DEVELOPMENT OF MICROMECHANICS BASED MATERIAL PROPERTY FIELDS FOR RANDOM COMPOSITES

S.C. Baxter, Assoc. M. ASCE
University of South Carolina, Columbia, SC 29208
baxter@engr.sc.edu

L.L. Graham, Assoc. M. ASCE
Johns Hopkins University, Baltimore, MD 21234
graham@virginia.edu

Abstract

The effective use of particulate reinforced composites requires an accurate characterization that includes the influence of their three dimensional microstructure. The extension of a two dimensional moving window technique to three dimensions is illustrated in this work with an application to a clustered microstructure. Constitutive properties are described by random material property fields that are directly linked to the material microstructure. Statistical characterizations on these fields quantify the variation of material properties due to random material microstructure. It is shown that the method captures the influence of clustering, a common microstructural feature which results from fabrication techniques.

Introduction

Short-fiber or particulate reinforced composites, like homogeneous materials, can be easily processed to near net shape and still have the higher specific stiffness, strength and fracture properties associated with continuously reinforced composites. Their effective use however, requires accurate characterization which should include the prediction of local behavior associated with the three dimensional spatial variation in the microstructure. This task is made difficult by random microstructures that can include clustering of the reinforcing phase.

Based on a digitized image of a microstructure, a microstructure-based moving window technique has been proposed for a two dimensional analysis of composite microstructure (continuously reinforced composites) by Baxter and Graham (2000). The technique develops computationally tractable, stochastic material property fields with a direct link to local composite microstructure. Statistical and probabilistic descriptions of the resulting property fields will ultimately be used to simulate additional material samples. Subsequent analysis of the mechanical behavior of these samples will aid in characterizations of variability of material response.

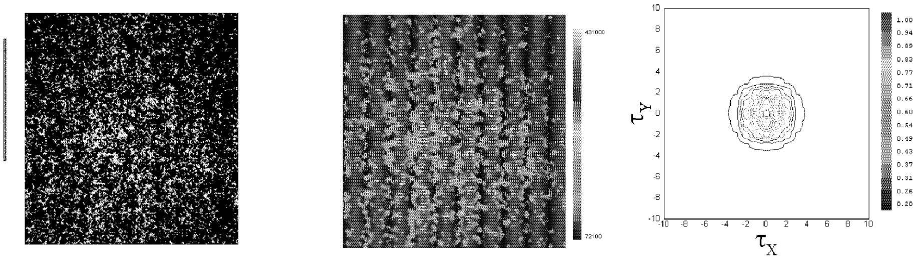
The focus of the present work is to illustrate the extension of the moving window technique to a three dimensional microstructure, specifically a particulate reinforced composite. To demonstrate the method and its extension, the analysis is performed on numerically generated composite micrographs. Comparison of a three dimensional analysis of the full sample with a two dimensional analysis, performed on a plane section of the microstructure, illustrates the additional information obtained through the use of a three dimensional analysis. The ability of the method to distinguish clustering, a common microstructural feature of these composites, is demonstrated by a comparison of selected material property fields and statistical properties of a uniform random microstructure with a clustered random microstructure.

The Moving Window Technique

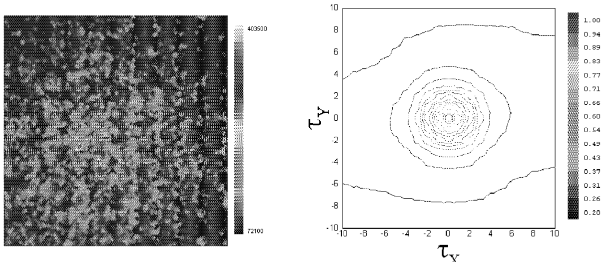
If the densities of the phases of a composite are distinct (at least 1-2 %) three dimensional digital images of the microstructure can be obtained through commercial CAT (computer aided tomography) x-ray scanning. The result is a three-dimensional array of pixels; gray levels are associated with individual phases of the composite and phase material properties. Converting the digital image of the composite into the numeric data based on the individual gray scale levels produces coarse material property fields in one-to-one correspondence with the digital representation of the microstructure. While these coarse fields are the most accurate representation based on the digitized record, they are extremely noisy; for a two phase composite, a two point field is generated. The statistics on such fields are difficult to develop and the cost of simulating these fields for use in a finite element context is likely to be prohibitive. The moving window technique was developed in order to produce more tractable fields for characterization and simulation. Small volumes of the full sample, called windows (a cube in three dimensions) are analyzed individually. The dimensions of the window, once selected, remain constant throughout the analysis, and are specified in units of pixels. The micromechanics model, Generalized Method of Cells, (Aboudi, 1989, Pindera and Bednarcyk 1999), is used to calculate the effective material properties for each window. The effective property of the window is assigned the spatial coordinates corresponding to the center-point of the window. The windows overlap one another, capturing the effect of neighboring microstructure on properties at a point. The procedure is similar to performing a moving average over a noisy signal, but for this particular application the “averaging” is based on the physical assumptions of a detailed micromechanical analysis. This procedure produces a three dimensional field for each material property. Periodic boundary conditions are imposed to allow for calculations of window approximations at grid points near the edge of the sample. If the original sample is presumed to capture the random behavior of the microstructure then generation of material property fields using these boundary conditions should not significantly affect the analysis, although any such assumption has the potential to artificially influence the statistical characterization.

Two-dimensional Analysis vs. Three-dimensional Analysis

Quantitative stereology techniques have traditionally been used to characterize geometric aspects of three dimensional microstructure through the analysis of two dimensional images. The goal is to reconstruct the three dimensional microstructure through an analysis of the two dimensional sections. These techniques are useful when the microstructure is spatially random. In some cases of random microstructure a single plane may be extensive enough to contain a statistically significant number of features and can be used to obtain valid results. In most cases though, reconstruction of the three-dimensional microstructure requires serial sectioning and an average analysis over all sections. If enough sections are examined, and the orientation of the sections is assumed to be the dominant plane for characterization of spatial differences, then the average analysis can be used to predict three dimensional characteristics. However, decisions as to the appropriate number of sections and their orientation are difficult to make, and in some cases serial sectioning may be physically impractical. The analysis of data obtained non-destructively via CAT scan techniques has the potential to provide a more accurate characterization of the material. Additionally, when the data is used in conjunction with the moving window technique, material property fields rather than complex geometric characteristics of the microstructure, become the basis of characterization. This significantly reduces the parameters involved in predictions of the response of the material.



(a) 2-D



(b) 3-D

Figure 1: (a) Plot of Clustered Microstructure; Plot of Elastic Modulus $E_{yy}(x, y)$, 2-D analysis, Auto-correlation of Modulus $E_{yy}(x, y)$, 2-D analysis, (b) Plot of Elastic Modulus $E_{yy}(x, y)$, 3-D analysis, Auto-correlation of Modulus $E_{yy}(x, y)$, 3-D analysis

The comparison of the extreme case of a two dimensional analysis a i.e., single plane, with a three-dimensional analysis of the same plane for a random composite microstructure is presented in Figure 1. The properties of each of the phases were assumed to be isotropic. The reinforcing phase was modeled as a silicon/carbide particulate with an elastic modulus of 431.0 GPa and a Poisson's ratio of 0.19; the matrix phase was modeled as aluminum with an elastic modulus of 72.1 GPa and a Poisson's ratio of 0.34. Figure 1(a) shows the center plane of the micrograph (microstructure), the corresponding elastic modulus E_{yy} field and a 2-D projection of the auto-correlation function calculated using the two dimensional analysis. Figure 1(b) shows the the property field and auto-correlation function for the center plane calculated using a three-dimensional analysis on the microstructure of

Parameter	2-D Analysis		3-D Analysis	
	19% volume fraction		15% volume fraction	
	Elastic Moduli			
	E_{yy}	E_{zz}	E_{yy}	E_{zz}
Minimum (GPa)	72.10	72.10	72.10	72.10
Maximum (GPa)	431.00	431.00	253.30	243.60
Mean (GPa)	102.02	101.94	84.10	84.13
Range (GPa)	358.90	358.90	181.20	171.50
C.O.V.	.36	.36	0.143	0.143

Table 1: Statistical characterization from two and three dimensional analysis

the plane. Table 1 provides details of the material property fields for the elastic moduli, E_{yy} and E_{zz}.

The predicted material property field from the three dimensional analysis shows more smoothing, suggesting the influence of microstructure out of the plane of the section. The most striking difference between the two fields is the perceived volume fraction. As calculated from a single plane section, the predicted volume fraction is much higher, $\approx 19\%$, than that of the full sample, $\approx 15\%$. This contributes to the wider range of values and higher mean found in the 2-D analysis. The two dimensional analysis also predicts a higher coefficient of variation. The correlation area for the elastic modulus E_{yy} is larger for the 3-D analysis, which again suggests the three dimensional influence of clustering. It is expected that if the statistical properties of multiple planes were averaged then the predicted characteristics would more closely match those of the three-dimensional analysis providing that no measurable bias of the microstructure existed associated with the orientation of the planes. A statistical analysis of multiple planes parallel to each of the coordinate directions would improve the analysis, but is not feasible using the results of destructive testing.

Clustered versus Non-Clustered Microstructures

Many real composite materials exhibit clustering of inclusions as a result of the fabrication process. While the distribution of particles is random, clustering can result in correlation areas larger than the inclusion size. There is evidence (Lewandowski et al., 1989, and Lloyd, 1991) that the local spatial distribution generated by clustering of the reinforcement phase can strongly affect static and dynamic mechanical properties.

To analyze this type of microstructure the following procedure was followed to simulate a digitized image of a particulate microstructure. A small percentage of particles, referred to as nucleation sites, were randomly placed on a (200×200×200) grid. In the first cycle a three dimensional random walk was initiated from each nucleation site. The random walk in each cycle consisted of movement right or left, up or down and front to back, i.e., in the positive or negative directions along the three coordinate axis. The final position, due to the random walk resulted in the placement of a particle in the array. Subsequent cycles

Parameter	Random		Clustered	
	Elastic Moduli			
	E_{yy}	E_{zz}	E_{yy}	E_{zz}
Minimum (GPa)	72.71	72.71	72.10	72.10
Maximum (GPa)	247.00	232.10	403.50	403.50
Mean (GPa)	89.17	89.18	88.39	84.13
Range (GPa)	174.90	160.00	331.40	331.40
C.O.V.	.179	.179	0.143	0.143

Table 2: Statistical characterization from uniform random and clustered-random microstructures

were started from the final positions of the previous cycles random walk. If the final grid point defined by a cycle was already occupied by a particle, the new particle was placed adjacent to this site to mimic the behavior of particles subject to similar physical forces but constrained not to occupy the same space.

To investigate the ability of the moving window technique to capture different random configurations the clustered microstructure was compared to a unclustered, (more uniformly random) microstructure in Figure 2. Figure 2 shows the unclustered microstructure, the material property field for the elastic modulus E_{yy} and the auto-correlation function. Table 2 provides details of the material property fields for the elastic moduli, E_{yy} and E_{zz} for the two microstructures.

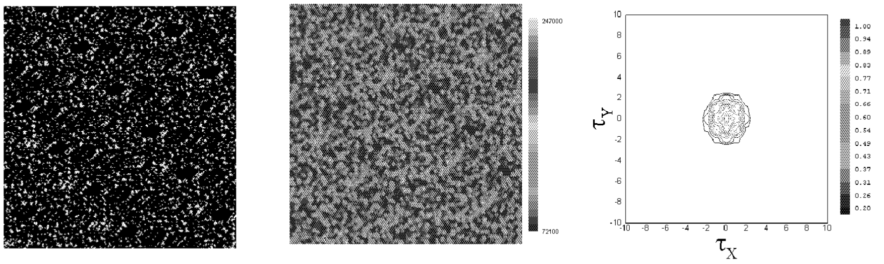


Figure 2: L-R: Random microstructure, Elastic Modulus $E_{zz}(x, y)$, and Auto-correlation function, E_{yy}.

The three dimensional analysis of the two microstructures shows similar values for the mean values but a slightly broader range for the clustered material. The influence of the clustering manifests itself in a larger correlation length as reflected by the larger spread of the correlation function in Fig. 1 versus Fig. 2.

Conclusions

Three dimensional microstructures have traditionally been characterized by an analysis of two dimensional sections. These procedures have mostly focussed on a simulated reconstruction of the microstructure. The difficulties in these methods are due to the destructive nature of sectioning methods and the lack of *a priori* knowledge of the number and orientation of sections required to capture the characteristics of the microstructure.

When the microstructure is clearly delineated in a micrograph image, non-destructive CAT scan techniques can produce a three dimensional digitized image of the microstructure. The proposed moving window technique uses this digitized image to construct material property fields with a direct connection to the microstructure. The strength of this approach, i.e., material property fields, is two-fold. First, it eliminates the need to provide a detailed geometric description of the microstructure for example, shapes of the included phase. Statistical descriptions are then based on the composite constitutive behavior rather than geometry. The second advantage of the method is that simulations of the material can be performed based on the characteristics of the material property fields. Again, analysis of material response requires a constitutive law, in this case a stochastic field of properties, which is the direct result of the method.

The moving window technique has been extended to three dimensional digital images and is illustrated in this work through an application to a particulate reinforced composite. Although the windowing scheme contributes a smoothing effect to the material property fields, the generated fields are sufficiently sensitive to distinguish the differnce between a clustered and non-clustered microstructure.

Acknowledgements

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