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Locally-exact homogenization of unidirectional composites with coated or hollow reinforcement

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ABSTRACT

Effects of coated and hollow reinforcement on homogenized moduli and stress fields in unidirectional composites are investigated using elasticity-based homogenization theory for periodic materials with hexagonal and tetragonal symmetries extended to accommodate coatings. The theory employs Fourier series representations for fiber, coating and matrix displacement fields in the cylindrical coordinate system that satisfy exactly equilibrium equations and continuity conditions in the interior of the unit cell. The inseparable exterior problem requires satisfaction of periodicity conditions efficiently accomplished using previously introduced balanced variational principle which ensures rapid displacement solution convergence in the presence of thick or very thin coatings with relatively few harmonic terms. The solution's stability facilitates rapid identification of coatings' impact on homogenized moduli and local fields in wide ranges of fiber volume fraction and coating thickness. Elastic response of unidirectional composites reinforced by hollow fibers may be obtained without specializing the theory's framework by appropriately adjusting input parameters. This is illustrated using alumina nanotubes as reinforcement, revealing new results of interest in the design of multifunctional porous materials. Equally important, the theory's analytical framework requires minimal effort in constructing input data file that defines the unit cell problem, facilitating use by researchers with little mechanics exposure.

1. Introduction

Interfaces play a key role in stress transfer between fiber and matrix phases of a fiber-reinforced composite, which is at the core of reinforcement principles in the mechanics of composite materials. They take different forms that depend on the fiber/matrix system and hence different names have been used to describe them. Examples include regions with variable properties, or interphases, due to altered chemical bond structure of the matrix phase adjacent to the fiber's surface in polymeric matrix composites; fabrication-induced reaction zones with degraded properties in metal matrix composites reinforced by ceramic fibers; as well as coatings that promote fiber/matrix adhesion, control fracture toughness or reduce residual stresses. The effect of interfaces or interphases on the homogenized and local response of unidirectional composites has been investigated by many researchers using different modeling approaches within various micromechanics or homogenization theories, including distinct interfacial layers with properties different from those of the adjacent fiber or matrix, and spring and cohesive zone models. For very thin interface/interphase regions the latter two models offer an attractive alternative to finite-thickness interfacial layers especially when variational techniques requiring detailed geometric discretization are employed.

Review of the early approaches based on simple geometric models of unidirectional composites such as the CCA (composite cylinder assemblage), Mori-Tanaka and GSC (generalized self-consistent) models was provided by [15]. A more recent discussion of the various approaches may be found in [8]. The simple geometric models based on a single fiber embedded in the matrix phase, which may in turn be embedded in the homogenized medium of sought properties, yield estimates of homogenized moduli in the presence of interphases or coatings with uniform or variable (so-called graded) properties, but do not provide accurate estimates of stress fields that account for adjacent fiber interaction. To gauge the effect of coatings or interphases on the homogenized moduli without sacrificing local stress field accuracy critical in failure analysis, the finite-element approach has been, and continues to be, employed by a number of investigators, cf. [17,31,1,26,21,35,27]. In the presence of thin coatings, however, detailed mesh discretization is required for converged stress fields. Alternative approaches to the homogenization of unidirectional composites include elasticity-based solutions for periodic microstructures, [23,19], and finite-volume techniques, cf. [24,5,4,29]. Interest in elasticity-based methods has revived within the past 15 years in light of advances in computational technology, as well as due to the potential advantages offered by these techniques, cf. [11,33,34,6,7,3], with a recent focus on the incorporation of interphase and spring models into elasticity-based solutions, [22,25,12]. Optimization of interfacial properties will profit from the use of analytical techniques in the solution of unit cell problems due to the significantly smaller design variable space, more efficient specification of objective functions and implementation of more efficient search procedures. Another benefit is the efficient reconstruction of local fields from

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homogenized-based results within a multi-scale analysis of local failure modes, [18], and material development which relies on rapid answers to what/if questions.

Herein, the elasticity based locally-exact homogenization theory proposed by [7] for rectangular and square periodic microstructures, and [32] for hexagonal arrays with transversely isotropic phases, is further extended to enable rapid calculation of homogenized moduli and stress fields in unidirectional composites with coated fibers. This enhanced capability may also be used for the analysis of unidirectional composites reinforced by hollow fibers, such as alumina nanotubes being developed for microelectronic, optical and potentially structural applications, [9]. The theory differs from other elasticity-based solutions of the local unit cell problem such as the eigenstrain expansion technique[3], the equivalent homogeneity method [22], or the eigenfunction expansion technique [25], in the manner of periodic boundary conditions implementation. While the eigenstrain and eigenfunction expansion techniques employ doubly-periodic displacement field representations that satisfy periodicity conditions a priori, the present theory employs a balanced variational principle in enforcing periodicity conditions along the boundary of a unit cell. This variational principle produces rapid convergence of the displacement field in cylindrical coordinates which satisfies both the Navier's equations and interfacial continuity conditions in the interior of the unit cell representative of rectangular, square or hexagonal periodic arrays of transversely isotropic inclusions. As a result, converged homogenized moduli and local stress fields alike are obtained with relatively few terms in the displacement field representation, in contrast with the eigenstrain expansion technique which requires substantially greater number of terms to obtain converged stress fields [3]. The extended locally-exact homogenization theory that accommodates coatings exhibits convergence of both homogenized moduli and local stress fields which is just as rapid in a wide range of coating thickness and coating/fiber/matrix modulus contrast. While the effect of coating on homogenized moduli has been documented by the above-mentioned elasticity-based unit cell solutions, no data is available on local stress fields which underpin stress transfer mechanisms and ensuing coating-driven modulus alteration.

Section 2 describes the locally-exact homogenization theory's extension which is validated in Section 3. In Section 4 we investigate the combined effects of coating thickness and elastic properties on the homogenized moduli and local stress fields, as well as the effect of emerging nanotube reinforcement of evolving interest in the nanotechnology areas. Specifically, we generate homogenized moduli of unidirectionally-reinforced composites with coated fibers in a wide range of inclusion volume fractions and coating/matrix modulus contrast, and illustrate new and unexpected results when nanotube reinforcement is employed. Conclusions are presented in Section 5.

2. Locally-exact homogenization theory for periodic arrays

2.1. Unit cell solution overview

We investigate the elastic response of periodic materials with continuous coated reinforcement along the x_1 axis, characterized by repeating unit cells representative of either hexagonal or rectangular microstructure, Fig. 1. The fibers are not centered to highlight the solution's insensitivity to fiber placement[7]. Loading the entire hexagonal or rectangular array of coated inclusions by uniform homogenized strain components ε_{ij} is equivalent to loading a single unit cell by the same components. The solution for the ensuing local stress fields is formulated in terms of displacements in the fiber, coating and matrix phases subject to interfacial continuity conditions and periodic boundary conditions on unit cell surface displacements and tractions.

$$u_i(\mathbf{x}_o + \mathbf{d}) = u_i(\mathbf{x}_o) + \overline{\varepsilon}_{ij} d_j, \qquad t_i(\mathbf{x}_o + \mathbf{d}) = -t_i(\mathbf{x}_o) \tag{1}$$

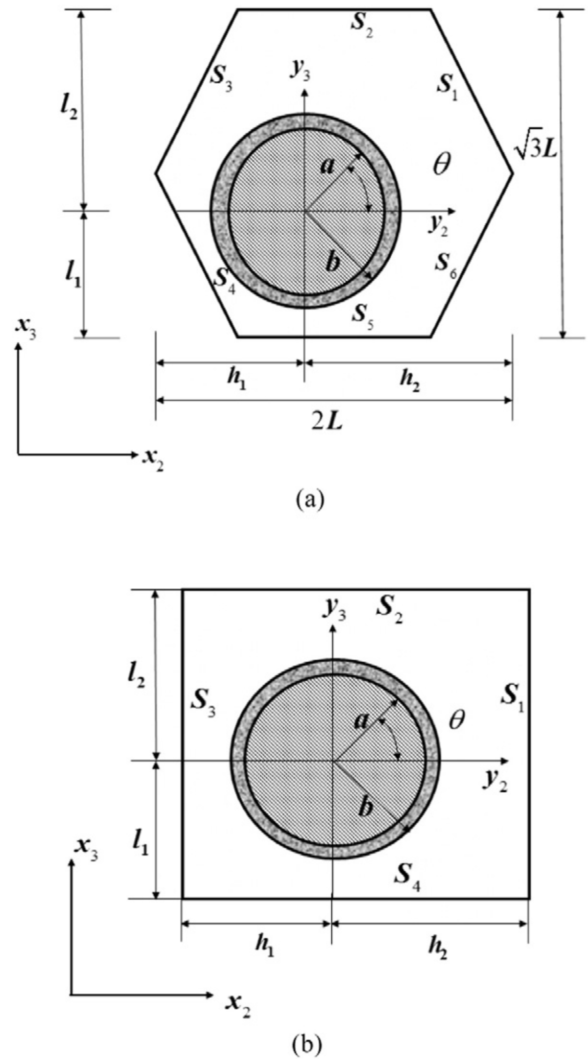

Fig. 1. Repeating unit cells of hexagonal (a) and rectangular (b) arrays of coated fibers.

where $(\mathbf{x}_o, \mathbf{x}_o + \mathbf{d}) \in S$, S is the unit cell boundary, $\mathbf{d}$ is a characteristic distance that defines the unit cell array microstructure, and $t_i = \sigma_{ji} n_j$ from Cauchy's relations, with n_j denoting the jth component of the unit normal to the boundary.

The solution for the displacement fields is carried out within the homogenization theory's framework wherein the global coordinates $\mathbf{x} = (x_1, x_2, x_3)$ describe the average response of the entire periodic array, and the local coordinates $\mathbf{y} = (y_1, y_2, y_3)$ describe the interior unit cell response, [2,28]. Accordingly, a two-scale displacement field representation is employed in the individual phases as follows.

$$u_i^{(k)}(\mathbf{x}, \mathbf{y}) = \overline{\varepsilon}_{ij} x_j + u'^{(k)}_i(\mathbf{y}) \tag{2}$$

where the fluctuating displacement components u_i' caused by the material's heterogeneity are functions of the local coordinates (y_2, y_3) given the unidirectional constraint along the x_1 direction by continuous reinforcement, and the superscripts $k = f, c, m$ denote fiber, coating and matrix phases, respectively. The above displacement field generates the local strains.

$$\varepsilon_{ij}^{(k)}(\mathbf{y}) = \overline{\varepsilon}_{ij} + \varepsilon'^{(k)}_{ij}(\mathbf{y}) \tag{3}$$

from which local stresses follow, with continuous reinforcement yielding the constraint $\overline{\varepsilon}_{11}^{(k)} = \overline{\varepsilon}_{11}$.