Effective Properties of Composites Whose Reinforcement has Microstructure

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Summary

A local averaging procedure is proposed for determining effective properties of a reinforcement that has microstructure. This allows reduction in the number of microstructural scales. Preliminary results emphasize the importance of in situ modeling when determining the effective properties.

Introduction

Generally, heterogeneous materials would be too computationally intensive to analyze if each homogeneous subregion had to be modeled discretely. If the microstructure is sufficiently periodic, effective material properties for a representative volume element (RVE) can be determined using micromechanics. The original heterogeneous material is "replaced" by a homogeneous material and the effective properties are used. A common application of this strategy is replacement of a composite lamina that has millions of individual fibers with a homogeneous orthotropic material. At a larger scale, one can expedite the analysis of thick composite laminates by homogenizing subgroups of the lamina such that a laminate with a hundred distinct plies might be modeled as an equivalent laminate with only ten equivalent homogenized plies. [1]

The application of micromechanics to expedite analysis of heterogeneous materials becomes more tenuous when there are multiple levels of heterogeneity. The original motivation for this investigation stemmed from an interest in describing the effective properties of a carbon nanotube in the context of a composite material. Nanotubes have attracted tremendous attention because they appear to have almost amazing properties that depend on the particular chirality, including extremely high strength, stiffness, thermal conductivity, and electrical conductivity, semi-conductivity, and unusual optical properties. When nanotubes are added to a matrix, there are multiple levels of microstructure. (Fig. 1)

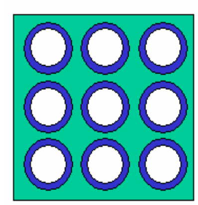

Figure 1 Nanotubes in matrix

The nanotube has "microstructure" in the sense that it is a tube, not a solid rod. The nanotubes are dispersed in the matrix,

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creating a second level of microstructure. Conventional micromechanics techniques would use effective properties for the nanotube in a model that includes two homogeneous phases: the matrix and solid fibers. This paper examines the accuracy of this strategy. As part of the study, the concept of effective in situ effective properties will be explored.

The complete paper will consider two basic configurations, which represent two different scales. The first consists of matrix with a fiber that is not solid, such as the carbon nanotube. The second consists of a laminated material in which the laminae contain transverse matrix cracks. (Fig. 2)

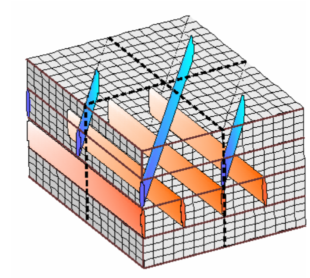


Figure 2: Transverse matrix cracks in a composite

In this second case, damage provides an additional level of inhomogeneity. Although they appear quite different, the challenge is similar. Because of space limitations in this brief abstract, only a simplified version of the first configuration will be considered. In particular, this paper will describe the analysis methodology and some preliminary results that show the effect of fiber fraction on the in situ properties of a fiber that is hollow.

Calculation of effective properties

Calculation of effective properties is straightforward when the microstructure can be approximated as periodic and heterogeneity is modeled discretely, such as in the finite element model in Figure 3.

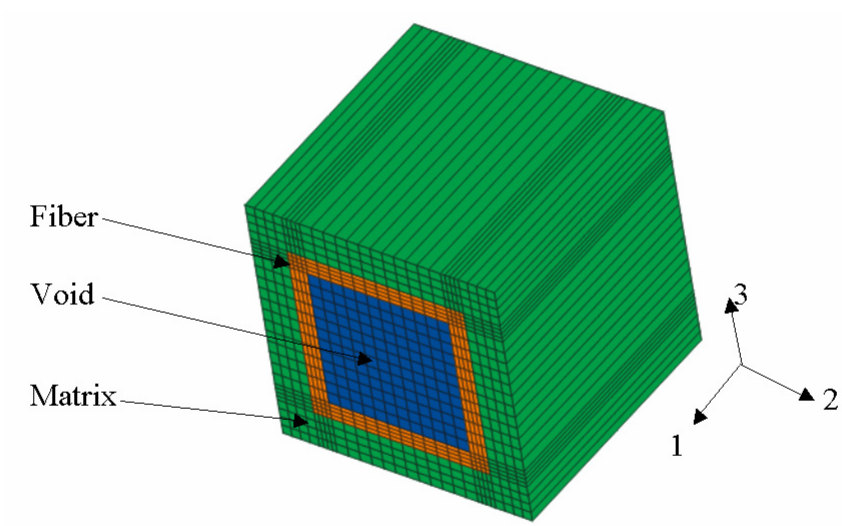


Figure 3: Three-phase analysis model

The periodicity requirements can be expressed as $u_i\left(x_\alpha + d_\alpha\right) = u_i\left(x_\alpha\right) + \left\langle \frac{\partial u_i}{\partial x_\beta} \right\rangle d_\beta$,

where u_i are the displacments, d_β is the vector of periodicity, and $\left\langle \frac{\partial u_i}{\partial x_\beta} \right\rangle$ are the volume averaged displacement gradients. The term $\left\langle \frac{\partial u_i}{\partial x_\beta} \right\rangle d_\beta$ appears because of rigid body motion. Derivatives with respect to the coordinates are zero, so the periodicity of strains is guaranteed and can be expressed as $\varepsilon_{ij}\left(x_\alpha + d_\alpha\right) = \varepsilon_{ij}\left(x_\alpha\right)$. Since the material properties are also assumed to be periodic, the stress fields are also periodic: $\sigma_{ij}\left(x_\alpha + d_\alpha\right) = \sigma_{ij}\left(x_\alpha\right)$. The analysis of an RVE using finite elements involves imposition of multi-point constraints (mpc's) on nodal displacements on the RVE boundaries. Of course, the forces must be self-equilibrating between adjacent RVE's. If transformation techniques are used to impose the mpc's, the transformed force vector includes terms that represent this sum of forces, so it is convenient to prescribe them to be zero. To calculate effective properties, the model is subjected to a series of loadings, each one with a single non-zero component of $\left\langle \frac{\partial u_i}{\partial x_\beta} \right\rangle$. The volume averaged strain and stresses and strains are calculated for each load case. Based on the requirement that $\left\langle \varepsilon_{ij} \right\rangle = \overline{S}_{ijkl} \left\langle \sigma_{kl} \right\rangle$, one can set up simultaneous equations to solve for the effective engineering properties.

The definition of effective properties is no longer so clear when there are multiple levels of microstructure. Suppose one desires to obtain the effective properties for the nanotube in Figure 1. The standard procedure would be to analyze a periodic array of tubes, like that in Fig. 4.

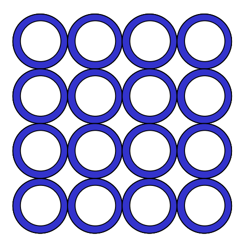


Figure 4: Periodic array of circular fibers

There is only point contact between the adjacent tubes. The interaction of one tube with the surrounding material is nothing like that in Fig. 1. There is little hope that the properties determined from analyzing such an array would produce useful results. Instead, one is faced with determining in situ properties. How does a typical tube behave when it is surrounded by matrix? Of course, when the fiber arrangement is changed (e.g. from a hexagonal to square array) or the fiber fraction is changed, the behavior of a typical tube also changes… i.e. the effective properties change.

The in situ effective properties are herein calculated by performing local volume averaging of stresses and strain in just the fiber for various load cases in contrast to the volume averaging for the entire RVE. This is not a rigorous procedure. One of the goals of this paper is to examine the error in this calculation for various situations.

Configurations

The tube chosen for this brief paper has a square cross-section. (Fig. 5) While this might seem somewhat unusual, there is an advantage for this fundamental study. The advantage of the square shape (and the other shapes shown in Fig. 5) is that it is space filling, which allows for a periodic array in which there is reasonable contact between

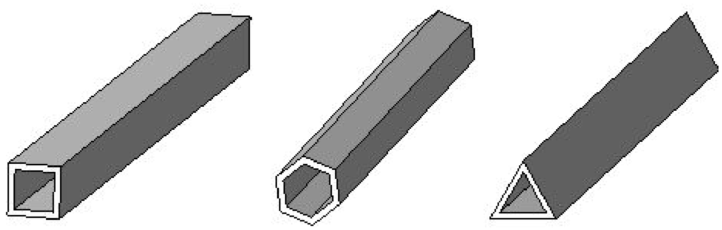


Figure 5: Space-filling fibers

adjacent RVE's, in contrast to the point contact for the circular fibers. As a result, one can calculate the in situ properties for the fiber from a very small fiber volume to 100 percent fiber volume without dealing with pathological configurations. The expanded version of this paper will consider the circular shape as well as other possibilities. Also, herein the tube wall thickness was assumed to be 10 percent of the outside width of the tube. Hence, 64% of the tube was void. The material properties for the matrix and fiber wall were assumed to be isotropic and were as follows

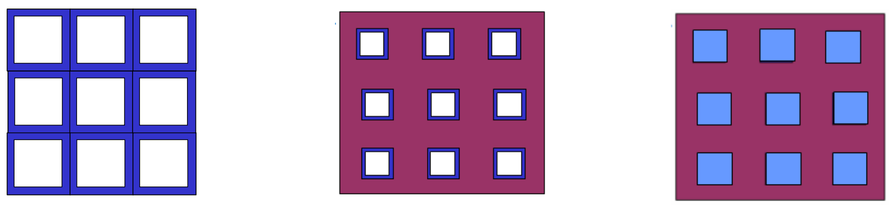
	E (in Gpa)	υ
Matrix	2.82	0.395
Fiber wall	200	0.3

Note that fairly extreme material properties and void percentage was used. Less extreme cases were also considered, but will not be discussed in this abstract.

Results and Discussion

There are various ways to characterize the adequacy of the effective properties calculated for the fiber. One way is to calculate the effective properties of the periodic array of just fibers (Fig. 6). Then matrix is placed between the fibers. This composite is then subjected to periodic loading. Local volume averaging of stresses and strains for the fiber is used to determine the in situ effective properties of the fiber. Characterization of the fiber behavior would be much easier if the effective properties from the model in Fig.6a agreed with the in situ properties from the model in Fig. 6b. Of course, one does not expect to be so lucky… so this paper will examine the differences.

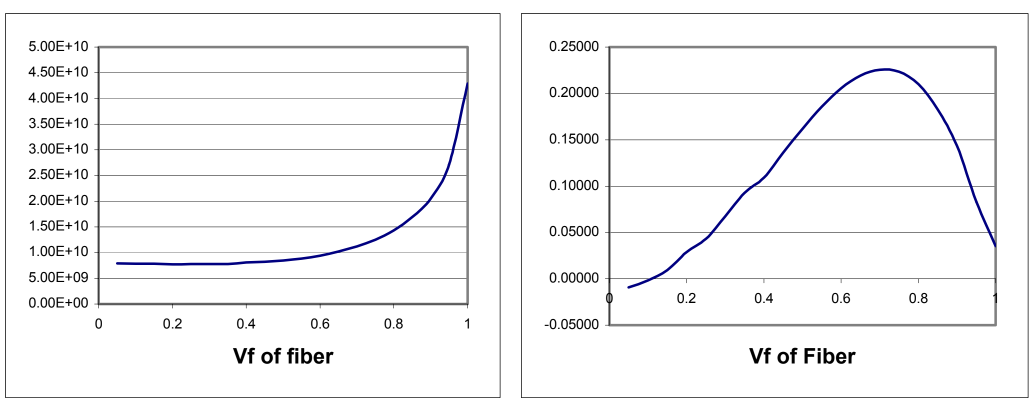
Figure 7 shows that the in situ fiber E_{22} and G_{12} are nearly constant up to about 50 %



a) Fibers only b) Fibers with discrete voids c) Homogenized fibers

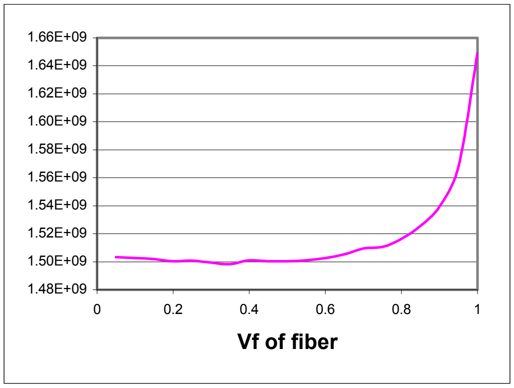
Figure 6: Different configurations of periodic arrays.

fiber fraction. The E_{22} then begins to rise quickly to a value more than four times as large. The Poisson's ratio ν_{23} changes significantly throughout the range of fiber fraction. The G_{23} decreases monotonically with fiber fraction for almost the entire range. It is clear that the properties obtained when the fiber fraction is 1.0 are usually irrelevant. To check whether the in situ properties could be used to replace a three-phase model with a two-phase mode, effective properties of the composite were calculated using the models shown in Fig. 6b and 6c, where the fiber properties in 6c are the in situ properties. This was done for fiber fractions = .1 and .9. The composite effective properties from the two-phase model agreed very well with the three phase predictions… the maximum error for any of the orthotropic properties was 2.3%.

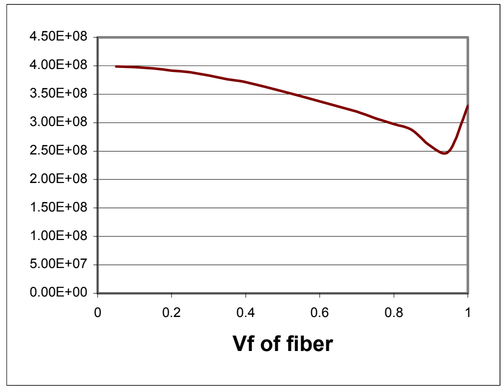


a) In situ E22 b) In situ υ23

Fig. 7: Variation of predicted in situ fiber properties with fiber fraction. Note that fiber fraction =1 corresponds to configuration in Fig. 6a.



c) In situ G12



d) In situ G23

Fig. 7. completed.

Conclusions

When multiple levels of microstructure exist, accurate micromechanics predictions become much more complicated. Initial results showed that in situ effective properties calculated using a simple local volume averaging procedure can give a good estimate of the behavior of a hollow fiber. These properties could potentially be used to eliminate one level of microstructure. At the same time, the in situ effective properties cannot be used to model the behavior of hollow fibers at any volume fraction in a composite. The in situ properties vary greatly with fiber fraction and properties obtained using an insitu analysis of 0.9 fiber fraction cannot be used in modeling composites with low fiber fraction. Much more investigation is required to outline the limits of the strategy proposed herein.

Acknowledgements

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