COBEM 99
XV Congresso Brasileiro de Engenharia Mecânica
15th Brazilian Congress of Mechanical Engineering
22 - 26 de Novembro de 1999 / November 22 - 26, 1999 Águas de Lindóia, São Paulo,

VARIATIONAL FORMULATION OF THE HEAT CONDUCTION PROBLEM IN COMPOSITES WITH AN INTERFACIAL THERMAL RESISTANCE

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Abstract. *In this paper we develop a continuous variational formulation of the heat conduction problem in composite materials with an interfacial thermal resistance between the constituent phases. The contact resistance is a freely variable parameter, representing the ratio of the temperature jump to the heat flux at the interface. The continuous equations are obtained by applying the method of homogenization to the variational form of the conduction boundary value problem for the multiscale composite medium. Our formulation is applicable to both ordered and random composites, and to two– and three–dimensional geometries; the variational form is well suited for subsequent numerical solution by the finite element method. We illustrate the capabilities of our approach by numerically calculating the effective conductivity of a laminated binary composite with contact resistance between the layers, and validate our results against the exact prediction.*

Keywords: *Heat conduction, Variational formulation, Composites, Contact resistance*

1. INTRODUCTION

The determination of the macroscopic behavior of composite materials is of fundamental and practical importance, even more so nowadays, as new composites are being continually developed for the automotive and aerospace industries, electronic packaging, thermal insulation and many other applications (Ayers & Fletcher, 1998; Furmañski, 1997). Typical composite microstructures consist of unidirectional long fibers, short chopped fibers, or particles or voids dispersed in a solid matrix. One of the most important macroscopic thermal properties of composites is the effective conductivity, which depends on the conductivities, relative amounts and geometric distributions of the constituent phases. A recent comprehensive review of heat conduction in composites is presented in Furmañski (1997).

Most manufacturing processes of composite materials do not ensure a perfect thermal contact between the constituent phases (Fadale & Taya, 1991; Hasselman & Johnson, 1987). Therefore, in practice, the effective conductivity also depends on the interfacial thermal resistance, or contact resistance, between the continuous phase (the matrix) and the dispersed phase. The nature, governing parameters and methods for quantitative evaluation of the contact resistance have been extensively studied, both theoretically and experimentally (Yovanovich, 1986; Madhusudana & Fletcher, 1985; Mikić, 1974). It turns out that the *a priori* determination of the contact resistance resulting from a certain composite manufacturing process is a very difficult, if not impossible, task.

The common practice in the literature is to model the interfacial thermal resistance as a freely variable parameter, representing the ratio of the temperature jump to the heat flux at the interface (Mikić, 1974). Such model is adopted in basically all the analytical (Auriault & Ene, 1994; Hasselman & Johnson, 1987) and phenomenological (Benveniste, 1987) studies of heat conduction in composites, which attempt to determine the effective conductivity accounting for the contact resistance between the phases; these studies are generally restricted to dilute concentrations and simple geometries, or to the validity of self–consistent assumptions. Comparison of calculated effective conductivity results to experimental measurements (Mirmira & Fletcher, 1999) may tentatively be effected by selecting values of the contact resistance which lead to better agreement. Mirmira & Fletcher (1999) point out that more flexible approaches, which can accomodate geometric and physical variations more easily, are needed in order to obtain more satisfactory comparison with experimental results. We believe the approach we describe in this paper has these characteristics.

Here we develop a continuous variational formulation of the heat conduction problem in composite materials with an interfacial thermal resistance. As in previous studies, the contact resistance is a freely variable parameter. Our equations are obtained by applying the method of homogenization (Bensoussan *et al.*, 1978; Auriault, 1991) to the variational form of the conduction boundary value problem for the composite medium; the medium is periodic in the mesoscale, to allow for application of homogenization techniques. Our formulation is applicable to both ordered and random composites, and to two– and three–dimensional geometries; the variational form is well suited for subsequent numerical solution by the finite element method. In fact, we apply the finite element method to numerically determine the effective conductivity of a simple laminated binary composite with contact resistance between the layers, and validate our results against the exact prediction of Auriault & Ene (1994). Our flexible analytico–numerical treatment is currently needed and lacking in the literature, and shall be appropriate for future calculations of the effective conductivity of more complex two– and three–dimensional composites.

2. CONTINUOUS PROBLEM FORMULATION

2.1. Strong Form of the Multiscale Periodic Problem

We consider a periodic composite whose continuous and distributed components are, respectively, a matrix of thermal conductivity k_c and inclusions (particles or fibers of arbitrary shape) of thermal conductivity k_d. As noted in the Introduction, the composite may be ordered or random, and two– or three–dimensional. It is assumed that both components are solid, homogeneous, and isotropic. The geometric regions occupied by the continuous and dispersed components are, respectively, Ω_c and Ω_d. A uniform thermal contact resistance, r, is present at the interface $\partial\Omega_s$ between the matrix and the inclusions. The composite extends throughout a macroscale region $\Omega_{ma} = \Omega_c \cup \Omega_d$ of characteristic dimension L, over which an external temperature gradient $\Delta T/L$ is imposed.

The representative periodic cell, Ω_{pc}, has area λ^2, and in general contains several dispersed inclusions of characteristic dimension d; d is the microscale, and λ is the mesoscale. We define the small parameter $\epsilon \equiv \lambda/L \ll 1$.

The multiscale periodic heat conduction problem in the medium described above, under steady–state conditions, can be mathematically expressed by:

$$-\frac{\partial}{\partial x_j^*}\left(k_c\,\frac{\partial T^c}{\partial x_j^*}\right) = \dot{g}_c \quad \text{in} \;\; \Omega_c\,, \tag{1}$$

$$-\frac{\partial}{\partial x_j^*}\left(k_d\,\frac{\partial T^d}{\partial x_j^*}\right) = \dot{g}_d \quad \text{in} \;\; \Omega_d\,, \tag{2}$$

$$-\,k_c\,\frac{\partial T^c}{\partial x_j^*}\,n_j^c = -\,k_d\,\frac{\partial T^d}{\partial x_j^*}\,n_j^c \quad \text{on} \;\; \partial\Omega_s\,, \tag{3}$$

$$-\,k_c\,\frac{\partial T^c}{\partial x_j^*}\,n_j^c = h\,(T^c - T^d) = h\,[T_\epsilon]_{\partial\Omega_s} \quad \text{on} \;\; \partial\Omega_s\,, \tag{4}$$

$$T_\epsilon \text{ subject to Dirichlet boundary conditions on } \partial\Omega_{ma}\,. \tag{5}$$

Here, x_j^*, $j = 1,\ldots,m$, are the components of $\mathbf{x}^* \in I\!R^m$, m is the number of spatial dimensions, and summation over repeated indices is implied; T_ϵ and $\dot{g}$ are, respectively, the temperature field and the volumetric rate of heat generation at the microscale; $T^c = T_{\epsilon|\Omega_c}$, $T^d = T_{\epsilon|\Omega_d}$, $\dot{g}_c = \dot{g}_{|\Omega_c}$, and $\dot{g}_d = \dot{g}_{|\Omega_d}$; $\mathbf{n}^c$ is the unit vector locally normal to $\partial\Omega_s$ and pointing to the outside of Ω_c; $h \equiv 1/r$ is the interfacial thermal conductance, expressing the ratio of the heat flux to the temperature jump at the interface $\partial\Omega_s$; the notation $[\phi]_{\partial\Omega_s}$ represents the discontinuity $(\phi^c - \phi^d)$ of the function ϕ at $\partial\Omega_s$ (henceforth, ϕ^c or ϕ_c and ϕ^d or ϕ_d refer, respectively, to $\phi_{|\Omega_c}$ and $\phi_{|\Omega_d}$); and, finally, $\partial\Omega_{ma}$ in Eq. (5) is the union of the external boundaries of Ω_{ma} where the temperature gradient is imposed.

Defining the non–dimensional quantities

$$\mathbf{y} \equiv \frac{\mathbf{x}^*}{\lambda}\,,\;\; \theta \equiv \frac{T_\epsilon}{\Delta T}\,,\;\; k \equiv \frac{k_d}{k_c}\,, \tag{6}$$

we can rewrite Eqs. (1)–(5) as

$$-\frac{\partial}{\partial y_j}\left(\frac{\partial \theta^c}{\partial y_j}\right) = G_c \quad \text{in} \;\; \Omega_c\,, \tag{7}$$

$$-\frac{\partial}{\partial y_j}\left(k\,\frac{\partial \theta^d}{\partial y_j}\right) = G_d \quad \text{in} \;\; \Omega_d\,, \tag{8}$$

$$-\frac{\partial \theta^c}{\partial y_j}\,n_j^c = -\,k\,\frac{\partial \theta^d}{\partial y_j}\,n_j^c \quad \text{on} \;\; \partial\Omega_s\,, \tag{9}$$

$$-\frac{\partial \theta^c}{\partial y_j}\,n_j^c = Bi\,(\theta^c - \theta^d) = Bi\,[\theta]_{\partial\Omega_s} \quad \text{on} \;\; \partial\Omega_s\,, \tag{10}$$

$$\theta \text{ subject to Dirichlet boundary conditions on } \partial\Omega_{ma}\,, \tag{11}$$

where $G_c \equiv \dot{g}_c \lambda^2 / k_c \Delta T$ and $G_d \equiv \dot{g}_d \lambda^2 / k_c \Delta T$ are the non–dimensional heat generation numbers, and $Bi \equiv h\lambda / k_c$ is the Biot number.

2.2. Variational Formulation

We now write the variational formulation of the heat conduction problem (7)–(11). The variational formulation, relative to the strong formulation (7)–(11), is advantageous because, first, it naturally enforces the flux continuity condition (9), and, second, it is appropriate for subsequent finite element treatment (see Section 5).

We consider the function space $X(\Omega_{ma}) = \{ w \mid w_{|\Omega_c} = w^c \in H_0^1(\Omega_c), w_{|\Omega_d} = w^d \in H_0^1(\Omega_d), [w]_{\partial\Omega_s} = s \in I\!R \}$, where $H_0^1(\Omega)$ is the space of all functions which vanish on the portions of $\partial\Omega$ in $\partial\Omega_{ma}$ (condition (11)), and for which both the function and derivative are square–integrable over Ω. Multiplying Eqs. (7) and (8) by $v \in X(\Omega_{ma})$, integrating, respectively, over Ω_c and Ω_d, and applying the first form of Green's theorem, we derive

$$\int_{\Omega_c} \frac{\partial v^c}{\partial y_j} \frac{\partial \theta^c}{\partial y_j} \, d\mathbf{y} - \int_{\partial\Omega_c} v^c \frac{\partial \theta^c}{\partial y_j} n_j^c \, ds = \int_{\Omega_c} G_c \, v^c \, d\mathbf{y} \qquad \forall v \in X(\Omega_{ma}) \,, \tag{12}$$

$$\int_{\Omega_d} k \frac{\partial v^d}{\partial y_j} \frac{\partial \theta^d}{\partial y_j} \, d\mathbf{y} - \int_{\partial\Omega_d} k \, v^d \frac{\partial \theta^d}{\partial y_j} n_j^d \, ds = \int_{\Omega_d} G_d \, v^d \, d\mathbf{y} \qquad \forall v \in X(\Omega_{ma}) \,, \tag{13}$$

where $\mathbf{n}^d = -\mathbf{n}^c$, and $d\mathbf{y} \equiv dy_1 \ldots dy_m$. Applying conditions (9) and (10) to Eqs. (12) and (13), using the definition of the space $X(\Omega_{ma})$, and summing the resulting equations, we obtain the variational (weak) form

$$\int_{\Omega_{ma}} \alpha \frac{\partial v}{\partial y_j} \frac{\partial \theta}{\partial y_j} \, d\mathbf{y} + \int_{\partial\Omega_s} Bi \; [v]_{\partial\Omega s} [\theta]_{\partial\Omega s} \, ds = \int_{\Omega_{ma}} G \, v \, d\mathbf{y} \qquad \forall v \in X(\Omega_{ma}) \,, \tag{14}$$

where $\alpha(\mathbf{y}) = 1$ if $\mathbf{y} \in \Omega_c$, and $\alpha(\mathbf{y}) = k$ if $\mathbf{y} \in \Omega_d$; the jump $s \in I\!R$ at $\partial\Omega_s$ allowed to a member of $X(\Omega_{ma})$ accomodates all possible values of the Biot number. In what follows, we assume that the conductivities of the two components are such that $k = O(\epsilon^0)$ (i.e., $\epsilon \ll k \ll 1/\epsilon$).

3. HOMOGENIZATION

In this Section, the method of homogenization (Bensoussan *et al.*, 1978; Auriault, 1991) is applied to the variational form (14) of the multiscale heat conduction problem. The method proceeds by writing the temperature field as a function of two space variables, $\theta = \theta(\mathbf{x}, \mathbf{y})$, where $\mathbf{y} \equiv \mathbf{x}^* / \lambda$ and $\mathbf{x} \equiv \mathbf{x}^* / L = \epsilon \mathbf{y}$ are, respectively, the fast (microscopic) and slow (macroscopic) variables. Next, the multiple–scale asymptotic expansions are introduced,

$$\theta(\mathbf{x}, \mathbf{y}) = \theta_0(\mathbf{x}, \mathbf{y}) + \epsilon \, \theta_1(\mathbf{x}, \mathbf{y}) + \epsilon^2 \, \theta_2(\mathbf{x}, \mathbf{y}) + O(\epsilon^3) \,, \tag{15}$$

$$v(\mathbf{x}, \mathbf{y}) = v_0(\mathbf{x}, \mathbf{y}) + \epsilon \, v_1(\mathbf{x}, \mathbf{y}) + \epsilon^2 \, v_2(\mathbf{x}, \mathbf{y}) + O(\epsilon^3), \quad v \in X(\Omega_{ma}) \,, \tag{16}$$

where all functions are λ–doubly periodic in $\mathbf{y}$. Inserting Eqs. (15)–(16) into Eq. (14), and using the chain rule $(\partial/\partial y_j) = (\partial/\partial y_j) + \epsilon\,(\partial/\partial x_j)$, we derive, $\forall v_0, v_1, v_2 \in X(\Omega_{ma})$,

$$\int_{\Omega_{ma}} \alpha \left(\frac{\partial v_0}{\partial y_j} + \epsilon \frac{\partial v_0}{\partial x_j} + \epsilon \frac{\partial v_1}{\partial y_j} + \epsilon^2 \frac{\partial v_1}{\partial x_j} + \epsilon^2 \frac{\partial v_2}{\partial y_j}\right)\left(\frac{\partial \theta_0}{\partial y_j} + \epsilon \frac{\partial \theta_0}{\partial x_j} + \epsilon \frac{\partial \theta_1}{\partial y_j} + \epsilon^2 \frac{\partial \theta_1}{\partial x_j} + \epsilon^2 \frac{\partial \theta_2}{\partial y_j}\right) d\mathbf{y}$$
$$+ \int_{\partial\Omega_s} Bi \left[v_0 + \epsilon\, v_1 + \epsilon^2\, v_2\right]_{\partial\Omega_s} \left[\theta_0 + \epsilon\, \theta_1 + \epsilon^2\, \theta_2\right]_{\partial\Omega_s} ds = \int_{\Omega_{ma}} G\,(v_0 + \epsilon\, v_1 + \epsilon^2\, v_2) d\mathbf{y}\ . \quad (17)$$

The last step in the homogenization process is to collect similar powers of ϵ, leading to two boundary value problems, one in a homogenized macroscale region, the *homogenized problem*, and one in a periodic cell, the *cell problem*. The process will be successful if $\theta_0 \neq 0$, which is the homogenization condition (Auriault, 1991; Auriault & Ene, 1994). For Eq. (17), it follows that the homogenization condition imposes the restriction $G = O(\epsilon^2)$ (Rocha, 1999); physically, this means that homogenization is possible when the amount of heat generated in the composite on the macroscale is of the same order of magnitude as the amount of heat conducted due to the external temperature gradient. Finally, as discussed in Auriault & Ene (1994), five different homogenization processes are possible, corresponding to five different orders of magnitude of the Biot number: $Bi = O(\epsilon^a)$, $a \in \{-1, 0, 1, 2, 3\}$. Here we only consider the more physically relevant Models I and II, respectively corresponding to $a \in \{-1, 0\}$; Models III, IV and V, respectively corresponding to $a \in \{1, 2, 3\}$, are presented in Auriault & Ene (1994) (in strong form) and in Rocha (1999) (in variational form). We now make two important remarks concerning the Models: first, Model II yields Model III on decreasing the Biot number; second, real composite materials often possess a dispersed phase and a continuous phase, such that the former is totally encapsulated by the latter. For such composites, Models III, IV and V are physically equivalent, corresponding to a perfectly insulated dispersed phase.

4. ANALYSIS OF MODELS I AND II

In the following two subsections we proceed to analyse Models I and II, whose related quantities are respectively designated by the superscripts I and II.

4.1. Model I

Considering $Bi = O(\epsilon^{-1})$ in Eq. (17), and collecting the terms of order ϵ^{-1}, we obtain

$$\int_{\partial\Omega_s} Bi \left[v_0^{\rm I}\right]_{\partial\Omega_s} \left[\theta_0^{\rm I}\right]_{\partial\Omega_s} ds \;=\; 0 \qquad \forall v_0^{\rm I} \in X(\Omega_{ma})\,. \quad (18)$$

We thus conclude from Eq. (18) that $\left[\theta_0^{\rm I}\right]_{\partial\Omega_s} = 0$, i.e., $\theta_0^{\rm I}$ is continuous across $\partial\Omega_s$ (and so $v_0^{\rm I} \in \tilde{X}(\Omega_{ma})$, where $\tilde{X}(\Omega_{ma}) \subset X(\Omega_{ma})$ does not allow jumps at $\partial\Omega_s$, i.e., $s = 0$).

Collecting now the non–zero terms of order ϵ^0 of Eq. (17), we obtain

$$\int_{\Omega_{ma}} \alpha\, \frac{\partial v_0^{\rm I}}{\partial y_j} \frac{\partial \theta_0^{\rm I}}{\partial y_j}\, d\mathbf{y} \;=\; 0 \qquad \forall v_0^{\rm I} \in \tilde{X}(\Omega_{ma})\,. \quad (19)$$

We thus conclude from Eq. (19) that $\partial\theta_0^{\rm I}/\partial y_j = 0$, i.e., $\theta_0^{\rm I} = \theta_0^{\rm I}(\mathbf{x})$ varies only on the macroscale. The non–zero terms of order ϵ^1 of Eq. (17) lead to $\int_{\partial\Omega_s} Bi \left[v_1^{\rm I}\right]_{\partial\Omega_s}\left[\theta_1^{\rm I}\right]_{\partial\Omega_s} ds = 0$ for all $v_1^{\rm I} \in X(\Omega_{ma})$, from which we conclude that $\left[\theta_1^{\rm I}\right]_{\partial\Omega_s} = 0$ (and so $v_1^{\rm I} \in \tilde{X}(\Omega_{ma})$).

Finally, collecting the terms of order ϵ^2 of Eq. (17), taking into account Eqs. (18) and (19), and choosing $v_0^{\rm I} = 0 \in \tilde{X}(\Omega_{ma})$, we arrive at

$$\int_{\Omega_{ma}} \alpha \left(\frac{\partial \theta_0^{\rm I}}{\partial x_j} + \frac{\partial \theta_1^{\rm I}}{\partial y_j}\right)\left(\frac{\partial v_1^{\rm I}}{\partial y_j}\right) d\mathbf{x} \;=\; 0 \qquad \forall v_1^{\rm I} \in \tilde{X}(\Omega_{ma})\,. \tag{20}$$

Equation (20) for $\theta_1^{\rm I}$ has already been solved in Cruz (1997), and corresponds to the heat conduction problem in composites for which the interfacial thermal resistance is negligible, such that the Biot number can be considered effectively infinite. Physically, Model I is appropriate for composites whose components have an excellent thermal contact.

4.2. Model II

Considering $Bi = O(\epsilon^0)$ in Eq. (17), and collecting the terms of order ϵ^0, we obtain

$$\int_{\Omega_{ma}} \alpha \frac{\partial v_0^{\rm II}}{\partial y_j}\frac{\partial \theta_0^{\rm II}}{\partial y_j}\, d\mathbf{y} + \int_{\partial\Omega_s} Bi \left[v_0^{\rm II}\right]_{\partial\Omega_s} \left[\theta_0^{\rm II}\right]_{\partial\Omega_s} ds \;=\; 0 \qquad \forall v_0^{\rm II} \in X(\Omega_{ma})\,. \tag{21}$$

Choosing $v_0^{\rm II} \in X(\Omega_{ma})$ such that $\left[v_0^{\rm II}\right]_{\partial\Omega_s} = 0$, we conclude from Eq. (21) that the temperature field $\theta_0^{\rm II}$ does not vary on the microscale, i.e., $\partial\theta_0^{\rm II}/\partial y_j = 0$. It thus also follows from Eq. (21) that $\left[\theta_0^{\rm II}\right]_{\partial\Omega_s} = 0$, i.e., $\theta_0^{\rm II}$ is continuous across the interface, $\theta_0^{\rm II} = \theta_0^{{\rm II},c} = \theta_0^{{\rm II},d} = \theta_0^{\rm II}(\mathbf{x})$ (Auriault & Ene, 1994; Auriault, 1983), and $v_0^{\rm II} \in \tilde{X}(\Omega_{ma})$.

Since the terms of order ϵ^1 of Eq. (17) lead to no additional information, we now collect the non–zero terms of order ϵ^2, to obtain

$$\int_{\Omega_{ma}} \alpha \left(\frac{\partial v_0^{\rm II}}{\partial x_j}\frac{\partial \theta_0^{\rm II}}{\partial x_j} + \frac{\partial v_0^{\rm II}}{\partial x_j}\frac{\partial \theta_1^{\rm II}}{\partial y_j} + \frac{\partial v_1^{\rm II}}{\partial y_j}\frac{\partial \theta_0^{\rm II}}{\partial x_j} + \frac{\partial v_1^{\rm II}}{\partial y_j}\frac{\partial \theta_1^{\rm II}}{\partial y_j}\right) d\mathbf{y} + \int_{\partial\Omega_s} Bi \left[v_1^{\rm II}\right]_{\partial\Omega_s}\left[\theta_1^{\rm II}\right]_{\partial\Omega_s} ds$$
$$= \int_{\Omega_{ma}} G\, v_0^{\rm II}\, d\mathbf{y} \qquad \forall v_0^{\rm II} \in \tilde{X}(\Omega_{ma}),\ \forall v_1^{\rm II} \in X(\Omega_{ma})\,. \tag{22}$$

We can break Eq. (22) into two equations by choosing, first, $v_1^{\rm II} = 0 \in X(\Omega_{ma})$ and, second, $v_0^{\rm II} = 0 \in \tilde{X}(\Omega_{ma})$, to obtain

$$\int_{\Omega_{ma}} \alpha \frac{\partial v_0^{\rm II}}{\partial x_j}\left(\frac{\partial \theta_0^{\rm II}}{\partial x_j} + \frac{\partial \theta_1^{\rm II}}{\partial y_j}\right) d\mathbf{y} \;=\; \int_{\Omega_{ma}} G\, v_0^{\rm II}\, d\mathbf{y} \qquad \forall v_0^{\rm II} \in \tilde{X}(\Omega_{ma})\,, \tag{23}$$

$$\int_{\Omega_{ma}} \alpha \frac{\partial v_1^{\rm II}}{\partial y_j}\left(\frac{\partial \theta_0^{\rm II}}{\partial x_j} + \frac{\partial \theta_1^{\rm II}}{\partial y_j}\right) d\mathbf{y} + \int_{\partial\Omega_s} Bi \left[v_1^{\rm II}\right]_{\partial\Omega_s} \left[\theta_1^{\rm II}\right]_{\partial\Omega_s} ds \;=\; 0 \qquad \forall v_1^{\rm II} \in X(\Omega_{ma})\,. \tag{24}$$

We next assume, motivated by solvability (Cruz, 1997; Auriault, 1983; Bensoussan *et al.*, 1978), that we can separate the functional dependence of $\theta_1^{\rm II}$ on the spatial variables $\mathbf{x}$ and $\mathbf{y}$:

$$\theta_1^{\rm II}(\mathbf{x},\mathbf{y}) \;=\; -\,\chi_p^{\rm II}(\mathbf{y})\,\frac{\partial \theta_0^{\rm II}(\mathbf{x})}{\partial x_p}\,, \tag{25}$$

where, by construction, the unknown function $\chi_p^{\rm II}$ is a λ–doubly periodic solution to Eq. (24) corresponding to a unit temperature gradient imposed in the x_p direction, and summation over p, $p = 1, \ldots, m$, is implied. Inserting Eq. (25) into Eq. (24), and given that $\theta_0^{\rm II}$ is continuous across the interface, we obtain

$$\int_{\Omega_{ma}} \alpha \left(\delta_{jp} - \frac{\partial \chi_p^{\rm II}}{\partial y_j} \right) \frac{\partial v_1^{\rm II}}{\partial y_j} \frac{\partial \theta_0^{\rm II}}{\partial x_p} \, d\mathbf{y} = \int_{\partial \Omega_s} Bi \left[v_1^{\rm II} \right]_{\partial \Omega_s} \left[\chi_p^{\rm II} \right]_{\partial \Omega_s} \frac{\partial \theta_0^{\rm II}}{\partial x_p} \, ds \quad \forall v_1^{\rm II} \in X(\Omega_{ma}), \quad (26)$$

where δ_{ij} is the Kronecker delta. At this point we need to invoke the *periodicity property* (Cruz, 1997; Auriault, 1983), which in our case transforms, as $\epsilon \to 0$: the integral of a quantity over Ω_{ma} into the integral, over Ω_{ma}, of the *average* of the quantity over a periodic cell, Ω_{pc}; and the integral of a quantity over $\partial \Omega_s$ into the integral, over $\partial \Omega_s$, of the *average* of the quantity over the portion of $\partial \Omega_s$ in a periodic cell. Applying the periodicity property to Eq. (26), we obtain

$$\int_{\Omega_{ma}} \left\{ \frac{1}{|\Omega_{pc}|} \int_{\Omega_{pc}} \alpha \left(\delta_{jp} - \frac{\partial \chi_p^{\rm II}}{\partial y_j} \right) \frac{\partial v_1^{\rm II}}{\partial y_j} \, d\mathbf{y} \right\} \frac{\partial \theta_0^{\rm II}}{\partial x_p} \, d\mathbf{y} \; = \; \int_{\partial \Omega_s} \left\{ \frac{1}{|\Gamma|} \int_{\Gamma} Bi \left[v_1^{\rm II} \right]_{\Gamma} \left[\chi_p^{\rm II} \right]_{\Gamma} ds \right\} \frac{\partial \theta_0^{\rm II}}{\partial x_p} \, ds \qquad \forall v_1^{\rm II} \in X(\Omega_{ma}) \, , \quad (27)$$

where Γ is the portion of $\partial \Omega_s$ in Ω_{pc}, $|\Omega_{pc}| \equiv \int_{\Omega_{pc}} d\mathbf{y}$ is the total volume measure of the cell Ω_{pc}, and $|\Gamma| \equiv \int_\Gamma ds$ is the total length of the surface Γ. Equation (27) must be true for all possible values of the Biot number, and for all $v_1^{\rm II} \in X(\Omega_{ma})$; we conclude that the outer integrands on both sides of Eq. (27) must be equal for any periodic test function over the cell, with period λ in all m directions, or

$$\int_{\Omega_{pc}} \alpha \left(\delta_{jp} - \frac{\partial \chi_p^{\rm II}}{\partial y_j} \right) \frac{\partial \tilde{v}}{\partial y_j} \, d\mathbf{y} \; = \; \frac{|\Omega_{pc}|}{|\Gamma|} \int_{\Gamma} Bi \, [\tilde{v}]_{\Gamma} \left[\chi_p^{\rm II} \right]_{\Gamma} ds \qquad \forall \tilde{v} \in \tilde{Y}(\Omega_{pc}) \, , \quad (28)$$

where $\tilde{Y}(\Omega_{pc}) = \{ w \mid w_{|\Omega_{pc,c}} = w^c \in H^1_\#(\Omega_{pc,c}), w_{|\Omega_{pc,d}} = w^d \in H^1_\#(\Omega_{pc,d}), [w]_\Gamma = s \in I\!R \}$, $H^1_\#(\Omega)$ is the space of all periodic functions in Ω (subscript $\#$) with period λ in all m directions, for which both the function and derivative are square–integrable over Ω, and $\Omega_{pc,c}$ and $\Omega_{pc,d}$ are, respectively, the portions of Ω_{pc} in the continuous and dispersed components. In Eq. (28), the function $\chi_p^{\rm II}$ is determined up to a constant; thus, we further require for uniqueness that $\chi_p^{\rm II}$ have zero volume average ($\int_{\Omega_{pc}} \chi_p^{\rm II} d\mathbf{y} = 0$). Choosing $[\tilde{v}]_\Gamma = (|\Gamma|/|\Omega_{pc}|) \, [v]_\Gamma$, $\tilde{v}, v \in \tilde{Y}(\Omega_{pc})$, we can finally rewrite Eq. (28) as

$$\int_{\Omega_{pc}} \alpha \frac{\partial \chi_p^{\rm II}}{\partial y_j} \frac{\partial v}{\partial y_j} \, d\mathbf{y} + \int_{\Gamma} Bi \, [v]_\Gamma \left[\chi_p^{\rm II} \right]_\Gamma ds \; = \; \int_{\Omega_{pc}} \alpha \frac{\partial v}{\partial y_p} \, d\mathbf{y} \qquad \forall v \in Y(\Omega_{pc}) \, , \quad (29)$$

where $Y(\Omega_{pc}) = \{ w \in \tilde{Y}(\Omega_{pc}) \mid \int_{\Omega_{pc}} w \, d\mathbf{y} = 0 \}$. Equation (29) is the appropriate *cell problem*, which is solvable for all possible values of the Biot number.

Finally, inserting Eq. (25) into Eq. (23) and applying the periodicity property, we derive the variational form of the *homogenized problem*: $\forall v_0^{\rm II} \in X(\Omega_{ma})$,

$$\int_{\Omega_{ma}} \left\{ \frac{1}{|\Omega_{pc}|} \int_{\Omega_{pc}} \alpha \left(\delta_{jp} - \frac{\partial \chi_p^{\rm II}}{\partial y_j} \right) d\mathbf{y} \right\} \frac{\partial v_0^{\rm II}}{\partial x_j} \frac{\partial \theta_0^{\rm II}}{\partial x_p} \, d\mathbf{y} \; = \; \int_{\Omega_{ma}} \left(\frac{1}{|\Omega_{pc}|} \int_{\Omega_{pc}} G \, v_0^{\rm II} \, d\mathbf{y} \right) d\mathbf{y} \, . \quad (30)$$

By simple inspection of Eq. (30), we recognize the *tensorial effective thermal conductivity* of the composite medium,

$$k_{e,pq} = \frac{1}{|\Omega_{pc}|}\int_{\Omega_{pc}} \alpha\left(\delta_{pq} - \frac{\partial \chi_q^{\mathrm{II}}}{\partial y_p}\right) d\mathbf{y} \quad (31)$$

$$= \frac{1}{|\Omega_{pc}|}\left\{\int_{\Omega_{pc,c}} \left(\delta_{pq} - \frac{\partial \chi_q^{\mathrm{II},c}}{\partial y_p}\right) d\mathbf{y} + \int_{\Omega_{pc,d}} k\left(\delta_{pq} - \frac{\partial \chi_q^{\mathrm{II},d}}{\partial y_p}\right) d\mathbf{y}\right\}. \quad (32)$$

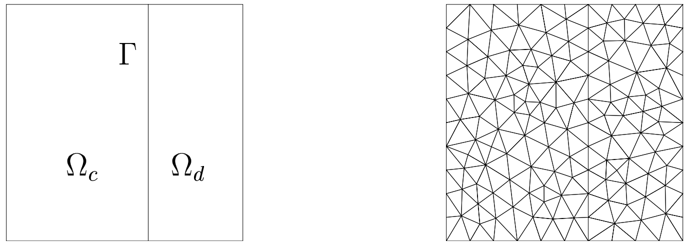
5. CASE STUDY: BILAMINATED COMPOSITE

In order to illustrate the capabilities of our approach, we now solve numerically the continuous variational cell problem, Eq. (29), via the finite element method, for the simple case study of heat conduction in a bilaminated composite with contact resistance between the two layers. The periodic cell domain consists of a unit square, as shown in Figure 1(a); we arbitrarily consider that one layer, the continuous component, encapsulates the other layer, the dispersed component, at infinity. The dispersed phase area fraction is the concentration c of the composite medium. We want to determine $k_{e,11}$, corresponding to an external temperature gradient imposed in the $p = 1$ direction, orthogonal to the interface Γ.

Numerical solution requires three steps: mesh generation, finite element discretization and solution of the resultant linear system of algebraic equations. Mesh generation is effected by, first, uniformly distributing finite–element corner–nodes on the boundaries of the cell and interface, and, next, generating the interior mesh using a third–party FORTRAN subroutine, MSHPTG (Cruz, 1997). Figure 1(b) shows a typical mesh for the cell, for the concentration $c = 0.4$ and uniform boundary mesh spacing of 0.1. The finite element discretization procedure to arrive at the discrete problem for χ_1^{II} is similar to the one described in Cruz (1997). The main complicating difference is the numerical treatment of the surface integral term in Eq. (29), due to the jump of χ_1^{II} at Γ because of the contact resistance between the phases. In order to handle this term using standard finite–element meshes and data structures, we must first duplicate the degrees–of–freedom corresponding to the global nodes belonging to the interface Γ, allowing for different values of the temperature χ_1^{II} at Γ (i.e., χ_1^{II} has different limiting values as the interface is approached from the continuous or the dispersed phase side). We then use discontinuous test functions at the degrees–of–freedom corresponding to nodes on Γ ($v \in Y(\Omega_{pc})$), so that (only) for such degrees–of–freedom the surface integral term generates non–zero contributions, which are dependent on the Biot number and on the lengths of the element sides on Γ. These contributions couple the degrees–of–freedom across and to the same side of Γ, and must thus be summed to the suitable elements of the global system matrix. As a consequence, such matrix, although still symmetric, is not positive–definite for arbitrary Bi. More details of the discretization procedure for Eq. (29) can be found in Rocha (1999). The resulting system of algebraic equations is then solved by a FORTRAN subroutine of the IMSL Library (1987), LSLSF. Finally, having determined the numerical approximation for the field χ_1^{II}, the numerical value of the effective thermal conductivity, $k_{e,N}$, is computed using the discrete equivalent to Eq. (32) (Cruz, 1997).

6. NUMERICAL RESULTS AND CONCLUSIONS

Our numerical results for the effective conductivity $k_{e,N}$ are presented in Table 1, for



(a) (b)

Figure 1: (a) Geometry of the cell domain for the bilaminated composite, $c = 0.4$. (b) Finite–element mesh for the cell domain, $c = 0.4$, boundary mesh spacing of 0.1, total of 254 triangles and 148 global nodes.

$c = 0.4$ and boundary mesh spacing of 0.1. The results are tabulated for various values of the Biot number, Bi, and two values of the ratio of component conductivities, $k = 2$ and $k = 10$. Also shown in the Table are the corresponding analytical results, $k_{e,A}$, derived by Auriault & Ene (1994), $k_{e,A}(c, k; Bi) = \{1/[\frac{c+(1-c)k}{k} + \frac{2}{Bi}]\}$. First, we see that our numerical results exactly match the analytical results for all tabulated values of Bi and k. Second, we observe that, as expected, the values of $k_{e,N}$ (and of $k_{e,A}$) asymptotically approach the value of the effective conductivity for the bilaminated composite with zero contact resistance, given by (Auriault, 1983) $k_{e,A}(c, k; Bi = \infty) = k/[c+(1-c)k]$. Finally, having successfully formulated the heat conduction problem in composite materials with an interfacial thermal resistance, we would like to remark that our approach shall be appropriate for future calculations of the effective conductivity of more complex two– and three–dimensional composites.

Table 1: Numerical, $k_{e,N}$, and analytical, $k_{e,A}$, effective conductivity results for the bilaminated composite, for $c = 0.4$, $k \in \{2, 10\}$, and various values of the Biot number, Bi.

Bi	$k = 2$		$k = 10$	
	$k_{e,N}$	$k_{e,A}$	$k_{e,N}$	$k_{e,A}$
10^{-5}	4.99998×10^{-6}	4.99998×10^{-6}	4.99998×10^{-6}	4.99998×10^{-6}
10^{-3}	4.99800×10^{-4}	4.99800×10^{-4}	4.99840×10^{-4}	4.99840×10^{-4}
10^{-2}	4.98008×10^{-3}	4.98008×10^{-3}	4.98405×10^{-3}	4.98405×10^{-3}
10^{-1}	4.80769×10^{-2}	4.80769×10^{-2}	4.84496×10^{-2}	4.84496×10^{-2}
1	3.57143×10^{-1}	3.57143×10^{-1}	3.78788×10^{-1}	3.78788×10^{-1}
10	1.00000	1.00000	1.19048	1.19048
10^2	1.21951	1.21951	1.51515	1.51515
10^3	1.24688	1.24688	1.55732	1.55732
10^5	1.24997	1.24997	1.56245	1.56245
∞	1.25000		1.56250	

Acknowledgements

The support of this work by the Brazilian agency CNPq through Grants 521002/97–4 and 131989/98–7 (M.Sc. stipend of R.P.A.R.), and by the State of Rio agency FAPERJ through Grant E–26/170.889/97–APQ1 is gratefully acknowledged.

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