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Numerical and analytical modeling of aligned short fiber composites including imperfect interfaces

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ABSTRACT

Finite element calculations were used to bound the modulus of aligned, short-fiber composites with randomly arranged fibers, including high fiber to matrix modulus ratios and high fiber aspect ratios. The bounds were narrow for low modulus ratio, but far apart for high ratio. These numerical experiments were used to evaluate prior numerical and analytical methods for modeling short-fiber composites. Prior numerical methods based on periodic boundary conditions were revealed as acceptable for low modulus ratio, but degenerate to lower bound modulus at high ratio. Numerical experiments were also compared to an Eshelby analysis and to an new, enhanced shear lag model. Both models could predict modulus for low modulus ratio, but also degenerated to lower bound modulus at high ratio. The new shear lag model accounts for stress transfer on fiber ends and includes imperfect interface effects; it was confirmed as accurate by comparison to finite element calculations.

1. Introduction

In mean-field modeling of short-fiber composite materials, a composite unit cell is subjected to mean stress or strain and the effective stiffness or compliance tensors are found by averaging strains and stresses throughout the composite [1]. This averaging is done over all unit cell orientations using a fiber orientation distribution function. The unit cell for this analysis is a short fiber composite with all fibers aligned in the same direction. Thus, the fundamental problem for analysis of short-fiber composites is to determine mechanical properties of an aligned, short-fiber composite.

One might think this problem is solved by methods such as Eshelby [2], Mori–Tanaka [3], modern shear-lag models [4–7], or numerical methods [8–13], but some gaps appear. First, most prior numerical studies have been limited to modest fiber/matrix modulus ratios of $R = E_f/E_m < 30$ and relatively short fiber aspect ratios, $\rho = l_f/d_f < 30$ [8,9,11,13]. Gusev and Lusti [10,12] looked at higher aspect ratios, but only for a narrow selection of R and fiber volume fraction, V_f. As a consequence, the validation of analytical models by these numerical studies [9] only validates them for the corresponding small range of properties.

A recent trend in composites research, especially in nanocomposites, is to reinforce soft polymers (*e.g.*, elastomers with $R > 10^4$) and isolate nano-fibers with aspect ratios higher then 30 [14–17]; the results of such work has been a challenge to model. Fig. 1 show some experimental results for reinforcement of an elastomer with nano-cellulose fibers [14] and compares them to an existing analytical model (labeled "Mori–Tanaka" [3]) and an existing numerical method based on large periodic representative volume elements (RVEs) with randomly placed fibers (labeled "Periodic RVE (FEA)" using approach of Gusev [8]). These experimental results are two to three orders of magnitude higher then existing models. The question arises—are these high reinforcements the discovery of a new nano-phenomenon that cannot be modeled with continuum mechanics or do continuum methods just need to be revised for high R? To explore this question, we developed a new numerical method to derive upper and lower bounds to the modulus. The sample calculation of bounds in Fig. 1 (see dashed lines) shows that experimental results fall within continuum mechanics bounds and that prior modeling methods all degenerate to lower bound results. In other words, the methods described here have new potential to guide expectations of properties for composites with high R.

To study composite modeling methods at high R and aspect ratio as well has how they relate to conventional methods at low R and aspect ratio, we ran numerical calculations for a very wide range of R (from 10 to 10^5) and aspect ratios (from 5 to 100). The calculations in this part of the study were based on novel methods that allowed us to numerically determine upper and lower bounds to the fiber-direction modulus. The shear number of calculations

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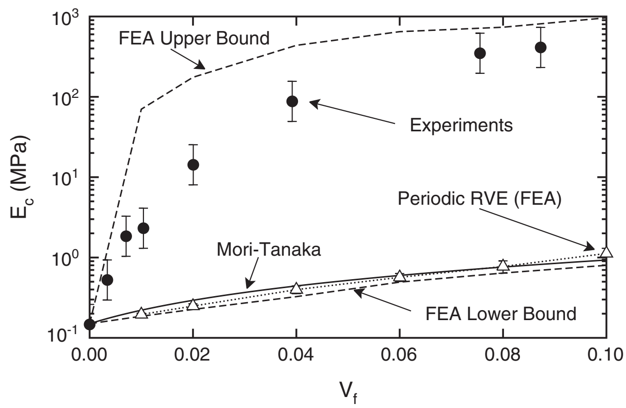

Fig. 1. The symbols are experimental results from Ref. [14] with $R = 9.5 \times 10^5$, which are compared to existing modeling methods (Mori–Tanaka and Periodic RVE (FEA)) and to upper and lower bounds described in this paper (dashed lines). The experiments are quasi-2D with fibers claimed to be randomly aligned in the plane of a film. The models are 2D calculations for aligned fibers. The comparison with experiments is only qualitative, but if experiments had aligned fibers, they would move toward the upper bound and still demonstrate that prior models are near the lower bound and far below experiments.

along with the size of mesh (particularly at high aspect ratio) precluded mesh refinement of numerical results. A powerful feature of the bounding method, however, is that it allows one to get definitive bounds even without mesh convergence. These numerical results provided input for considering four questions:

What is correct modulus? One of the best ways to judge the accuracy of modeling methods is to compare them to numerical results [9], but what numerical method gives the correct modulus? Here we derived numerical bounds using Monte Carlo methods with randomly placed and well-dispersed, aligned fibers. We used bounding methods to define limits on the modulus for R up to 10^5 and ρ up to 100. The separation of the bounds shows that the calculated modulus depends on boundary conditions, especially for large R.

How do periodic RVE calculations compare to numerical bounds? Most numerical models use periodic RVEs and assume analysis results with periodic boundary conditions are equivalent to bulk composite properties. To test this hypothesis, we compared the new numerical bounds to both small periodic RVEs (using either cylindrical (rectangles in 2D) or elliptical fibers) and large RVEs with random fibers. All periodic RVE methods work well for low R, but degenerate to lower bound results at high R.

Can an analytical model sufficiently capture the results of periodic RVE composites? Given the capabilities (and limitations) of periodic RVE analysis, an analytical model that agrees with those numerical results would have those same capabilities (and limitations). We developed an improved shear-lag model for short composite fibers that explicitly includes stress transfer on the fiber ends and imperfect interfaces. The new model, along with an Eshelby [2] analysis, were compared to numerical results on the same geometries. These analytical methods can reproduce numerical methods based on periodic conditions, which means they give good prediction for low R, but degenerate to lower bound results for high R.

Can an analytical model account for 3D fibers and for imperfect interfaces? The first three questions used 2D calculations and assumed perfect fiber/matrix interfaces. Real composites are 3D and may have imperfect interfaces. We lastly considered 3D single fiber RVE results by comparing axisymmetric numerical calculations with imperfect interfaces to the new shear lag analysis with concentric cylinders that also includes imperfect interface effects. The new model accurately reproduces all numerical results including the role of imperfect interfaces.

2. Methods

All finite element calculations (FEA) were linear elastic, static, and two dimensional. Most simulations were plain strain analyses although some 3D results were generated using axisymmetric simulations. All calculations were done using the open source code NairnFEA [18] with 8-node quadrilateral elements. Issues involving convergence are discussed in Section 3. By using script control, we automated the thousands of FEA calculations needed to get sufficient results for answering the posed questions. The FEA calculations were run on either desktop computers or Linux nodes in a cluster. The main requirement for the largest calculations was to have sufficient memory (more than 5 GB).

3. Results and discussion

3.1. What is the Correct Modulus?

To run numerical experiments for the "correct" modulus of aligned short fiber composites, we ran FEA calculations on representative composites with randomly placed fibers. The fibers were all aligned in one direction, placed using a random sequential adsorption (RSA) method [11], and well dispersed (separated by at least one element in the mesh). The numerical experiments were done for fiber to matrix modulus ratios of $R = 10$, 100, 1000, 10^4, and 10^5, for fiber aspect ratios of $\rho = 5$, 10, 20, 40, 70, and 100, and for fiber volume fractions of $V_f = 0.01$, 0.02, 0.05, 0.1, 0.15, 0.2, and 0.25. Monte Carlo methods were used to account for the random structures. For each combination of R, ρ, and V_f, we ran FEA calculations for 20 random structures and averaged the results for mean and standard deviation of the modulus. For most property settings, the 20 replicates gave sufficiently narrow errors bars on the results. The total number of FEA calculations required to map the parameter space exceeded 15,000.

The first issue was the mesh. To deal with randomly placed fibers with randomly situated stress concentrations, the modeling used a regular mesh. A quick calculation showed that a 3D mesh for the largest aspect ratio would have over a billion degrees of freedom, which is infeasible for the 15,000 calculations we needed to run. 3D calculations by Gusev [8] required 30 processor-hours per calculation and that was for spherical inclusions ($\rho = 1$) which can use much smaller RVEs then needed here. We therefore switched to 2D, plain-strain FEA (which still can be used to evaluate other methods provided comparisons are made to 2D versions of those methods). Even in 2D, the mesh could not be highly refined. We used the crudest mesh possible where the element size was equal to the fiber diameter. Thus each fiber had one element across its width and the well-dispersed fibers were separated by at least one fiber diameter (*i.e.*, one mesh element). With this mesh, the largest calculation had about 200,000 degrees of freedom and could be completed in 5–30 min (depending on computer speed).

Because we were limited to a crude mesh, we could not refine the mesh for convergence. To allow definitive results with such a mesh, we adopted a bounding method. In composite variational mechanics, upper and lower bound results are found by the solving the two problems in Fig. 2 [1,19–21]. First, the composite is subjected to constant tractions, $\boldsymbol{T}$, over the entire surface of

$$\boldsymbol{T} = \boldsymbol{\sigma}_0 \cdot \hat{n} \tag{1}$$

where $\boldsymbol{\sigma}_0$ is the uniform applied stress and $\hat{n}$ is surface normal. For stress corresponding to axial loading in the fiber direction (see Fig. 2A), the complementary energy, as approximated by FEA strain energy (Γ_{FEA}), must be greater than or equal to the exact complementary energy, Γ, leading to