PERGAMON

International Journal of Solids and Structures 38 (2001) 9209–9220

INTERNATIONAL JOURNAL OF SOLIDS and STRUCTURES

www.elsevier.com/locate/ijsolstr

Micromechanics based random material property fields for particulate reinforced composites

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Received 26 September 2000; in revised form 15 March 2001

Abstract

Particle reinforced metal matrix composites offer a number of advantages over continuously reinforced composites. They generally can be made using conventional metal-working processes and often fabricated to near net shape. Like continuously reinforced composites though, the potential exists to tailor these materials for higher specific stiffnesses, greater strength and improved fracture properties over their homogeneous counterparts. Their effective use requires an accurate characterization, which is made difficult by a three-dimensional (3D) random microstructure. A micromechanics based moving window technique, used to develop material property fields associated with the random 3D microstructure of a particulate reinforced composite, is described in this paper. The resulting sample material property fields are computationally tractable and have a direct link to the composite microstructure. The method can be used to generate material property fields for elastic or inelastic properties. Statistical and probabilistic descriptions of these property fields can subsequently be used to simulate the material and characterize the variability of the material response. The method is illustrated in this paper by generating fields for selected elastic moduli developed from a numerically simulated microstructure.

Keywords: Microstructure; Micromechanics modeling; Random composites; Particulate composites

1. Introduction

For many applications high cost and difficulty of fabrication limit the use of continuous fiber reinforced composites. These limitations, coupled with current research into functionally graded microstructures, have fostered a renewed interest in particulate reinforced composites. Short-fiber or particulate reinforced composites, like homogeneous materials, can be easily processed to near net shape. They have the potential to be designed for specific applications which require a higher specific stiffness, greater strength and/or improved fracture properties than the traditional homogeneous material.

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0020-7683/01/$ - see front matter
PII: S0020-7683(01)00076-2

Reliable design and use of these materials requires an accurate characterization. The traditional approach to characterization of composite materials has been to develop effective properties based on the constitutive properties of the phases, relative volume fractions and a generalization of the microstructure. For many engineering applications this is a valid assumption; when examining displacements, average stresses or average strains it can be assumed that small-scale fluctuations in material properties are averaged when evaluating macroscopic behavior. The advantage of an effective property is that it can be assumed valid for a large selection of material samples. The disadvantage of an effective property is that it smooths or averages local response.

Many critical damage phenomena in composite materials are linked to local stresses that can be associated with local variations in material properties due to variations in the composite microstructure. Additionally, variations in the microstructure and the resulting local material response, a function of the consistency of the fabrication process as well as the heterogeneous nature of the composite, must also be considered in any analysis of material reliability. This analysis of local behavior requires a method of characterizing material properties in terms of material microstructure. For particle reinforced composites this characterization can be made difficult by the inherent microstructural randomness.

While many issues in the modeling and characterization of the effects of randomness on the behavior of heterogeneous solid materials remain open, fundamental research does exist in the literature. There is a substantial body of work dealing with the establishment of bounds on the effective properties of random heterogeneous media, for example, Gibiansky and Torquato (1995), who developed bounds on effective properties based on geometrical parameters associated with the microstructure, and Roberts and Knackstedt (1996), who developed rigorous bounds of effective properties of model random fields based on statistical correlation functions. Criteria for the evaluation of stochastic methods for modeling the constitutive behavior of heterogeneous solids have been proposed by Frantziskonis (1998). Ostoja-Starzewski (1994), proposed micromechanics as the basis for the development of continuum random fields and the approximation of material properties at the meso-scale. Povirk (1995), showed that representative volume elements for periodic microstructures could be found that are statistically similar to more complex random microstructures and could be used efficiently in finite element models to predict effective elastic properties of the composite.

Researchers characterizing the microstructure of porous or cellular solids have made major contributions to investigations of local behavior. Much of their work has focused on reconstructing microstructure since transport phenomena in porous media depend on specific aspects of the microstructural geometry, e.g., the degree of interconnectedness. These characterizations are often based on digitized images of two-dimensional (2D) material sections (see Adler and Thovert, 1998; Roberts, 1997; Kwiecien et al., 1990; Quibler, 1983). Traditional stereological techniques (Underwood, 1981) and statistical analyses are employed in the characterization and reconstruction process. These methods provide a direct link to real microstructures but must often make assumptions, e.g., isotropy, to extend the 2D sectional analysis to three dimensions, and generalize specific features, i.e, shapes, of the microstructural geometry.

For composite materials another approach to investigating the effect and influence of microstructure is available. For composites the description and reconstruction of the microstructure is often of less interest than the characterization of the local material response that results from the microstructure. Thus, if the microstructure can be linked to material property fields, then characterization and simulations can be done of properties rather than the geometry and architecture of the microstructure. The focus of this work is the development of a link between 3D microstructures and material properties.

Using the generalized method of cells (GMC) micromechanics model, (Aboudi, 1989; Paley and Aboudi, 1992; Pindera and Bednarcyk, 1999) in conjunction with a moving window concept, a methodology known as moving window-GMC (MW-GMC) has been proposed by Baxter and Graham (2000). This procedure develops 2D material property fields from digitized descriptions of real microstructures, using a local micromechanical analysis. In this paper, the methodology is extended to three dimensions in order to predict, more accurately, material property fields due to 3D microstructures.

Digitized images are a powerful tool in providing records of material microstructure. For composite materials, commercial computer aided tomography (CAT) scans can distinguish differences in density on the order of 2%, and can produce a 3D array of pixels representing phases of the microstructure. While the use of this technology is limited by the availability of the equipment, the viability of large image files on many computer platforms coupled with the fact that the range of materials that can be distinguished is relatively broad, make it an excellent tool for the examination of materials whose microstructures require a 3D description (see for example Bart-Smith et al., 1998). Where a digital record of the microstructure is available, no a priori assumptions are required regarding the stochastic material properties associated with the random microstructure.

The moving window methodology produces material property fields from digitized images. The material property fields describe the spatially dependent constitutive behavior of the composite. The fields are suitable input for other computational models, such as finite element analysis, and a statistical analysis of these fields can be used to provide insight into the response of other similarly fabricated samples of the material through stochastic simulations (Graham and Baxter, 2001).

In what follows, details of the MW-GMC technique are presented. The extension of the moving window technique to three dimensions is illustrated by an application to a numerically generated 3D digital microstructure. Property fields and associated statistical descriptions for selected elastic properties of the sample are also generated. Results from the 3D windowing analysis are compared with those of a 2D windowing analysis.

2. Moving window micromechanics technique

If the phases of a composite are clearly delineated, i.e., if different phases can be distinquished on the basis of gray scale levels, then the composite microstructure can be recorded as a discrete 3D array. Using the gray scales, each pixel can then be associated with a phase of the composite and assigned the material properties of that phase. The total image size, $N_x \times N_y \times N_z$, is then defined in units of pixels. Each pixel, designated by i, j, k, where $i = 1, 2, \ldots, N_x$ and $j = 1, 2, \ldots, N_y$, $k = 1, 2, \ldots, N_z$, represents an integer coordinate in a 3D space field. Converting the digital image of the composite into numeric data based on the individual gray scale levels that are associated with each of the composite phases, results in coarse material property fields, in one-to-one correspondence with the image 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-value field is generated. The statistics on such fields are difficult to develop and there is no consistent methodology recommended in the literature for simulating such stochastic fields. Further, the cost of implementing these fields 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 remain constant throughout the analysis and are also specified in units of pixels. GMC is used to calculate the effective material properties for each window. The effective property of the window, as calculated by GMC, is then assigned the spatial coordinates of the center point of the window. For example, for the elastic modulus E_{yy}:

$$E_{yy}(i,j,k) = E_{yy}^{\mathrm{GMC}}(\mathbf{A}^{(ijk)}) \tag{1}$$

where $E_{yy}^{\mathrm{GMC}}(\mathbf{A}^{(ijk)})$ is the value of the elastic modulus E_{yy} calculated by GMC for the window, $\mathbf{A}^{(ijk)}$, centered at i, j, k with length l, width w and height h, defined by the dimensions of the window. As material properties are calculated for each window centered at i, j, k, for all values $i = 1, 2, \ldots, N_x$ and $j = 1, 2, \ldots, N_y$, $k = 1, 2, \ldots, N_z$, a 3D field for each material property is generated. The windows for adjacent grid points will overlap. Since grid points near the edges of the sample will not be surrounded by a full window these points were not included in the windowing analysis and the resulting material property field corresponds to a cropped microstructure. The moving window technique is analogous to the calculation of a moving average over a noisy signal; however the "averaging" is physically based on the detailed micromechanical analysis provided by the generalized method of cells micromechanics model.

Fig. 1 shows a schematic of the moving window procedure. The resulting property fields, while smoother than the original digitized input, still reflect the influence of local variations and correlated features of the microstructure. These fields are less noisy than the original digitized record, allowing a statistical and probabilistic analysis of the randomness of the property fields due to the random microstructure.

The micromechanics model chosen for this work is an extension of the original method of cells developed by Aboudi (1989) and can be used to predict the response of doubly or triply periodic microstructures. It uses a repeating unit cell, divided into rectangular subcells, to characterize the microstructure. Periodic boundary conditions are enforced on the unit cell and, under the assumption of perfect bonding, displacements are assumed continuous across subcell boundaries. The requirements for equilibrium are satisfied by also requiring continuity of tractions across these micro-level boundaries. The homogenization process in GMC then connects the material microstructure to an equivalent homogeneous material through a set of continuum level equations, which result from the continuity conditions, and effective properties are

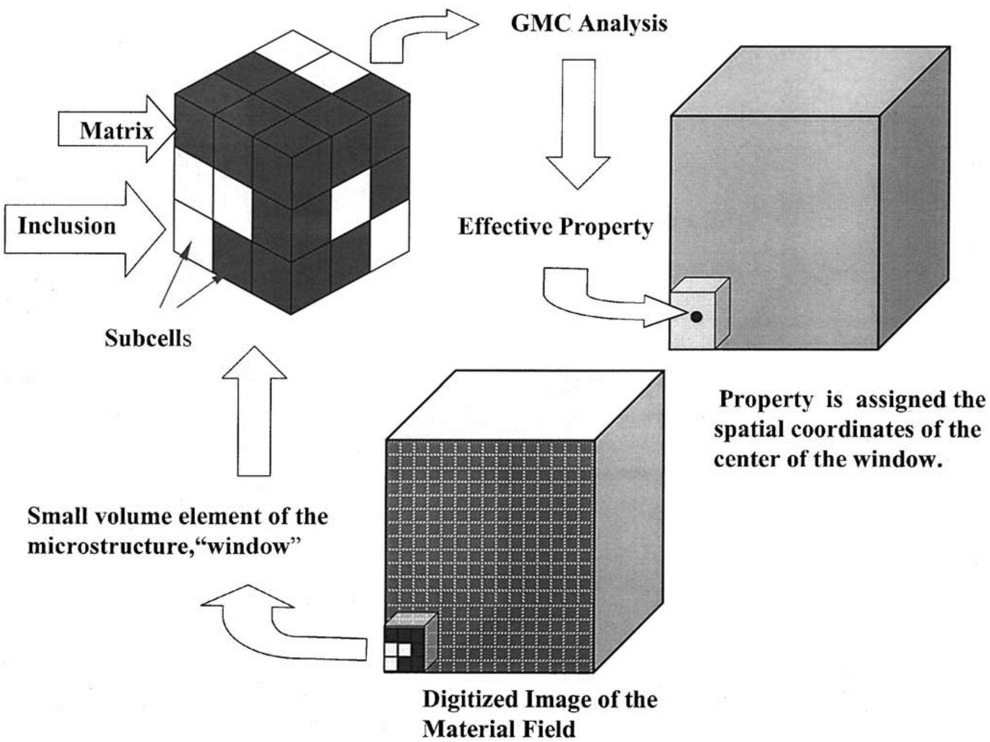

Fig. 1. Schematic of 3D moving window technique. (clockwise from bottom center) Small volumes of the sample, "windows" are selected. Each window serves as the repeating volume element for GMC, which is used to calculate the effective properties. Effective properties are assigned the spatial coordinates of the center of the window. Process is repeated for overlapping windows moving through the full array of the microstructure.

predicted in an average sense. GMC is capable of calculating effective elastic and shear moduli, Poisson's ratio, yield stress as well as hardening behavior, for the microstructure in each window, based on the known constitutive behavior of the individual phases.

The 2D formulation of GMC models fiber reinforced composites; a 3D version (Aboudi, 1995) models short fiber or particulate reinforced composites. GMC has been used to model the effective elastic and inelastic properties of continuously reinforced metal matrix composites, (Salzar et al., 1996), intermetallic matrix composites, (Baxter and Pindera, 1999), porous media, (Herakovich and Baxter, 1999; Aboudi, 1984), and functionally graded materials (Aboudi et al., 1996). A more efficient implementation of GMC, developed by Pindera and Bednarcyk (1999), has significantly reduced computation time for complex microstructures, and a more complete description of the method can be found in this article.

There are two immediate advantages to using GMC to calculate the effective properties in each window. First, because GMC uses a Cartesian geometry for its microstructural descriptions, the image array data of the digitized microstructure maps directly into the micromechanical analysis. Second, in finite element methods the material response depends specifically on the boundary condition imposed, either prescribed displacements or prescribed tractions, (Ostoja-Starzewski, 1994), making the resulting constitutive law non-unique. GMC circumvents the problem of boundary conditions through its assumption of periodicity. This undoubtedly contributes an additional level of smoothing to the property fields. Periodic boundary conditions can also be implemented using finite element methods, but additional requirements on the mesh size must be imposed in order to achieve convergence and will increase the computational time.

3. Sample material system

To illustrate the 3D moving window technique 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 in a 3D array of 200 planes, 200 rows and 200 columns, i.e., a $200 \times 200 \times 200$ grid. For the first cycle a 3D grid spaced random walk was initiated from each nucleation site. Three sequences of random numbers, with uniform distribution, were generated using a psuedo-random number generator code. Each sequence was mapped to the integer interval $(-5, 5)$ corresponding to steps along each of the three coordinate axes. Each resulting ordered triple, a cycle of the random walk, specified the placement of the next particle of the reinforcing phase in the array. Subsequent cycles were started from the final positions of the previous cycles. 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.

Sections of the simulated microstructure are shown in Fig. 2. They represent, from left to right, sections centrally located in the sample and orthogonal to the three coordinate axes. The white represents the particles of the reinforcing phase, the black is the surrounding matrix material. The phases of the composite were assigned the properties of a silicon carbide particle reinforced aluminum matrix. To illustrate the method, property fields for selected elastic moduli were generated. The method, however, can be used to develop material property fields for a complete set of elastic and inelastic properties. The constituent properties in the sample material were assumed deterministic and isotropic; the elastic modulus of aluminum was assumed to be 72.1 GPa and the elastic modulus of the silicon carbide particles, 431.0 GPa.

4. Property characterization

Material property fields were developed for the central plane, perpendicular to the z-axis, of the digital image of the microstructure shown in Fig. 2(a). The fields were developed using a window of dimension

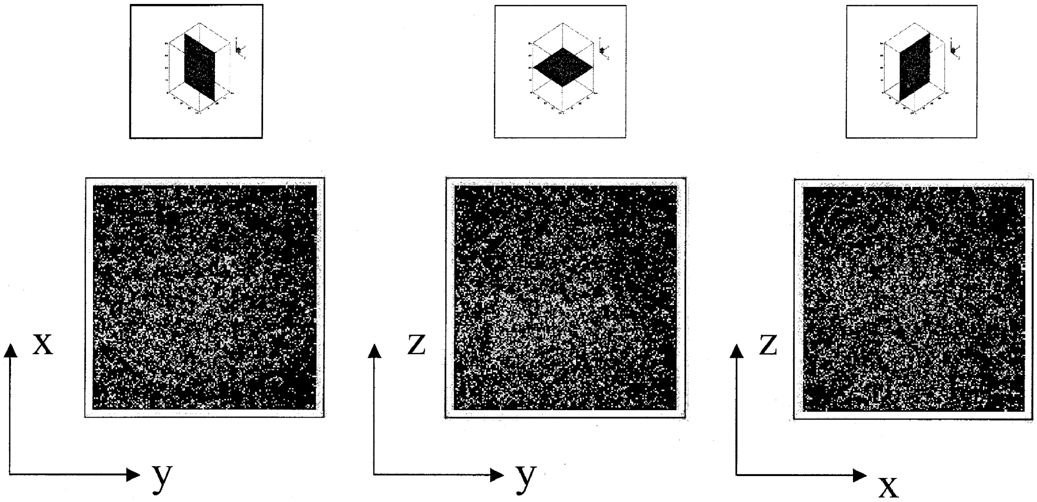

Fig. 2. Orthogonal cross-sections of the microstructure. Black is the aluminum matrix material, white represents the silicon carbide particles.

$(3 \times 3 \times 3)$ pixels. Fig. 3 shows (a) the 2D plane of material microstructure (b) the field of local volume fractions of the included phase and (c) and (d) corresponding property fields, for the elastic moduli, E_{xx} and E_{yy}, calculated using the 3D windowing procedure. For the microstructure, the white corresponds to the included particulate phase and the black to the matrix material. In the volume fraction and property fields, higher values of volume fraction and modulus are represented by darker shades.

To illustrate the influence of the 3D microstructure/micromechanics analysis on the calculation of local properties, Fig. 3(e)–(g) show the corresponding fields calculated using a 2D windowing scheme with (3×3) pixel windows. The mean volume fraction within the volume fraction field from the 2D analysis is 19.7%, with a minimum value 0% and a maximum of 100%. For the 3D volume fraction field the mean is approximately the same, 19.6%, but the range runs from a minimum of 0% to a maximum 88.9%. Table 1 lists the statistical characteristics associated with the material property fields shown in Fig. 3.

Both windowing schemes produce material property fields in which the minimum value of the modulus is 72.1 GPa (see Table 1). This corresponds to the modulus of the aluminum matrix, so for both schemes the window size is small enough to select window volumes which are pure matrix. The maximum values are higher in the fields generated using 2D windowing which is largely a confirmation of the expected higher probability of getting a window composed of pure particulate from a window with nine elements, (3×3), than from a window with 27 elements, $(3 \times 3 \times 3)$. This shows that the contribution of the out-of-plane microstructure has a significant influence on the predicted properties at a point. In addition to the reduced range of properties in the fields generated using the 3D windowing scheme, the material property fields have slightly lower means and smaller standard deviations when compared to the 2D windowed versions.

In both the 2D and 3D cases the two transverse moduli, E_{xx} and E_{yy}, are extremely well correlated with one another; 0.921 for 3D and 0.908 for 2D. Despite qualitatively different fields, the elastic moduli are also well correlated to their respective fields of volume fraction, $\mathrm{corr}(v.f., E_{xx}) = 0.91$ (2D) and $\mathrm{corr}(v.f., E_{xx}) = 0.92$ (3D). This is expected since areas with a high volume fraction of the stiffer particulate material should have correspondingly higher moduli, but the visual differences between the property fields and the field of local volume fractions (see Fig. 3(b) and (d)) illustrate the difference between the micro-

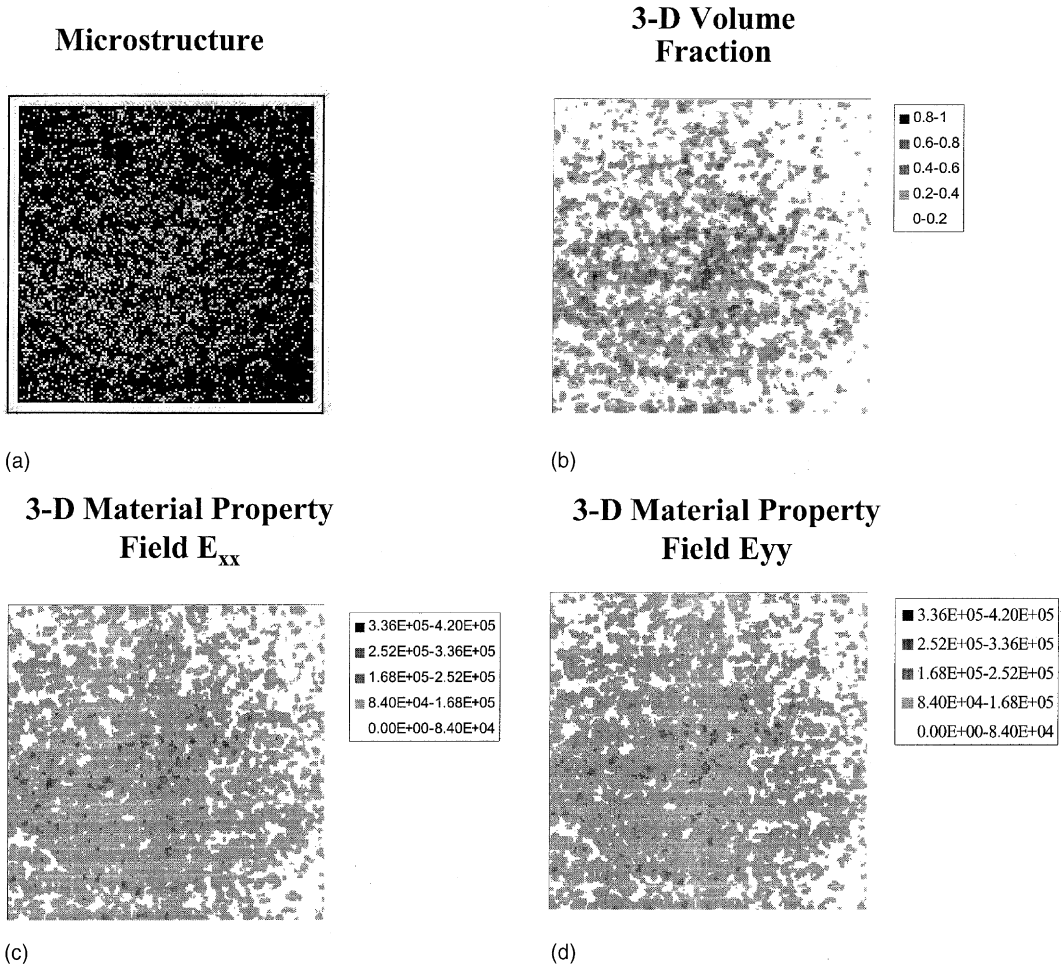

Fig. 3. Material property fields for elastic moduli generated using 3D ($3 \times 3 \times 3$), and 2D (3×3), windowing schemes: (a) microstructure, white particles, black matrix material; (b) field of local particulate volume fractions; (c) E_{xx} (d) E_{yy}, 3D windowing; (e) field of local particulate volume fractions; (f) E_{xx} (g) E_{yy}, 2D windowing. Darker colors denote higher volume fractions and moduli.

mechanical analysis and composite models which follow a rule-of-mixture formulation and mimic the trends in the volume fraction field. There is less correlation between the two schemes for the same modulus, i.e., the degree of correlation between E_{xx} (2D) and E_{xx} (3D) is 0.73 and that between E_{yy} (2D) and E_{yy} (3D), is 0.74. This indicates a significant change in the statistics of the generated fields due to the windowing scheme.

As a further illustration of the differences between the 2D and 3D material property fields for the sample material system histograms are given, in Fig. 4, corresponding to the elastic moduli E_{xx} and E_{yy} under both the 2D and 3D windowing schemes. These histograms show very similar frequency distributions between the two moduli, for each of the 2D and 3D results. However, the histograms resulting from the 2D windowing scheme indicate a much higher percentage of the values in the smallest range than those resulting from the 3D windowing scheme ($\approx$68% vs. 60%).

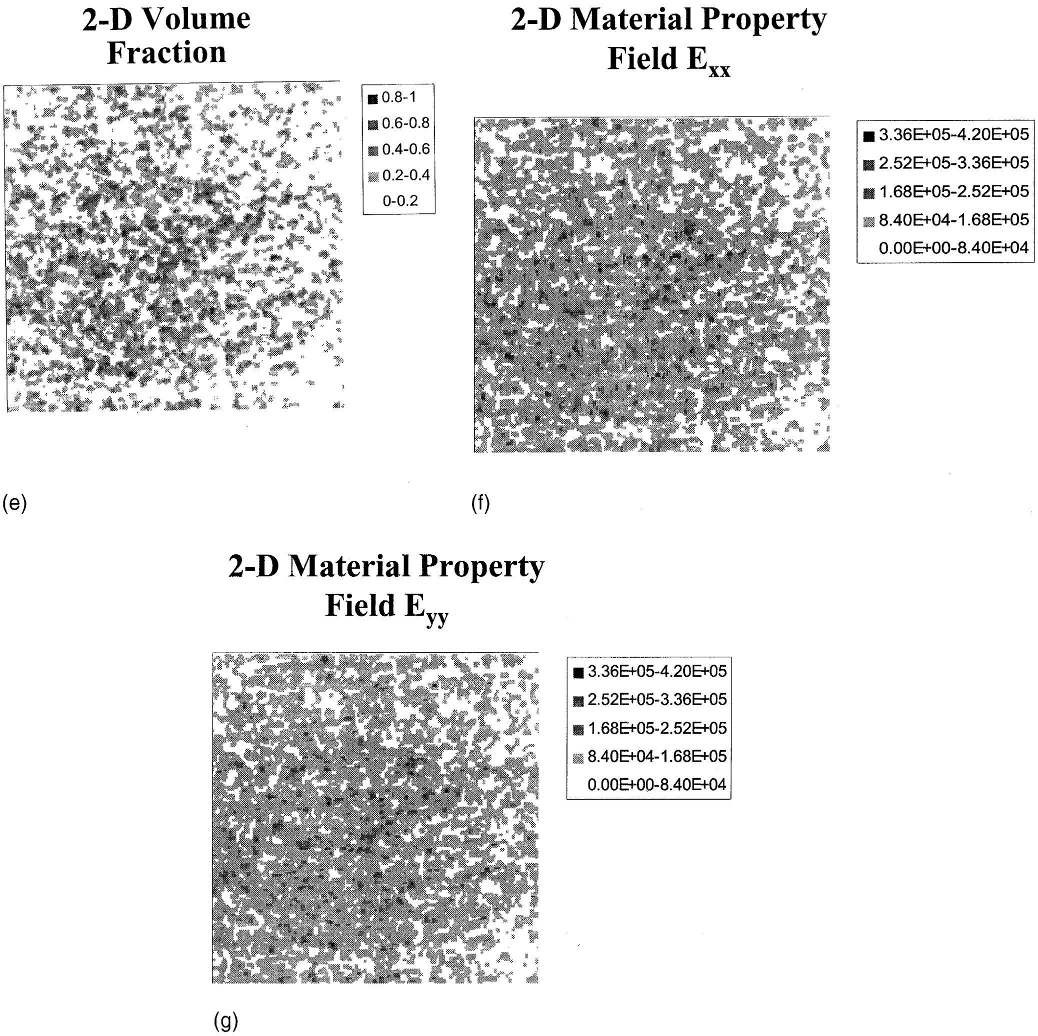

Fig. 3 (*continued*)

Table 1
Statistical characteristics of the 2D and 3D material property fields shown in Fig. 3

Parameter	Elastic moduli			
	2D windowing		3D windowing	
	E_{xx}	E_{yy}	E_{xx}	E_{yy}
Minimum (GPa)	72.1	72.1	72.1	72.1
Maximum (GPa)	431.0	431.0	348.1	348.1
Mean (GPa)	103.0	102.7	98.9	98.6
Range (GPa)	358.9	358.9	276.0	276.0
COV	0.36	0.36	0.26	0.26

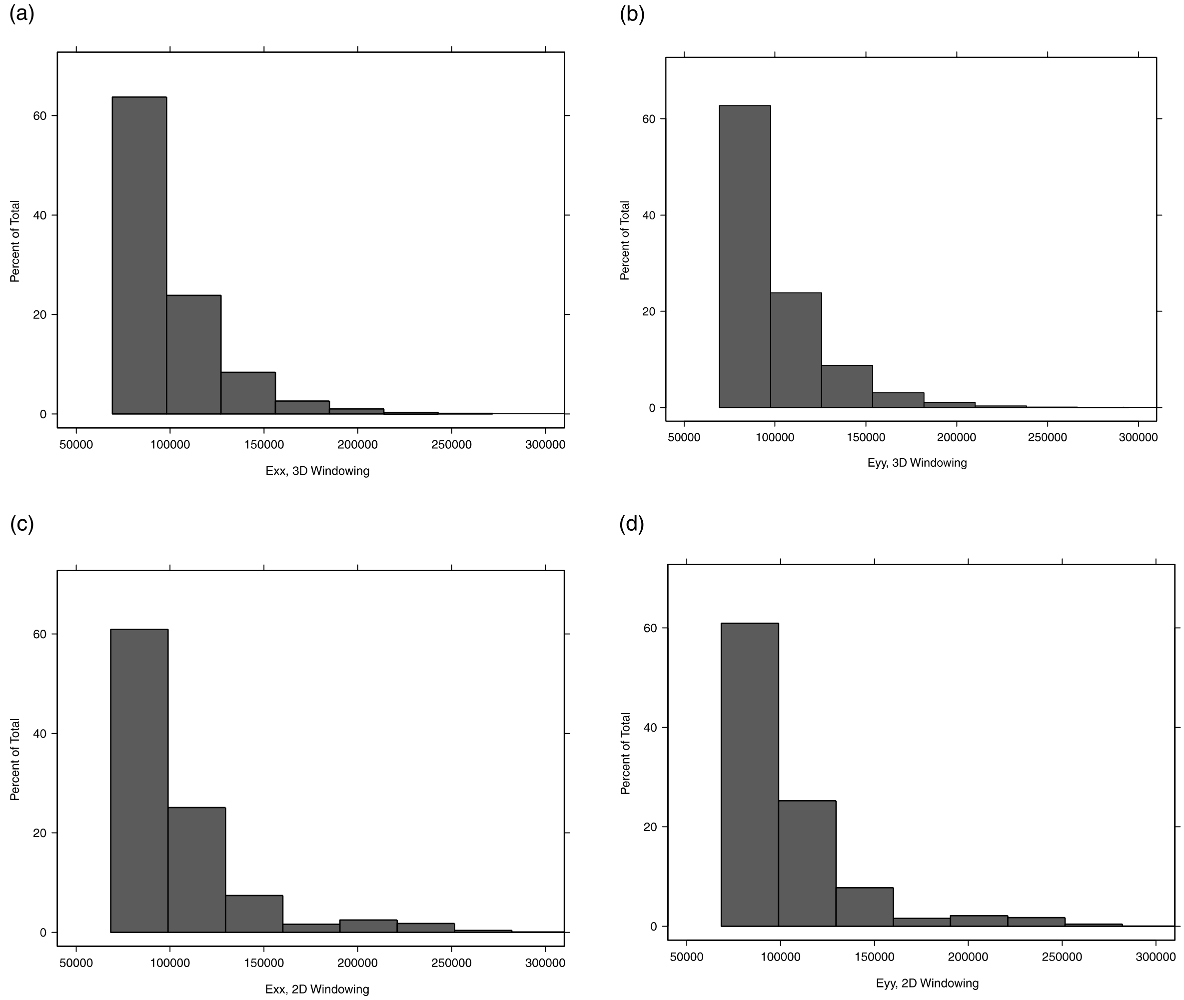

Fig. 4. Histograms calculated from fields shown in Fig. 3: (a) E_{xx} (b) E_{yy}, 3D windowing, (c) E_{xx} (d) E_{yy}, 2D windowing.

5. Effect of window size

Property fields and their statistics are not only affected by the choice of 2D or 3D windowing but will also depend significantly on window size. Table 2 compares the statistics for the E_{xx} field generated using 3D windowing for three window sizes $(2 \times 2 \times 2)$, $(3 \times 3 \times 3)$, $(5 \times 5 \times 5)$ and $(7 \times 7 \times 7)$ pixels. It is clear that in each case as the window dimension increases, the field becomes smoother in that the mean value, the coefficient of variation (COV) and the range of values for each modulus decreases.

Fig. 5 shows histograms based on the material property fields developed using each of the window sizes. Each set of data was modeled using approximately the same number of histogram classes (bars), to compare the shape of the distribution relatively independent of the decrease in the range. The effect of increasing the window size is a smoother and more symmetric histogram.

A strength of the MW-GMC method is that the level of smoothing, corresponding to the size of the window, is adjustable. This will allow the method to adapt to different levels of magnification/resolution in

Table 2
Statistical characteristics of property fields generated using different size windows

Window size parameter	Elastic modulus E_{yy}			
	$(2 \times 2 \times 2)$	$(3 \times 3 \times 3)$	$(5 \times 5 \times 5)$	$(7 \times 7 \times 7)$
Minimum (GPa)	72.1	72.1	72.1	72.1
Maximum (GPa)	431.0	348.1	189.8	149.8
Mean (GPa)	108.0	98.9	92.6	90.7
COV	0.44	0.26	0.15	0.11

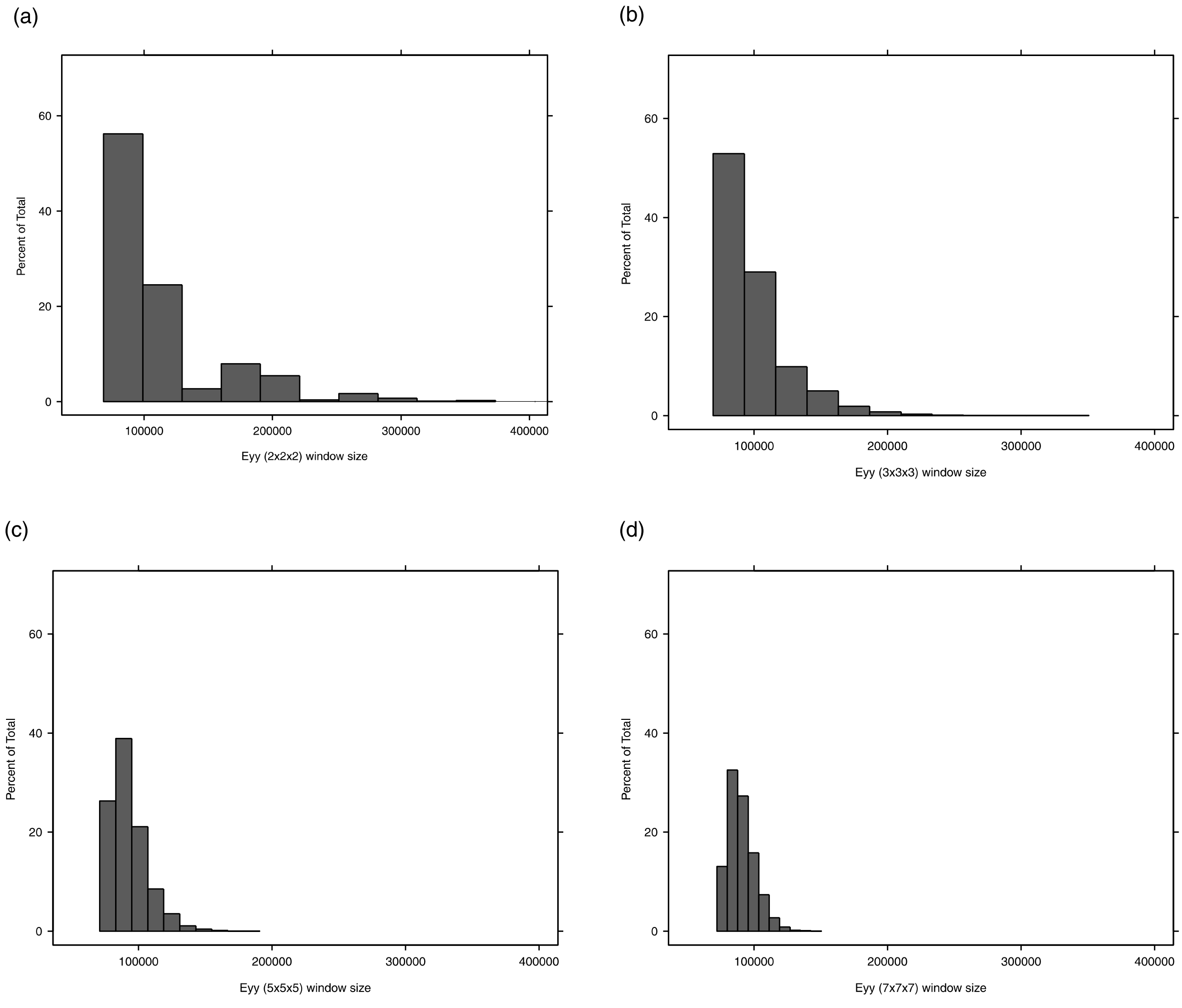

Fig. 5. (a) Histogram calculated from property fields developed from 3D windowing based on window sizes of (a) $(2 \times 2 \times 2)$ (b) $(3 \times 3 \times 3)$ (c) $(5 \times 5 \times 5)$ and (d) $(7 \times 7 \times 7)$. Horizontal axis plots the value of the modulus, vertical axis plots the percent of the total.

the image as well as relative sizes of the inclusions. Small windows share the drawbacks of the original digitized field, they are noisy and computationally difficult. Larger window sizes will lead to more "smoothing" of the properties and smaller values for the variance. If the window size becomes too large, then the material property variability approaches zero and the properties approach the effective properties of an equivalent homogeneous medium. The choice of a window size must be made carefully, in order to develop consistent models based on different images of the same material and to avoid these extremes.

In this work, the approximate size of the inclusion was used to define the window size. For the current material system the inclusions were of dimension $(1 \times 1 \times 1)$ pixels, however the effect of the random walk generation of the microstructure was to produce clustering of the included phase. This may have resulted in an average effective size larger than the individual pixels. To estimate this effective cluster size, the range of the material property fields was used. Using a window size of $(2 \times 2 \times 2)$ the maximum value of the modulus observed in the fields was 431.0 GPa, the modulus of the silicon carbide particles, indicating the presence of windows that were composed only of the particle phase. The next larger window size, $(3 \times 3 \times 3)$, showed a decrease in the maximum modulus value to 348.1 GPa, i.e. no windows of pure particulate. This suggested that the effective size of the particles (or clusters) was between the two window sizes. Since the larger windowing field produces a less noisy field, the $(3 \times 3 \times 3)$ window was used for the purpose of illustration in this paper.

6. Conclusions

The MW-GMC methodology can be extended to an analysis using 3D windows resulting in a descriptive characterization, in the form of material property fields, that is directly linked to the material microstructure. The method is computationally efficient and requires no a priori assumptions about the random distribution of microstructure or details of microstructural geometry to characterize local material properties.

By using 3D windows, the resulting material property fields reflect the influence of neighboring microstructure both in and out of the plane of a specific spatial position. For a particulate reinforced composite this may represent a more consistent characterization of local material properties. In particular, a comparison of fields produced using 2D and 3D windowing show more smoothing using the 3D scheme, in particular a smaller range of values of the modulus and a slightly lower mean value.

The size of the window also has a significant effect on the moving window characterization. Criteria for window size should be able to be applied independent of the resolution/magnification of material micrographs.

The material property fields produced using MW-GMC are suitable for application in a stochastic finite element sense. Because these fields are substantially less noisy than the original digitized image, statistical measurements can be used to characterize the fields for use in simulations of the material and additional analysis of material behavior.

Acknowledgements

This work was supported by the National Science Foundation under Grant # CE-NSF-7899-98, with Dr. Sunil Saigal as Program Director

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