COMPOSITES WITH FUNCTIONALLY GRADED INTERPHASES: MESOCONTINUUM CONCEPT AND EFFECTIVE TRANSVERSE Conductivity

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(Received 6 January 1995; in revised form 19 June 1995)

Abstract—We consider a unidirectional fiber-reinforced composite with an interphase between the fiber and matrix taken as a graded zone of two randomly interpenetrating phases of these materials. In particular, we take this interphase as a functionally graded material (FGM). The objective of this paper is to present a micromechanics based method to treat FGM and to calculate the effective macroscopic properties (transverse conductivity, or, equivalently, axial shear modulus) of such a composite material. This problem requires the treatment of several length scales: the fine interphase microstructure, its mesocontinuum representation, the fiber size, and the macroscale level (of many fibers) at which the effective properties are defined. It is shown through an example that a convergent hierarchy of bounds on the effective response is obtained with systematically increasing mesoscale resolutions.

1. INTRODUCTION

Interfaces in composite materials influence their local fields and effective properties [1-3]. Theoretical studies in this area represent the interface as either a two dimensional bounding surface, or as a three dimensional region of certain microstructure, called an interphase [4]. In this paper we focus on the effective transverse conductivity of unidirectional composite materials with interphases having functionally graded properties. It can be noted that this problem is mathematically equivalent to other phenomena governed locally by Laplace's equation, such as electrical conductivity or anti-plane elasticity [5]; see Table 3 in the Appendix. The inhomogeneity of the interphase may be due, for example, to the chemical reaction(s) or diffusion.

Composites with inhomogeneous interphases have been studied by several researchers recently. These works include the studies of local fields due to thermal [6-10] and mechanical [11] loadings and the evaluation of effective elastic moduli of composites [12-17]. However, in these studies the interphase region is assumed to be isotropic with one property, typically Young's modulus, varying linearly, as a power law, or as a polynomial, and in general the Poisson's ratio is taken as a constant. The anisotropy of the interphase is considered in [18, 19] where the anisotropic constants are assumed to vary as a power law. Also, several studies represent the inhomogeneous interphase by a number of layers, e.g. [20]. For additional references on the subject see also [21].

Functionally graded materials (FGM in current terminology), or materials with spatially varying properties, present new theoretical challenges in mechanics and micromechanics of solids. The fundamental problem is how to predict the effective properties of such materials given the spatially inhomogeneous distribution of phases. Zuiker and Dvorak [22, 23] generalized the Mori-Tanaka method to account for the variable reinforcement density and thus to linearly varying local and global fields. An alternate approach was considered by Aboudi and co-workers [24, 25] who employed a modified method of cells to study an FGM model system. Recently, a study of elastoplastic phenomena in FGM has been presented in [26].

In this paper we approach this complicated problem in a new way which explicitly deals with spatially random graded microstructures. We begin by considering the microstructure of the interphase, which we represent as a zone of two randomly interpenetrating phases with radially dependent statistics. We admit two generic models of the microstructure: a fine-grained model with a topology of a random chessboard, and a coarser-grained model with a topology of a Voronoi tessellation, whose cells are occupied by either one of the phases. While we choose these material systems for simplicity, it has been noted that the presented model and method admit any type of FGM microstructure. Ideally, the input on details of microstructure should come from experimental observations; this however still remains a challenge [27-29].
The analysis is based on a mesoscale window finitely larger than the scale of a heterogeneity in the FGM medium. In order to define the effective properties of this mesoscale window, we introduce two types of boundary conditions: essential (temperature- or displacement-controlled) and natural (flux- or traction-controlled). It follows that, at a given mesoscale resolution and any location, we obtain two bounds on the scale-dependent properties of interphase. As a result local properties of interphase are anisotropic in nature and are given as a continuous differentiable tensor function which we approximate by polynomials. This is used as input in the effective medium theory allowing the prediction of the transverse conductivity of the composite. In this latter stage of the analysis we use the “composite cylinders assemblage” model [30] to account for the fiber interactions in the numerical examples shown; we choose this model for simplicity. Some preliminary results of the present study were given in [31,39].

2. PROBLEM STATEMENT

In this paper we are concerned with computing the effective transverse thermal conductivity of a unidirectional fiber-reinforced composite with continuous and aligned fibers, which are in a shape of circular cylinders. In this composite the fiber-matrix interface is explicitly taken as a finite thickness zone of two randomly mixed phases of the matrix and the fiber; we refer to it as an interphase (Fig. 1). We assume that the fiber (f) and the matrix (m) phases are homogeneous and isotropic, that is, they are described by two constant isotropic conductivities $C^{(f)}$ and $C^{(m)}$. A second rank conductivity tensor $C^{(s)}_{ij}$, $s = f$ or $m$, is defined as a mapping of temperature gradient into heat flux: $q_{ij} = -C^{(s)}_{ij}T_{ij}$; for an isotropic material $C^{(s)}_{ij} = \delta_{ij}C^{(s)}$. We will also employ a resistivity tensor $S_{ij} = (C^{(s)})^{-1}$.

Noting that the objective is to calculate the effective (i.e. macroscopic) response of the composite, a particular obstacle is posed by the presence of three different length-scales: (i) the fine structure of the interphase region, (ii) size and spacing of fibers, and (iii) the macroscopic dimension of the composite. In addition we need to address the randomness on the first two length-scales: of the grains in the interphase, and of the fibers. In the following we outline the analytical treatment of these length-scales and randomness.

3. SOLUTION PROCEDURE

3.1. Passage from the micro to meso level

We employ a cylindrical coordinate system $r$, $\theta$, $z$, such that the $z$-axis is parallel to the axes of the fibers and the $r-\theta$ plane is a transverse plane, which becomes the plane of our two-dimensional (2-D) problem [Fig. 2(a)]. The random mixture of two types of phase ($f =$ fiber, and $m =$ matrix) in the interphase is represented either by a random chessboard [Fig. 2(b)], or by a Voronoi mosaic [Fig. 2(c)]. We choose these two geometrically well-defined models for our examples for the sake of numerical convenience. Other microstructures can be treated by our approach in the same manner. It is seen that the random chessboard model represents an extreme of a fine-grained microstructure, albeit with a square, rather than Voroni mosaic topology. In both cases
Fig. 2. (a) Sketch of the fiber-interphase-matrix system, and the window concept shown for a random chessboard model (b) and a Voronoi model (c).

cells are occupied at random by either one of the phases according to a so-called indicator function:

$$\chi_L(\omega) = \begin{cases} 1 & \text{if } L \in V_I \\ 0 & \text{if } L \in V_m \end{cases} \quad \omega \in \Omega$$  

where

- $V_I$ = domain occupied by a phase $s =f$ or $m$;
- $\Omega$ = sample space,
- $\omega$ = one realization of an interphase.

In the above we employ an established model of description of random media [32,33], whereby $B = \{ B(\omega); \omega \in \Omega \}$ is a random microstructure. Two typical realizations of $B(\omega)$ for both models of the interphase are shown in Fig. 2(b) and (c).

In what follows we characterize $\chi$ probabilistically in terms of a distribution $P\{\chi(\Omega)\}$. For a functionally graded interphase we assume $P\{\chi(\Omega)\}$ to be axisymmetric

$$P\{\chi(\Omega) = 1\} = P\{\chi(r) = 1\} \quad \forall r$$  

and monotonic

$$P\{\chi(r) = 1\} \leq P\{\chi(r') = 1\} \quad \forall r > r'.$$  

Also, $P\{\chi(\Omega)\}$ satisfies two boundary conditions

$$P\{\chi(a_o) = 1\} = 1 \quad \text{and} \quad P\{\chi(b_o) = 1\} = 0$$  

where $a_o$ is the radius of the fiber (i.e. the inner radius of the interphase), while $b_o$ is the outer radius of interphase. The fiber and matrix phases are both taken as locally isotropic, and hence statement (4) implies that the conductivity $C_{ik}$ equals $\delta_{ik}C^{(0)}$ at $r \leq a_o$, and $\delta_{ik}C^{(m)}$ at $r \geq b_o$.

The highly heterogeneous interphase microstructure—piecewise-constant (non-differentiable) and random—poses a major problem in the analysis. Actually, one needs a differentiable distribution for input to the field equation $q_{ij} = 0$, where $q_i$ is a heat flux. Following a procedure developed for random media [33–35], this obstacle is now overcome by introducing an approximating mesocontinuum—a random conductivity tensor field $C_{ik}^{(i)}(r, \theta, \omega)$, where the superscript $i$ denotes the interphase. This field is defined with the help of a window of size $L$, with $(b_o - a_o) \geq L > d$, where $d$ denotes the average heterogeneity (i.e. micrograin) size. At this point it is convenient to introduce a nondimensional parameter $\tilde{\delta} = L/d$ that specifies the actual mesocontinuum resolution.

More specifically, the mesocontinuum conductivity field is obtained by employing the window as a scale-dependent analogue of an RVE characterizing the material response $C_{ik}^{(0)}(r, \theta, \omega)$, as a transformation from the temperature gradient $\nabla T = \tilde{\nabla}$ into the heat flux $\tilde{q}_i$, or vice versa. It is very important to note here that a conventional, unique, deterministic continuum cannot be set up in the FGM interphase since a passage $\delta \to \infty$ is not attainable. Hereinafter overbars indicate volume averages over the volume (i.e. area) of the window.

It follows that, in order to define the effective conductivity, we may use two types of boundary conditions:

(a) essential (temperature-controlled)

$$T = \tilde{\beta}_i x_i$$  

which yield $C_3^\delta$, and

(b) natural (flux-controlled):

$$q = \tilde{q}_k n_k$$  

which yield $C_3^\delta = (\bar{S})^{-1}$. In the above $\tilde{\beta}_i$ is a uniform temperature gradient, $\tilde{q}_i$ is a uniform heat flux, $x_i$ is a spatial position, and $n_k$ is the outer normal vector to the boundary. Here we use the superscripts $e$ and
n to denote results obtained under the essential and the natural boundary conditions, respectively. Of course, in case of elasticity, (a) and (b) correspond to the displacement-controlled and traction-controlled conditions, respectively (see Table 3 in the Appendix).

It can be shown from the principles of minimum potential energy and complementary energy that the effective conductivity tensor is bounded, at any given radius \( r \) and on scale \( \delta \), by two locally anisotropic (l) tensor fields \( \langle C_l(r) \rangle \) and \( \langle S_l(r) \rangle^{-1} \), where \( \langle \cdot \rangle \) signifies the ensemble averaging, i.e. averaging over \( \Omega \). Indeed, we may recall here a hierarchy of bounds [36]

\[
C^R \equiv \langle C^R \rangle^{-1} \leq \langle S^R \rangle^{-1} \leq \langle S^V \rangle^{-1} \leq \langle C^V \rangle \quad \forall \delta < \delta_0
\]

on the effective response tensor \( C^e \) on the infinite scale \( (\delta \to \infty) \) for a statistically homogeneous medium; \( C^V \) and \( C^R \) denote the Voigt and Reuss bounds. In other words, effective response depends on the boundary conditions, and the influence of the latter disappears as the body becomes infinite. In case of an interface, however, the limit \( \delta \to \infty \) does not make much sense, and, hence, the concept of \( C^e \) is understood only as an effective response bounded by two types of boundary conditions. The problem is similar to the one encountered in stochastic finite elements (and differences), where an effective stiffness matrix for a given finite element not infinitely larger than the heterogeneity size is required, see [37, 38].

It turns out that both these tensors are orthotropic as can heuristically be seen from Fig. 2(b) and (c) by noting a gradient in the radial direction. Indeed, the \( \theta \theta \)-component is larger than the \( r r \)-component. As can be seen from Fig. 2(b) and (c) by noting a gradient in the radial direction. Indeed, the \( \theta \theta \)-component is larger than the \( r r \)-component. This is due to the fact that the first window is placed wholly in the matrix region with its side just touching the interphase region. Its center is at \( r = a_0 - L/2 \), we denote this position by \( a \). At this location the effective property is the one of the fiber. However, as the window is moved a small distance into the interphase zone, but with its center still being in the fiber region, the effective property of this window is already different than the one of the fiber. We move this window along \( r \) and evaluate its properties at \( n \) points. The final window considered is the one that is completely in the matrix region and its center is at the location \( r = b_0 + L/2 \), which we denote by \( b \). Thus the properties of interphase change continuously in the interval \( a < r < b \). At each point considered, except for the end points, we find two different values for the property of the interphase. In further analysis we will use both these bounds as the input for \( C^e \), and thus will obtain bounds on the effective property of the composite. The question yet to be answered is this: "Which \( \delta \) should be chosen?"

### 3.2. Passage from the meso to the macro level

We find the effective properties \( C^e \) of the composite using the Composite Cylinder Assemblage model (CCA) of Hashin and Rosen [30]. We choose this model for simplicity, noting that any other rigorous, or less rigorous, method accounting for fiber interaction at this meso-to-macro stage could be used. As this problem is well understood we choose the simplest method. In the CCA model the unidirectional composite is represented as a set of composite cylinders which completely fill the space. Each composite cylinder consists of a cylindrical fiber enclosed in two concentric cylinders, the inner one representing the interphase and the outer one the matrix. Furthermore, each composite cylinder has a similar geometry such that \( a/b \) and \( a/c \) are constant, where \( a, b \) and \( c \) are—the in the mesocontinuum approximation—the fictitious radius of the fiber, the fictitious...
outside radius of the interphase, and the outside radius of the matrix (and of the composite cylinder), respectively. Note that \(a\) and \(b\) are not the actual radii but new quantities that arose from the analysis in Section 3.1.

When calculating the effective conductivity of the composite we can apply, in principle, either essential or natural boundary conditions, but for the composite cylinder assemblage model both will yield identical results. In this presentation we choose to apply a uniform temperature gradient field \(T_{\text{bc}} = f, \theta = 0\) such that on the boundary of the composite we have

\[
T_{\text{bc}} = \tilde{p}c \cos \theta. \tag{8}
\]

The governing equation for our problem is the heat equation which for a case of no coupling between mechanical and thermal fields and steady state condition is

\[
-q_{k} = C^{(s)} T_{,\theta} = 0 \quad s = f, m \tag{9}
\]

for two homogeneous and isotropic regions of fiber and matrix, and

\[
-q_{k,s} = (C^{(s)} T_{,s})_{,s} = 0 \tag{10}
\]

in the inhomogeneous and anisotropic interphase; \(k, l = 1, 2\). Equation (9) is the Laplace's equation which yields the temperature fields in the fiber as

\[
T^{(f)} = A^{(f)} r \cos \theta \quad 0 < r < a \tag{11}
\]

and in the matrix as

\[
T^{(m)} = A^{(m)} r + B^{(m)} r \cos \theta \tag{12}
\]

Equation (10) for the interphase region takes the following form in polar coordinates

\[
\begin{aligned}
C^{(s)}_{\rho} \frac{\partial^2 T}{\partial \rho^2} + \left[ \frac{\partial C^{(s)}_{\rho}}{\partial \rho} + \frac{1}{\rho} C^{(s)}_{\phi} \right] \frac{\partial T}{\partial \rho} + \frac{1}{\rho} \frac{\partial C^{(s)}_{\rho}}{\partial \rho} \frac{\partial T}{\partial \phi} \\
+ \frac{1}{\rho^2} \frac{\partial^2 C^{(s)}_{\rho}}{\partial \phi^2} \left( \frac{\partial T}{\partial \rho} + \frac{1}{\rho} \frac{\partial T}{\partial \phi} \right) = 0
\end{aligned} \tag{13}
\]

for \(a \leq r \leq b\) with the \(C^{(s)}(r)\) tensor being either \(\langle C^{(s)}(r) \rangle\) or \(\langle S^{(s)}(r) \rangle^{-1}\) for a given \(\delta\). Recognizing that they both are orthotropic, i.e. \(C^{(f)}_{\rho} = 0\), we develop polynomial fits for \(C^{(f)}_{\phi}, C^{(m)}_{\phi}, C^{(f)}_{\rho}, \) and \(C^{(m)}_{\rho}\) of the form

\[
C^{(s)}_{\phi} = k_{0} + k_{1} r + k_{2} r^{2} + k_{3} r^{3} + \ldots \tag{14}
\]

Next, using the separation of variables we find a solution to (13) in terms of series

\[
T = \left[ A^{(s)} \sum_{n=0}^{N} d_{n}(r - r_{0})^{n} + B^{(s)} \sum_{n=0}^{N} e_{n}(r - r_{0})^{n} \right] \cos \theta \tag{15}
\]

which involves two new unknown constants \(A^{(s)}\) and \(B^{(s)}\); the constants \(d_{n}\) and \(e_{n}\) are known. We take \(r_{0} = (a_{0} + h_{0})/2\) for best convergence.

Finally, we evaluate the five unknown constants \(A^{(s)}, A^{(m)}, B^{(s)}, B^{(m)}\) by using the boundary conditions

\[
\begin{align*}
T^{(s)} &= T^{(s)} \quad \text{at } r = a \\
q^{(s)} &= q^{(s)} \quad \text{at } r = a \\
T^{(m)} &= T^{(m)} \quad \text{at } r = b \\
q^{(m)} &= q^{(m)} \quad \text{at } r = b \\
T^{(m)} &= p_{c} \cos \theta \quad \text{at } r = c \tag{18}
\end{align*}
\]

where we note that

\[
q^{(s)} = -C^{(s)} \frac{\partial T^{(s)}}{\partial r} \quad s = f, m. \tag{19}
\]

This permits the determination of the effective conductivity \(C^{\text{eff}}\) from equating the normal component of flux on the boundary of our composite cylinder \(q^{(m)}(c)\) with the normal flux in the equivalent homogeneous cylinder having the effective properties

\[
q^{(m)}(c) = -C^{\text{eff}} p_{c} \cos \theta \tag{20}
\]

which yields

\[
C^{\text{eff}} = \delta_{s} C^{\text{eff}} \quad C^{\text{eff}} = \frac{C^{(m)}}{p} \left( A^{(m)} - B^{(m)} \right) \tag{21}
\]

As pointed out at the end of Section 3.1, we note again that we actually conduct this procedure twice, for \(C^{(s)}(r)\) equal to either \(\langle C^{(s)}(r) \rangle\) or \(\langle S^{(s)}(r) \rangle^{-1}\).

4. NUMERICAL RESULTS AND DISCUSSION

The foregoing theoretical formulation is illustrated through numerical results for a composite having a random chessboard interphase. We take the following basic parameters: contrast ratio \(C^{(f)}/C^{(m)} = 10\), and \(a_{0} = 1.0\), \(b_{0} = 1.1\) implying that the interphase thickness is 10% of the fiber radius. We assume a linear distribution

\[
P_{\{X(r) = 1\}} = A_{1} r + A_{2} \tag{22}
\]

where \(A_{1} = -10.0\) and \(A_{2} = 11.0\) are found from the end conditions (4). We choose a linear function in (22) because of a lack of any experimentally based data. It has to be pointed out, however, that the mesocontinuum concepts and the entire analysis are applicable, without any complication, to deal with nonlinear \(P_{\{X(r)\}}\) distributions as well as multiple inhomogeneous interphases.

We take the interphase to have the thickness of one hundred squares (i.e. micrograins), and consider three window sizes: \(\delta = 10, 20, 40\) which thus span \(10 \times 10, 20 \times 20, \text{ and } 40 \times 40\) micrograins, respectively. Now, for each \(\delta\), for each specific \(B(\omega)\), and at \(n\) radial locations we obtain bounds \(C^{(s)}(\omega)\) and \(\langle S^{(s)}(\omega) \rangle^{-1}\) according as the boundary conditions (5) and (6), respectively, are employed. In order to solve these two boundary value problems of thermal conductivity of a two-phase composite in the interior of a given window, we employ a finite difference scheme. The idea is to approximate the planar continuum by a very fine mesh, and, in the following, we assume...
that a square mesh for the temperature field $T$ is used. The governing equations are thus

$$T(i,j)[k_r + k_i + k_u + k_d] - T(i+1,j)k_r,$$

$$-T(i-1,j)k_i - T(i,j+1)k_u,$$

$$-T(i,j-1)k_d = 0.$$  \hspace{1cm} (23)

Here $i$ and $j$ are the coordinates of mesh points, and $k_r$, $k_i$, $k_u$ and $k_d$ are defined from the series spring model

$$k_r = [1/C(i,j) + 1/C(i+1,j)]^{-1},$$

$$k_i = [1/C(i,j) + 1/C(i-1,j)]^{-1},$$

$$k_u = [1/C(i,j) + 1/C(i,j+1)]^{-1},$$

$$k_d = [1/C(i,j) + 1/C(i,j-1)]^{-1}.$$ \hspace{1cm} (24)

where $C(i,j)$ is the property (thermal conductivity) at a point $(i,j)$. Calculation of these two tensors is conducted by using a fine finite difference mesh with one node representing a single micrograin of the chessboard. This method—equivalently called a spring network—offers a possibility of a rapid assignment of configurations and solution for the said bounds.

It is noted here, following Section 3.1, that the mesocontinuum interphase ranges from $a$ through $b$, the inner and outer radii of the interphase, which depend on the actual choice of $\delta$. Specific values of $n$, $a$, and $b$, as well as the number $N$ of random configurations $\omega$ simulated in a Monte Carlo sense, of the interphase are given in Table 1; note that the scatter decreases with increasing scale $\delta$, and hence a smaller $N$ is needed.

Upon ensemble averaging of both response tensors at any given radial location we obtain two...
orthotropic tensors $\langle C^r \rangle$ and $\langle S^r \rangle^{-1}$ at all the points (see Figs 4, 5, and 6); calculation of all points of each figure was on the order of a few hours on a modern workstation. Let us note here that although $C_{\alpha\beta}$ and $S_{\alpha\beta}$ are, in general, different from zero for any given realization $B_{\alpha\beta}$, the ensemble averages of these tensors' components are zero due to the assumption of axisymmetry of $F_{\alpha\beta}(\xi)$, recall equation (2). More specifically, these figures illustrate:

- averages for $C_{\alpha\beta}$ and $C_{\gamma\delta}$ components of $\langle C^r \rangle$ and $\langle S^r \rangle^{-1}$;
- polynomial approximations of type (14) for each component of these tensors. Several observations are in order here:

(i) larger $\delta$ leads to a higher anisotropy, while for the smallest $\delta = 10$ the anisotropy is almost non-existent,
(ii) smaller $\delta$ results in wider bounds, since this tends to a limiting case of Voigt and Reuss bounds at $\delta = 1$ [recall equation (8)],
(iii) strength of fluctuations goes inversely with $\delta$, and hence there is a need for a large number of simulated configurations $N$ at $\delta = 10$,
(iv) generating a good fit to the data requires polynomials (14) with 16 terms for $\delta = 20$ and 40, and up to 32 terms for $\delta = 10$; however, generating fits which would have a zero slope at $r = a$—as should be the case—proved virtually impossible for $\delta = 10$ and 40; thus, the “lip” produced just to the right of $a$ is an artifact of the fitting.

With the mesocontinuum approximation at hand, we can now proceed to the calculation of macroscopic effective moduli via the CCA model. The CCA model, which we employ to pass from the meso to macro scale, is used for simplicity. A more accurate treatment of the inclusions’ interactions can be done by an extensive computer simulation involving a composite such as in Fig. 1 with many inclusions (fifty, say) all having functionally graded interphases; this has been done in [39], and the results were very close to the ones discussed below.

Figures 7, 8, and 9 give the plots as functions of volume fractions, up to 60%, for three cases of $\delta$. Each figure shows two curves, one corresponding to the $\langle C^r \rangle$, and another to the $\langle S^r \rangle^{-1}$ input. Also, each figure contains a magnification of these curves at right about 60% volume fraction. By comparing all the numbers we note that an increase in $\delta$ leads to ever closer bounds $C^{(\text{Voigt})}_{\text{eff}}$ and $C^{(\text{Reuss})}_{\text{eff}}$—the first corresponding to $C_{\alpha\beta}$ and the second to $S_{\alpha\beta}$—on the effective macroscopic response $C_{\text{eff}}$. This is also illustrated in Table 2 for a specific case of volume fraction 0.599, which is chosen for an easy reference to Figs 7, 8, and 9. We may therefore conclude by proposing a following hierarchy of bounds

\[
\begin{align*}
-C^{(\text{Voigt})}_{\text{eff}} & \approx C^{(\text{Reuss})}_{\text{eff}} \\
C^{(\text{Voigt})}_{\text{eff}} & \approx C^{(\text{Reuss})}_{\text{eff}} \\
C^{(\text{Voigt})}_{\text{eff}} & \approx C^{(\text{Reuss})}_{\text{eff}} \quad \forall \delta' < \delta. \quad (25)
\end{align*}
\]
Fig. 9. Effective conductivity of the composite as a function of volume fraction for the mesocontinuum approximation at $\delta = 40$.

The fact that the difference between the $\theta \theta$ and $rr$ components of $\langle C(r) \rangle$ or $\langle S(r) \rangle^{-1}$ is small raises a possibility of taking their average, and thus, effectively, replacing the anisotropic interphase by an isotropic one. This option was explored with the CCA model, so that the magnifications of Figs 7, 8, and 9 also show a pair of bounds (upper and lower) which were obtained by using such an isotropic mesocontinuum input. Examination of all the values indicates that: (i) for each $\delta$ these new upper and lower bounds are contained within the previous ones based on the more correct anisotropic models, and (ii) the new bounds also follow a convergent pattern of hierarchy (25). The hierarchy of bounds is also illustrated in Table 2.

Let us recall from the Introduction, that in conventional approaches, the interphase properties have typically been assumed in a simple form (e.g. linear, or power law). Here, we end our investigation by using an alternate continuum approximation for the interphase property, namely by employing directly the CCA pointwise along the radius $r$; see Fig. 10.

Table 2. $C^{\text{eff}}$ as predicted for various $\delta$

<table>
<thead>
<tr>
<th>$C^{\text{eff}}$</th>
<th>Window size $\delta$</th>
<th>Bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.639</td>
<td>10 x 10</td>
<td>Upper</td>
</tr>
<tr>
<td>1.634</td>
<td>20 x 20</td>
<td>Upper</td>
</tr>
<tr>
<td>1.623</td>
<td>40 x 40</td>
<td>Upper</td>
</tr>
<tr>
<td>1.614</td>
<td>40 x 40</td>
<td>Lower</td>
</tr>
<tr>
<td>1.607</td>
<td>20 x 20</td>
<td>Lower</td>
</tr>
<tr>
<td>1.592</td>
<td>10 x 10</td>
<td>Lower</td>
</tr>
</tbody>
</table>

Fig. 10. Properties of the interphase calculated using the CCA model.

That is, the CCA model is used at any $r$—with a corresponding volume fraction of both phases—as if one had a practically infinite medium there. Let us keep in mind that the CCA model is very crude at high volume fractions, which corresponds here to the $r$ close to $a_0$. Note that the resulting curve differs qualitatively from the curves of Figs 4, 5, and 6 in that it ranges from $a_0$ through $b_0$ only, and it has a kink—rather than zero gradients—at $a_0$.

Thus obtained effective conductivity distribution has then been employed in the CCA model calculation of composite's moduli, with the result depicted as curve #5 in Fig. 9. Note that the difference between both calculations is small for this example. However, it has to be kept in mind that this result—which, in effect, justifies the simplistic mixture treatment of the interphase—has been established here for a specific case of material parameters, a specific interphase thickness, a specific distribution of phases in the interphase region, and the inhomogeneous interphase represents a relatively small component of the composite. Also, this result is for effective properties of the composite; in this situation the details of microstructure are averaged (smeared out). Considering a problem of local (e.g. mesoscale) fields in and around the fiber, one has to note that these would be much more correctly brought out through an analysis based on scale-dependent windows.

Thus, if the FGM range extends over a larger region, the differences that arise between the rigorous approach presented here and the simplified models are expected to be more pronounced. Clearly, as seen
from our example, the continuum representations of the heterogeneous material are different from these two approaches, and thus they will, in general, have an influence on the predicted mesoscale and macroscale responses. This illustrates a need for a more complete study on functionally graded materials, which will consider a larger parameter space, will include different types of spatial inhomogeneity, will explore the effects of material geometry, and will focus on the local fields.

5. CLOSURE

In this paper we propose a new way to treat functionally graded materials which uses the microstructure information and involves several length scales. This is displayed on an example of a fiber composite, whose highly heterogeneous nature of the fiber–matrix interphase necessitates the introduction of a mesocontinuum concept; however any other transport or elasticity problem of FGM can be treated by this method. The scale $\delta$ of an RVE of the latter may be set up quite arbitrarily over a wide range of values. In contrast to the passage to an infinite scale as commonly employed in many other problems of micromechanics, the finite size of interphase precludes this possibility. As a result, two random fields bounding the effective response at any given $\delta$ may be introduced. This provides a first micromechanics-based derivation of the profile of material characteristics across the interphase. Both random fields are averaged in the ensemble sense to provide two mesocontinuum approximations for input to the effective medium calculations, that are based here on the CCA model. The convergent nature of resulting bounds on effective modulus $C_\nu$, with increasing $\delta$, suggests a $\delta$-dependent hierarchy of such bounds (25). This provides an answer to the question posed at the end of Section 3.1 concerning the choice of $\delta$.

It is finally of interest to mention here a need for mesocontinuum approximations in various other problems of mechanics—e.g. in stochastic versions of finite elements (or finite differences) aiming at inclusion of microstructural fluctuations on the scale of a finite element cell. As shown in a recent paper on this subject [37], one needs to solve the global boundary value problem—i.e. the finite element problem—twice with either type of input: once with $C_\nu$ and next with $(\frac{\partial}{\partial x})$−1. As a result one obtains the same type of convergent bounds as in (25) on the global response; see also [38] for a discussion of a micromechanically based variational formulation of stochastic finite elements and several related issues.

Acknowledgements—This research was funded by the NSF grants MSS-9202772 and MSS-9402285, and the Research for Excellence Fund from State of Michigan. Comments of anonymous reviewers have proved helpful in finalizing the paper.

**APPENDIX**

For a quick reference of the reader Table 3 gives the conceptual analogy between out-of-plane elasticity (i.e. anti-plane elasticity) and thermal conductivity.

<table>
<thead>
<tr>
<th>Out-of-plane elasticity</th>
<th>Thermal conductivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u$ = out-of-plane displacement</td>
<td>$T$ = temperature</td>
</tr>
<tr>
<td>$\epsilon_i$ = strains ($\epsilon_{11}$ and $\epsilon_{22}$) ($\delta$)</td>
<td>$T_\gamma$ = temperature gradient ($VT$)</td>
</tr>
<tr>
<td>$\sigma_i$ = stresses ($\sigma_{11}$ and $\sigma_{22}$) ($\gamma$)</td>
<td>$q_\gamma$ = heat flux vector ($q$)</td>
</tr>
<tr>
<td>$t$ = traction</td>
<td>$q$ = normal flux component</td>
</tr>
<tr>
<td>$C_o$ = out-of-plane stiffness tensor ($C$)</td>
<td>$C_i$ = conductivity tensor ($C$)</td>
</tr>
<tr>
<td>$S_o$ = out-of-plane compliance tensor ($S$)</td>
<td>$S_i$ = resistivity tensor ($S$)</td>
</tr>
</tbody>
</table>