted, in which short circular cylindrical fibers are placed at their centers; the axes of the fibers lie in the same plane, but are not (necessarily) parallel to each other. The steady heat conduction problem is numerically solved by first applying a recently implemented semi-automatic procedure to generate unstructured tetrahedral meshes in the overall periodic-cell microstructures. Next, the meshes are used in a finite-element code to obtain the effective conductivities as a function of the fiber volume fraction, ratio of phase conductivities and geometry of the microstructure, characterized by the aspect ratio and distribution of the fibers inside the matrix. Results such as these, originating from an attempt to model real microstructures, are needed in the literature. At the present time, an interfacial thermal resistance between the phases is not considered, and neither is the presence of voids and cracks (porosity) in the matrix.

2. BRIEF LITERATURE REVIEW

A large number of publications dedicated to the analytical, semi-analytical or numerical study of the heat conduction problem in composite materials deal with geometrically simple microstructures, constituted by a single particle or fiber embedded in the matrix. The dispersed phase is often modeled as spherical particles or (long or short) fibers, the latter in the form of ellipsoids of revolution or circular cylinders. Many analytical treatments do not take into account the effects of the thermal interactions between neighboring particles. Therefore, the analytical expressions derived are valid only for low (to moderate) volume fractions of the dispersed phase. In general, for short-fiber composites, analytical and numerical predictions for the effective thermal conductivity found in the literature are not in good agreement with experimental data. Much work needs to be done to narrow this gap. Currently, there is no single approach based on first principles which simultaneously treats three-dimensional microstructures, anisotropic phases, interactions between neighboring fibers, interfacial thermal resistance, presence of voids and/or cracks in the matrix, and distributions for the size, shape, position and orientation of the fibers. Comments on some previous works that are used later in this paper for comparison with the numerical results are now made.

Perrins *et al.* (1979) used a Rayleigh-type analytical method to determine transport properties of unidirectional fibrous composites, in which the long cylindrical fibers are arranged in the square or hexagonal array. The expression derived for the calculation of the transverse effective thermal conductivity of the square array, k_T^P, nondimensionalized with respect to the matrix conductivity, is

$$k_T^P = 1 - \frac{2c}{T + c - \dfrac{0.305827c^4 T}{T^2 - 1.402958c^8} - \dfrac{0.013362c^8}{T}}, \tag{1}$$

where $T \equiv \frac{1+\alpha}{1-\alpha}$, and c and α represent, respectively, the fiber volume fraction and the fiber-to-matrix ratio of phase conductivities. Nomura and Chou (1980) derived upper and lower bounds for the transverse effective thermal conductivity of unidirectional composites with ellipsoidal short fibers. The approach is based on a perturbation technique using a Green's function tensor, and the correlation functions used to calculate the bounds are evaluated up to the third order term.

Mirmira (1999) and Mirmira and Fletcher (1999) carried out an experimental study of the heat conduction problem in short-fiber composites, and at the same time developed an analytical expression for the transverse effective thermal conductivity based on a phenomenological micromechanical model which considers the fibers as circular cylinders. Mirmira (1999) and Mirmira and Fletcher (1999) focused their study on graphite fiber organic matrix (GFOM) composites with one of three kinds of fibers, denoted DKE X, DKA X and K22 XX. Their expression for the transverse effective thermal conductivity, k_T^M, nondimensionalized with respect to the matrix conductivity, is

$$k_T^M = \left[\frac{\left(\dfrac{(k_r k_\varphi)^{0.5}}{k_m} + \dfrac{(k_r k_\varphi)^{0.5}}{(d/2)(1/R)} + 1\right) + c\left(\dfrac{(k_r k_\varphi)^{0.5}}{k_m} - \dfrac{(k_r k_\varphi)^{0.5}}{(d/2)(1/R)} - 1\right)}{\left(\dfrac{(k_r k_\varphi)^{0.5}}{k_m} + \dfrac{(k_r k_\varphi)^{0.5}}{(d/2)(1/R)} + 1\right) + c\left(\dfrac{(k_r k_\varphi)^{0.5}}{(d/2)(1/R)} - \dfrac{(k_r k_\varphi)^{0.5}}{k_m} + 1\right)}\right](1 - V_p)^2, \tag{2}$$

where k_r and k_φ are the fiber conductivities in the radial and tangential directions, respectively, k_m is the matrix conductivity, d is the fiber diameter, R is the interfacial thermal resistance, and V_p is the porosity content. Expression (2) takes into account, in an ad-hoc fashion, the influence on k_T^M of the thermal properties of the phases, fiber volume fraction, fiber anisotropy, interfacial thermal resistance, and presence of voids in the matrix. However, the fibers are seemingly assumed to be longitudinally aligned, a less likely and less complex configuration than transversely aligned short fibers.

Cruz (2001) reviewed the application of computational methods to the study of heat conduction in composite materials. In particular, it was argued that approaches which combine homogenization theory with finite elements offered great geometrical and physical flexibility to rigorously treat complex microstructural configurations and phenomena. In fact, Rocha and Cruz (2001) accounted for the interfacial thermal resistance in disordered unidirectional fibrous composites, while Matt (2003) and Matt and Cruz (2002, 2001), respectively considering and not considering an interfacial thermal resistance, predicted the effective thermal conductivity of three-dimensional composites with spherical particles and with longitudinally aligned short fibers. The results obtained by Matt and Cruz (2001) are used here for validation purposes.

The present work extends the one by Matt and Cruz (2001) to three-dimensional composites with transversely aligned short fibers. Differently from many works found in the literature, the effects due to variable fiber orientation and to the interactions between neighboring fibers are taken into account. Other relevant physical parameters previously mentioned shall be progressively incorporated in future extentions of this work.

3. METHODOLOGY

The methodology employed in this work consists of two main steps:

- application of the homogenization method to the variational form of the steady three-dimensional heat conduction problem in the composite medium;
- numerical solution of the derived cell problem, defined in a representative volume element of the composite microstructure, using the finite element method; once the temperature distribution in the cell has been determined, the components of the effective thermal conductivity tensor can be calculated.

The continuous and discrete formulations of the problem (i.e., the homogenization procedure and the discretization by finite elements) and the mesh generation schemes are described in detail elsewhere (Matt and Cruz, 2001; Matt and Cruz, 2002; Matt *et al.*, 2003; Hirata, 2003).

The first model – Model I – for the composite microstructure consists of a periodic cell composed of four equal cubic subcells, in which four short circular cylindrical fibers are placed at the centers of the cubes. The axes of the fibers lie in the same vertical y_1-y_2 plane, but are not (necessarily) parallel to each other. Therefore, the so-constructed cell can represent composites with both longitudinally aligned and transversely aligned short fibers. Each cubic subcell has sides of length λ. The four cylinders have the same diameter d and length δ, and their axes lie in the y_1-y_2 plane located at $y_3 = \lambda/2$. To represent transversely aligned fibers, the angles φ_i, i=1,2,3,4, formed by the i-th fiber axis and the y_1 axis, are chosen randomly (i.e., drawn from a uniform probability density function) in the interval $0^o \leq \varphi_i < 180^o$. The nondimensional diameter d/λ and the nondimensional length δ/λ of the cylindrical fibers are determined as functions of the user-specified fiber volume fraction, c, and aspect ratio, ρ, respectively defined by

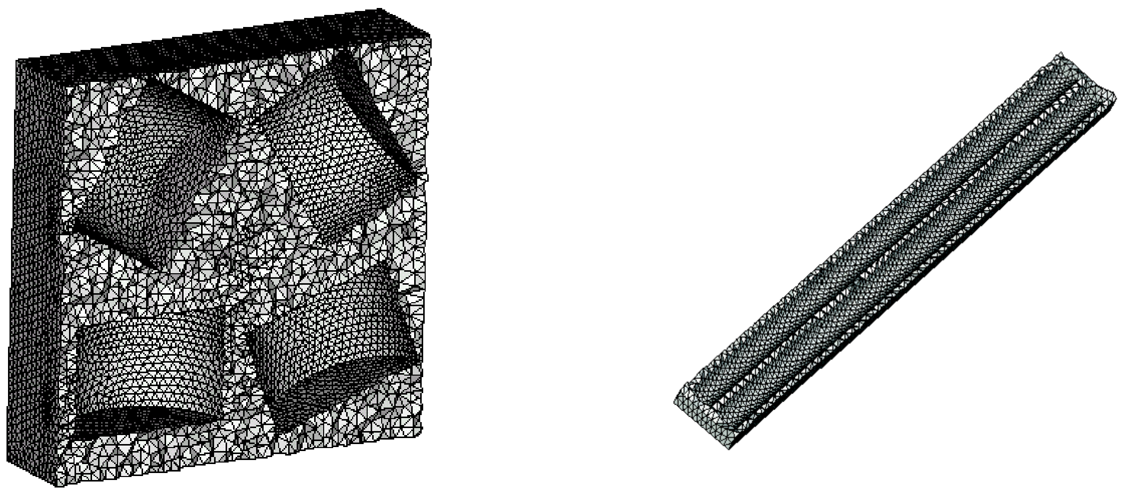
$$c = \frac{\pi d^2 \delta}{4\lambda^3} \quad \text{and} \quad \rho = \frac{\delta}{d}. \tag{3}$$

It is important to remark that, for an arbitrary value of the angle φ_i of a fiber, the geometry of the periodic cell leads to a limitation on the range of values of the fiber aspect ratio ρ for a given value of c (Matt *et al.*, 2003; Hirata, 2003). This limitation is due to the restriction that a fiber must not touch the faces of its enclosing subcell, or

$$\sqrt{d^2 + \delta^2} < \lambda . \tag{4}$$

The second model – Model II – for the composite microstructure consists of a parallelepipedonal periodic cell in which two circular cylindrical fibers are placed (slightly) oblique to each other. With this new model, it is possible to simulate the high fiber volume fractions and aspect ratios of some short-fiber composites used in practice. Nevertheless, another geometric limitation is imposed: the axes of the fibers tend to be practically parallel to each other, with angles of only a few degrees.

Representative examples of volume meshes in the periodic cells of Models I and II are shown in Fig. (1). The schemes for the generation of the unstructured tetrahedral finite-element meshes of this work rely on the software NETGEN (Schöberl, 2001), and are described elsewhere (Matt and Cruz, 2001; Matt *et al.*, 2003; Hirata, 2003). Effective conductivity results for Models I and II are presented, respectively, in sections 5 and 6.



(a) (b)

Figure 1. Representative examples of volume meshes in the periodic cells of (a) Model I, and (b) Model II.

4. VALIDATION

In this section, the implementation of the methodology is validated by comparing (nondimensional) numerical and analytical results for the longitudinal and transverse effective thermal conductivities of unidirectional fibrous composites, constituted by infinite circular cylindrical fibers arranged in a regular square array. In order to reproduce the microstructure of such composites, the angles φ_i, i=1,2,3,4, are set equal to zero, and ρ is progressively increased to approach the maximum value, $\rho_{max} = \sqrt{\pi/4c}$, for which the planar surfaces of the fibers are tangent to the y_2-y_3 faces of the cube. The numerical results (indicated by superscript ^{N}), k_L^N and k_T^N (subscript $_L$ for longitudinal conductivity, and $_T$ for transverse), are respectively compared to the analytical ones, k_L^{RM} and k_T^P. Values of k_L^{RM} are calculated using the well-known rule of mixtures, $k_L^{RM} = 1–c+\alpha\, c$. Values of k_T^P are calculated using expression (1), derived by Perrins *et al.* (1979).

Sample results for k_L^N, k_T^N and k_L^{RM}, k_T^P are shown in Tab. (1). We can clearly observe that the numerical results are in excellent agreement with the analytical ones. It is worth noting that, as an additional validation test, numerical results for the effective thermal conductivities of composites with longitudinally aligned short fibers have been compared to the ones obtained by Matt (2003) and Matt and Cruz (2001), and the agreement is again excellent. Having, thus, successfully validated the implementation of the methodology for the cases of unidirectional fibrous composites and composites with longitudinally aligned short fibers, numerical results for the effective conductivities of composites with transversely aligned short fibers are presented in the next two sections.

Table 1. Validation of numerical scheme: effective conductivities, k_L^N, k_T^N and k_L^{RM}, k_T^P, of unidirectional fibrous composites, for fixed ratio of fiber-to-matrix conductivities, α=2.

$\rho = 2$					
c	ρ_{max}	k_L^N	k_L^{RM}	k_T^N	k_T^P
0.1	2.802	1.1000	1.1000	1.0690	1.0690
0.3	1.618	1.3000	1.3000	1.2223	1.2223

5. NUMERICAL RESULTS FOR THE EFFECTIVE THERMAL CONDUCTIVITIES OF COMPOSITES WITH TRANSVERSELY ALIGNED SHORT FIBERS – MODEL I

New numerical values are now presented for the effective thermal conductivities of composites with transversely aligned short fibers in cubic subcells. For these composites, each value of $k_{T,i}^{N}$, i=1,2 (orthogonal directions in the plane of the axes of the fibers), is the arithmetic average of fifteen different arrangements constructed with random values for the angles φ_j, j=1,2,3,4. As one might expect, the average values of $k_{T,1}^{N}$ and $k_{T,2}^{N}$ are the same. Table 2 shows the variation of $k_{T,i}^{N}$ as ρ is increased, for fixed values of the fiber volume fraction, c, and ratio of phase conductivities, α. Table 3 shows the variation of $k_{T,i}^{N}$ as α is increased, for fixed values of the fiber volume fraction, c, and aspect ratio of the fibers, ρ.

Table 2. Effective conductivities $k_{T,i}^{N}$, i=1,2, of composites with transversely aligned short fibers, for increasing ρ and fixed values of c and α.

$c = 0.1$ and $\alpha = 2$				$c = 0.2$ and $\alpha = 2$		
ρ	$k_{T,1}^{N}$	$k_{T,2}^{N}$		ρ	$k_{T,1}^{N}$	$k_{T,2}^{N}$
0.5	1.0760	1.0760		0.5	1.1412	1.1412
1.0	1.0781	1.0781		1.0	1.1605	1.1605
1.5	1.0948	1.0948		1.5	1.1648	1.1648

Table 3. Effective conductivities $k_{T,i}^{N}$, i=1,2, of composites with transversely aligned short fibers, for increasing α and fixed values of c and ρ.

c=0.1 and ρ=1				c=0.2 and ρ=1		
α	$k_{T,1}^{N}$	$k_{T,2}^{N}$		α	$k_{T,1}^{N}$	$k_{T,2}^{N}$
2	1.0781	1.0781		2	1.1605	1.1605
5	1.1930	1.1930		5	1.4150	1.4150
50	1.3622	1.3622		50	1.8412	1.8412

The analysis of Tabs. (2) and (3) reveals that the values of the effective thermal conductivities increase when ρ (fixed c and α) and α (fixed c and ρ) are increased. Also, because the fibers are more conducting than the matrix and perfect thermal contact is assumed, the effective conductivities also increase when c (fixed α and ρ) is increased. The values of $k_{T,1}^{N}$ and $k_{T,2}^{N}$, for the same parameter set $\{c, \rho, \alpha\}$, agree up to the fourth decimal digit when the sample size contains at least fifteen different configurations.

6. NUMERICAL RESULTS FOR THE EFFECTIVE THERMAL CONDUCTIVITIES OF COMPOSITES WITH TRANSVERSELY ALIGNED SHORT FIBERS – MODEL II

Sample numerical values are now presented for the effective thermal conductivities of composites with transversely aligned short fibers in parallelepipedonal cells. For these composites, each effective conductivity value is the arithmetic average of three different configurations constructed with random values for the angles φ_j, j=1,2.

The GFOM composites used by Mirmira (1999) and Mirmira and Fletcher (1999) contain one of three types of fibers: DKA X, DKE X or K22 XX fibers. The diameter and aspect ratio of such fibers are d=10^{-5} m and ρ=20, respectively. The variation of the thermal conductivity of the pure cyanate ester resin matrix, measured by those authors as a function of temperature, is shown in Tab. (4). Mirmira (1999) and Mirmira and Fletcher (1999) conducted an uncertainty analysis of their experimental results. The uncertainty obtained for the longitudinal and transverse effective thermal conductivities were 12.6% and 11.8%, respectively.

Table 4. Thermal conductivity of the resin matrix as a function of temperature θ for the GFOM composites used by Mirmira (1999) and Mirmira and Fletcher (1999).

θ [°C]	20	40	60	80	100	120	140	160	180	200
k_m [W/m·K]	0.93	0.84	0.87	0.90	0.99	1.01	1.01	1.02	1.02	1.02

To tentatively compare numerical results with some experimental measurements by Mirmira (1999) and Mirmira and Fletcher (1999), values of ρ and $\alpha = k_f/k_m$ are chosen so as to match the corresponding values of the composites with DKA X and K22 XX fibers. The influence of the temperature θ in the numerical results is not explicit, but is taken into account through the variation of the thermal conductivity of the matrix, k_m. As Mirmira (1999) reports, for K22 XX fibers, $k_f = k_\varphi = 617$ W/m·K and $k_r = 2.4$ W/m·K, for DKA X fibers, $k_f = k_\varphi = 900$ W/m·K and $k_r = 2.5$ W/m·K, $R = 10^{-5}$ m^2·K/W, $V_p = 0.03$. Tables (5) and (6) show the comparison between the experimental data and the present numerical results.

Table 5. Experimental ($k_L^{M,exp}$, $k_T^{M,exp}$) and numerical (k_L^N, k_T^N) results for the longitudinal and transverse effective conductivities of the K22 XX composites, for $c \in \{0.55, 0.65\}$.

K22 XX, c=0.55						K22 XX, c=0.65			
θ [°C]	$k_L^{M,exp}$	$k_T^{M,exp}$	k_L^N	k_T^N		$k_L^{M,exp}$	$k_T^{M,exp}$	k_L^N	k_T^N
20	27.6452	3.3333	33.8484	4.0139		30.4086	4.8495	74.2294	6.1011
40	30.0952	3.7738	34.1388	4.0165		33.2262	5.3690	75.4586	6.1076
60	28.8046	3.6782	34.0414	4.0156		31.5402	5.2988	75.0443	6.1055
80	27.4889	3.4889	33.9446	4.0148		29.9667	5.0667	74.6346	6.1033
100	24.2020	3.1010	33.6576	4.0122		26.7778	4.5050	73.4320	6.0967
120	22.9109	3.0297	33.5944	4.0117		24.4455	4.4158	73.1701	6.0953
140	22.8317	3.0297	33.5944	4.0117		24.1287	4.4158	73.1701	6.0953
160	22.3726	3.0000	33.5630	4.0114		23.8137	4.4020	73.0398	6.0946
180	22.1569	2.9902	33.5630	4.0114		23.6961	4.4020	73.0398	6.0946
200	22.0490	2.9706	33.5630	4.0114		23.5882	4.4020	73.0398	6.0946

Table 6. Experimental ($k_L^{M,exp}$, $k_T^{M,exp}$) and numerical (k_L^N, k_T^N) results for the longitudinal and transverse effective conductivities of the DKA X composites, for $c \in \{0.55, 0.65\}$.

DKA X, c=0.55						DKA X, c=0.65			
θ [°C]	$k_L^{M,exp}$	$k_T^{M,exp}$	k_L^N	k_T^N		$k_L^{M,exp}$	$k_T^{M,exp}$	k_L^N	k_T^N
20	53.8925	7.3118	34.8108	4.0223		71.5914	9.7850	78.3786	6.1224
40	59.0952	8.0952	35.0210	4.0240		78.6429	10.810	79.3143	6.1270
60	56.4828	7.7701	34.9506	4.0234		74.8161	10.310	79.0000	6.1254
80	53.5778	7.5000	34.8806	4.0228		71.8889	9.7778	78.6880	6.1239
100	46.9596	6.7172	34.6721	4.0211		62.7576	8.8889	77.7671	6.1194
120	42.7723	6.5248	34.6261	4.0207		60.9010	8.6931	77.5653	6.1184
140	40.5050	6.3366	34.6261	4.0207		59.4753	8.6634	77.5653	6.1184
160	37.8627	6.0980	34.6031	4.0205		57.3431	8.5490	77.4648	6.1179
180	25.7647	5.9902	34.6031	4.0205		56.0294	8.3824	77.4648	6.1179
200	33.2451	5.8823	34.6031	4.0205		53.9314	8.0882	77.4648	6.1179

From Tabs. (5) and (6) it is observed that reasonable agreement is obtained in some instances, and poor agreement in others. Still, the numerical results - k_T^N - seem to be in better agreement with the data - $k_T^{M,exp}$ - than the results predicted by expression (2) (Hirata, 2003). The observed discrepancies between numerical results and experimental data vary quite a bit, and probably stem from inaccuracies in the microstructural model and from effects that are not accounted for, such as the presence of an interfacial thermal resistance and matrix porosity.

7. FINAL CONSIDERATIONS

Different from most of the previous analytical and numerical studies dedicated to the determination of the macroscopic thermal conductivity of short-fiber composites, the present work incorporates collectively the influence of relevant effects, namely the interaction between neighboring fibers and variable fiber orientation. With the current microstructural models, composites with both longitudinally and transversely aligned short fibers can be simulated. As expected, only a fraction of the numerical results are in reasonable agreement with the experimental measurements. Therefore, the results of this work encourage not only further improvements in the microstructural models, but, also, the incorporation of effects due to the presence of an interfacial thermal resistance and matrix porosity. It is believed that, in this way, more representative results of the macroscopic thermal behavior of short-fiber composites will be obtained.

8. ACKNOWLEDGEMENT

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