

*Journal of*  
***Mechanics of***  
***Materials and Structures***

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TWO-PHASE COMPOSITES USING TWO-POINT STATISTICAL  
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***Volume 3, N° 1***

***January 2008***



mathematical sciences publishers

# HOMOGENIZATION RELATIONS FOR ELASTIC PROPERTIES OF TWO-PHASE COMPOSITES USING TWO-POINT STATISTICAL FUNCTIONS

GHAZAL SAHELI, HAMID GARMESTANI AND ARUN GOKHALE

In this research we focus on studying the effect of anisotropy on the homogenization technique based on two-point statistics. We will investigate how the one-point and two-point statistical information from the microstructure can contribute in the calculation of elastic properties of isotropic and anisotropic composites. For this purpose, the homogenization relations will be studied in detail and the technique will be applied to two samples of anisotropic Al-SiC composite that were fabricated through extrusion with two different particle size ratios (PSR). The results show that two-point statistics is capable of capturing the effect of clustering of SiC particles in evaluating elastic properties for anisotropic composites. Although the two samples have the same volume fraction (difference less than 1%), the calculated elastic constants for both samples are different. The validity of the results will be investigated by direct comparison with experimental results.

## 1. Introduction

Materials science always looks for establishing a relationship between the internal structures of materials and their properties. In polycrystals, internal structure refers to the size and shape of crystallites (grains), the distribution of their crystallographic orientations (texture), and the spatial correlations between these geometrical and crystallographic features. However, in composites, internal structure refers to spatial correlations between geometrical features of the two phases.

The prediction of mechanical properties from details of the microstructure such as phase, crystalline grain orientation distribution, and microstructural morphology has received a special attention in the mechanics and materials community [Torquato and Stell 1982; Adams et al. 1987]. The mathematical description of heterogeneity has received some breakthroughs in the last few decades with the works [Beran 1968; Kröner 1972; 1977]. More progress has been achieved in calculating the effective properties by making simple assumptions about the microstructure distribution (random, isotropic, and periodic microstructures) or the shape of the second phase (spherical, ellipsoidal, etc.). These studies have relied primarily on the one-point probability functions (number or volume fractions of individual states within the microstructure), which ignored shape and geometric characteristics of the microstructure. It was realized that in order to use the measured materials' heterogeneity it is necessary to incorporate two and higher order probability functions. Progress was hindered due to lack of experimental techniques to obtain two and three-point correlation functions. These techniques are now available, which makes

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*Keywords:* statistical mechanics, microstructure, elastic moduli, composite.

This work has been funded under the AFOSR grant # F49620-03-1-0011 and Army Research Lab contracts # DAAD17-02-P-0398 and DAAD 19-01-1-0742. AMG gratefully acknowledges financial support of the grant from the Air Force Office of Scientific Research (AFOSR grant number 04-NA-152).

it possible to measure individual crystalline orientation in polycrystalline materials. Extension of this effort to nonrandom microstructures requires proper definition of  $n$ -th degree statistical correlation functions. For a detailed description of the theoretical discussion and the derivations please refer to [Adams et al. 1987; 1989; Beran et al. 1996; Garmestani et al. 1998b; 2001; Garmestani and Lin 2000; Saheli et al. 2004]. A statistical continuum mechanics approach for both elastic and inelastic deformation of composites was introduced earlier [Garmestani et al. 1998b; 1998a; 2001; Garmestani and Lin 2000]. In this research, the elastic formulation for the isotropic distribution will be extended to include anisotropy.

In this work a microstructure will be represented by a set of two-point correlation functions for a variety of states. In a polycrystalline material, each orientation is considered a different state and an  $n$ -dimensional space is then formulated for the homogenization relation [Garmestani et al. 2001; Adams et al. 2002]. However, a two-phase composite that consists of only two phases and the  $n$ -dimensional space is reduced to a two-dimensional state, assuming that the anisotropy within each phase is ignored. It is clear that such a construction that uses volume fraction of the second phase can only present a limited description of the composite. In this paper, two-point correlation functions are used as additional parameters for the description of a composite. Two-point statistics can incorporate not only the distribution and interaction of the two phases but also information on the shape and morphology of each individual phase.

The orientation distribution function (ODF) is a one-point statistical distribution function that only considers volume fractions (or number fractions) of crystallites with the same orientation. Two-point statistical functions can be used as a first order correction to the average (volume fraction) representation. Two-point correlation functions [Torquato and Stell 1982; Adams et al. 1987; Garmestani et al. 1998b; 1998a; 2001; Garmestani and Lin 2000; Lin et al. 2000] provide information about near neighbor and far field effects and allow the defect sensitive properties to be incorporated in the analysis. The composite formulation will be markedly enhanced by the use of empirical or spectral form of the two-point correlations [Corson 1974a; 1974b; Torquato and Stell 1982; Garmestani et al. 1998b; 2001].

Recent improvements in electron microscopy and image analysis have led to new techniques for analyzing the structure of polycrystalline materials at the scale of the crystalline grains. Orientation imaging microscopy (OIM) provides information on the spatial arrangement of lattice orientations in polycrystalline structures and is based on Kikuchi diffractometry [Garmestani et al. 1998a]. Measurements of the local orientation and misorientation of polycrystalline materials are now possible. However, for the composite, if the orientation of each phase is ignored, the correlation functions can be measured using imaging techniques (optical, SEM, etc.). The use of OIM for the measurement of orientation for a multiphase composite can introduce a large amount of detail and complexity. Higher order statistical formulations will be needed to incorporate such information for each phase as well as the interaction of the two phases.

For two-phase composite structures, the application of two-point statistics requires two different sets of probability functions. The first set can be chosen to describe the probability distribution functions for the interaction of the two phases. This reduces the problem to a composite formulation ignoring the crystalline phase for each component. The two phases can then be taken as isotropic (or anisotropic) phases, and the effect of texture can be incorporated in the anisotropy parameters in the constitutive relations. The second set can consist of the probability distribution functions for the individual crystalline phases. This means incorporating the effect of orientation for each phase.

## 2. Two-point distribution functions

The statistical details of a microstructure can be represented by an  $n$ -point probability distribution function. Volume fraction  $v_i$  is a one-point probability distribution function that is usually used to give an estimate of the effective properties. The details of the shape and morphology of the microstructure, including the interaction of the second phase in the composite and orientation distribution of crystallographic grains (texture), can only be realized by using higher order distribution functions [Corson 1974a; 1974b; Torquato and Stell 1982; Mason and Adams 1999]. A two-point distribution function can be defined as a conditional probability function when the statistics of a three-dimensional vector  $r$  is investigated once attached to each set of random points in a particular microstructure (One-point and two-point statistics functions are defined in Appendix A).

The exponential form of the distribution function, as proposed by [Corson 1974a; 1974b], has been shown to be appropriate for random microstructures. It is represented as

$$P_{ij}(r) = \alpha_{ij} + \beta_{ij} \exp(-c_{ij} r^{n_{ij}}), \quad (1)$$

where  $\alpha_{ij}$  and  $\beta_{ij}$  are components including volume fraction of phases. For a polycrystalline microstructure,  $i$  and  $j$  can vary from 1 to  $M$ .  $M$  is the total number of grains (or states); for a two-phase composite  $i$  and  $j$  correspond to phases 1 and 2. This reduces the number of two-point functions to four,  $P_{11}(r)$ ,  $P_{12}(r)$ ,  $P_{21}(r)$ , and  $P_{22}(r)$ , in the case of two-phase composites where normality relations require that only  $P_{11}$  be treated as an independent variable. The values of  $\alpha_{ij}$  and  $\beta_{ij}$  are summarized for a two-phase composite in Table 1.

In this equation  $r$  can generally be a vector which has been thrown in the microstructure to measure two-point probability functions. The other constants  $c_{ij}$  and  $n_{ij}$  are also microstructure parameters:  $n_{ij} = 1$  [Tewari et al. 2004], and  $c_{ij}$  is a scaling parameter representing the correlation distance. These empirical coefficients can be reformulated into an anisotropic form [Saheli et al. 2004],

$$c_{ij}(\theta, A) = c_{ij}^0 (1 + (1 - A) \sin \phi), \quad (2)$$

where  $A$  is a material parameter that represents the degree of anisotropy in a microstructure, such that  $A = 1$  corresponds to an isotropic microstructure and  $c_{ij}^0$  is the reference empirical coefficient.  $\phi$  represents the angle of the vectors thrown in the microstructures to measure two-point probabilities in different directions. The present form of Equation (1) is sufficient for a two-phase composite when the statistical information is uniform in all directions. However, a three-dimensional form of the distribution can also be introduced when the microstructure includes anisotropy. This requires data from a variety of sections through the sample.

	$i = 1; j = 1$	$i = 1; j = 2$	$i = 2; j = 1$	$i = 2; j = 2$
$\alpha_{ij}$	$v_1 v_1$	$v_1 v_2$	$v_2 v_1$	$v_2 v_2$
$\beta_{ij}$	$v_1 v_2$	$-v_1 v_2$	$-v_2 v_1$	$v_1 v_2$

**Table 1.** The empirical coefficients in Corson's equation for a two-phase composite.

An alternative form of the probability function was suggested in [Torquato 2002] for random and homogeneous systems of impenetrable spheres:

$$\begin{aligned} P_{11} &= 1 - \rho V(r) + \rho^2 M(r), \\ P_{12} &= P_{21} = v_1 - P_{11}, \\ P_{22} &= v_2 - v_1 + P_{11}, \end{aligned} \quad (3)$$

where  $\rho$  is the number density of spheres,  $v_1$  and  $v_2$  are the volume fractions of phases,  $r$  is the distance between two points, and  $V(r)$  and  $M(r)$  are functions of  $r$  as defined in Appendix B.

In Figure 1 Corson's equation and the Torquato equation are compared to real data of two-point statistics for a random microstructure.

### 3. Homogenization relations for elastic properties of composites

In the following section, the full homogenization relations for an elastic medium are reviewed for a representative volume element. The equilibrium equation is defined by

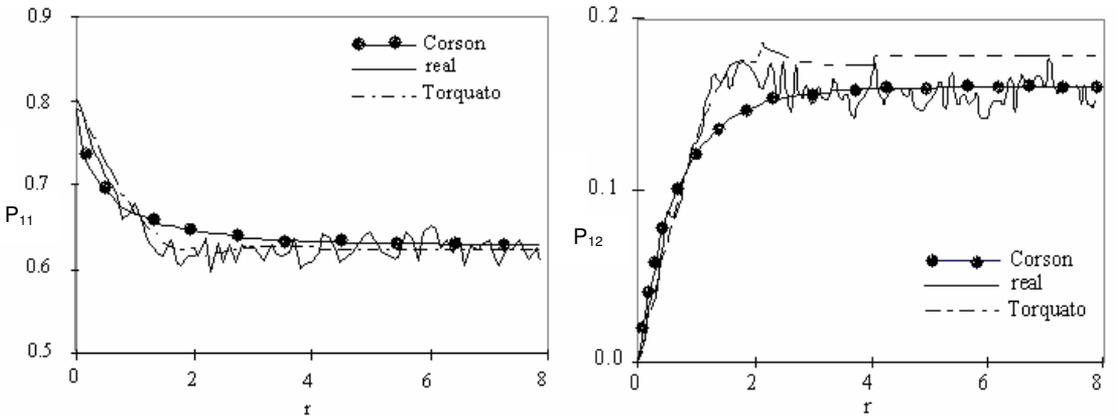
$$\sigma_{ij,j} = 0, \quad (4)$$

where  $\sigma_{ij}(x)$  is the local stress field. The elastic constitutive relations are satisfied locally throughout the heterogeneous medium as

$$\sigma_{ij}(x) = c_{ijkl}(x)\varepsilon_{kl}(x); \quad (5)$$

$c_{ijkl}(x)$ ,  $\sigma_{ij}(x)$ , and  $\varepsilon_{ij}(x)$  are local values of stiffness, stress and strain respectively. Let us define an effective elastic modulus  $C_{ijkl}$  such that [Beran et al. 1996; Garmestani and Lin 2000],

$$\langle \sigma_{ij} \rangle = C_{ijkl} \langle \varepsilon_{kl} \rangle. \quad (6)$$



**Figure 1.** Comparison of different models for two-point probability functions for a two-phase composite with random distribution of the second phase. Note that  $c_{ij}$  and  $n_{ij}$  are fitted to the measured (real) data in Corson's equation.

Symbol  $\langle h \rangle$  denotes the ensemble average over grains (phases, components, etc.) at state  $h$ . Assuming ergodic hypothesis, the average of the local stiffness  $\langle c_{ijkl} \rangle$  is defined as [Kröner 1972]

$$\langle c_{ijkl} \rangle = \langle c_{ijkl}(x) \rangle = \frac{1}{V} \int_V c_{ijkl}(x) dV. \quad (7)$$

The same definition is applicable for stress, strain and compliance. The local moduli and compliance, as well as the local stress and strain, can be defined as a perturbation from the average values  $\langle \dots \rangle$  by defining a new parameter ( $\tilde{\dots}$ ) as in [Beran et al. 1996; Garmestani and Lin 2000]

$$\begin{aligned} c_{ijkl}(x) &= \langle c_{ijkl} \rangle + \tilde{c}_{ijkl}(x), \\ s_{ijkl}(x) &= \langle s_{ijkl} \rangle + \tilde{s}_{ijkl}(x), \end{aligned} \quad (8)$$

$$\begin{aligned} \sigma_{ij}(x) &= \langle \sigma_{ij} \rangle + \tilde{\sigma}_{ij}(x), \\ \varepsilon_{ij}(x) &= \langle \varepsilon_{ij} \rangle + \tilde{\varepsilon}_{ij}(x), \end{aligned} \quad (9)$$

where  $\tilde{c}_{ijkl}(x)$ ,  $\tilde{s}_{ijkl}(x)$ ,  $\tilde{\sigma}_{ij}(x)$ , and  $\tilde{\varepsilon}_{ij}(x)$  are, respectively, the deviation from the mean value at each point of stiffness, compliance, stress and strain. Therefore, the following are satisfied:

$$\begin{aligned} \langle \tilde{c}_{ijkl}(x) \rangle &= 0, & \langle \tilde{s}_{ijkl}(x) \rangle &= 0, \\ \langle \tilde{\sigma}_{ij}(x) \rangle &= 0, & \langle \tilde{\varepsilon}_{ij}(x) \rangle &= 0. \end{aligned} \quad (10)$$

In the following, statistical continuum mechanics analysis is applied to a two-phase composite for the prediction of elastic properties. A theoretical framework has already been developed for isotropic distributions in composites, by [Garmestani et al. 1998b; Garmestani and Lin 2000], and for a textured polycrystalline material, by [Beran et al. 1996]. Here, a brief discussion is provided for the calculation of the effective elastic constants for isotropic distribution and will be extended to anisotropic distributions in later sections.

Substituting local moduli (Equation (9)) in the equilibrium equations (Equation (4)) and rewriting the equation as a function of displacement, the following equations will be obtained:

$$\langle c_{ijkm} \rangle \frac{\partial^2 \tilde{u}_k}{\partial x_j \partial x_m} + \frac{\partial}{\partial x_j} [\tilde{c}_{ijkm}(x) \varepsilon_{km}(x)] = 0. \quad (11)$$

The solution for this PDE can be written as an integral equation using the Green's function, defined by the PDE

$$\langle c_{ijkm} \rangle \frac{\partial^2 G_{kp}(x, x')}{\partial x_j \partial x_m} + \delta_{ip} \delta(x - x') = 0, \quad (12)$$

where  $\delta(x - x')$  is the Dirac's delta function for the vector relating any two points in the microstructure, and the term  $\delta_{ip} \delta(x - x')$  represents the  $i$ -th component of a unit force acting parallel to the direction  $p$  for a fixed point,  $p$  [Kröner et al. 1987; Willis 1965]. Green's function in the case of isotropy can be defined by a closed form, and for the case of anisotropy has to be calculated numerically. The details of the calculations of Green's functions for both cases are presented in Appendix C [Bacon et al. 1980; Mason and Adams 1999]. Substituting the values of local stress and strain in Equation (5), after some

manipulation, the effective elastic constants (in Equation (6)) can be calculated as (for details see paper by [Garmestani and Lin 2000])

$$C_{ijkl} = \langle c_{ijkl} \rangle + \langle \tilde{c}_{ijmn}(x) a_{mnkl}(x) \rangle, \quad (13)$$

where  $a_{mnkl}$  is a matrix defined to show the heterogeneity in the strain field as [Garmestani and Lin 2000, Equation (4)]

$$\tilde{\varepsilon}_{kl} = a_{mnkl} \langle \varepsilon_{kl} \rangle. \quad (14)$$

By substituting local stress from Equation (5) into the equilibrium Equation (4) an equation for displacement is obtained. Differentiating this equation and multiplying the result by  $c_{ijkl}$ , the second term in Equation (13) can be derived as [Saheli 2006], (details in Appendix D)

$$\begin{aligned} \langle \tilde{c}_{ijku}(x) a_{kurs}(x) \rangle = & \int_V \frac{\partial [K_{kpu}(x, x') \langle \tilde{c}_{ijku}(x) \tilde{c}_{pmrs}(x') \rangle]}{\partial x'_m dX'} \\ & - \int_V K_{kpum}(x, x') \langle \tilde{c}_{ijku}(x) \tilde{c}_{pmrs}(x') \rangle dX', \quad (15) \end{aligned}$$

where  $x$  and  $x'$  are two different positions in the media,  $dX'$  is the volume integral on the volume element around position  $x'$ , and  $K_{kpu}$  and  $K_{kpum}$  are calculated through

$$\begin{aligned} K_{kpu} &= \frac{(G_{kp,u} + G_{up,k})}{2}, \\ K_{kpum} &= \frac{(G_{kp,um} + G_{up,km})}{2}. \end{aligned} \quad (16)$$

$G_{kp,u}$  and  $G_{up,km}$  are, respectively, the first and the second derivative of the Green's function that solves Equation (12).

The two-point correlation function is defined through the equation

$$\langle \tilde{c}_{ijku}(x) \tilde{c}_{pmrs}(x') \rangle = \iint \tilde{c}_{ijku}(x) \tilde{c}_{pmrs}(x') P_2(x|h, x'|h') dh dh', \quad (17)$$

where  $P_2$  is a correlation function for two states of  $h$  and  $h'$ , and is defined in Appendix A. Equation (17) can be derived for composites by the relationship

$$\langle \tilde{c}_{ijku}(x) \tilde{c}_{pmrs}(x') \rangle = \tilde{c}_{ijku}^1 \tilde{c}_{pmrs}^1 P_{11} + \tilde{c}_{ijku}^1 \tilde{c}_{pmrs}^2 P_{12} + \tilde{c}_{ijku}^2 \tilde{c}_{pmrs}^1 P_{21} + \tilde{c}_{ijku}^2 \tilde{c}_{pmrs}^2 P_{22}, \quad (18)$$

where  $c^1, c^2$  are the local elastic moduli for the two individual phases.

#### 4. Analytical procedure

It was shown earlier that the effective modulus  $C$  can be calculated through Equation (13), which includes the correlation term (Equation (15)). This term will be analyzed analytically in this section to observe the effect of one-point and two-point statistics. This term is composed of two parts, or

$$\langle \tilde{c}_{ijku}(x) a_{kurs}(x) \rangle = I_{ijrs}^1 + I_{ijrs}^2, \quad (19)$$

where the first term is

$$I_{ijrs}^1 = \int_V \frac{\partial [K_{kpu}(x, x') \langle \tilde{c}_{ijk}(x) \tilde{c}_{pmrs}(x') \rangle]}{\partial x'_m dX'} \quad (20)$$

and can be converted to a surface integral by applying Gauss' theorem (for additional information see [mathworld.wolfram.com/DivergenceTheorem.html](http://mathworld.wolfram.com/DivergenceTheorem.html)). Gauss' theorem converts the volume integral in a sphere with infinite radius to a surface integral with the boundary of this sphere. The resulting surface integral requires evaluation on a surface at infinity and on a surface enclosing the singularity of  $K_{kpu}$  at  $x = 0$ .

Choosing both surfaces as spheres and applying Gauss' theorem, the following integral is obtained:

$$I_{ijrs}^1 = \left( \int_{x-x' \rightarrow 0} \langle \tilde{c}_{ijkl}(x) \tilde{c}_{pmrs}(x') \rangle K_{kpu} d\hat{A}_m \right) + \left( \int_{x-x' \rightarrow \infty} \langle \tilde{c}_{ijkl}(x) \tilde{c}_{pmrs}(x') \rangle K_{kpu} d\hat{A}_m \right) \quad (21)$$

To calculate the two surface integrals, the correlation term shown by  $\langle \tilde{c}_{ijk}(x) \tilde{c}_{pmrs}(x') \rangle$  has to be evaluated when  $x - x' \rightarrow 0$  and  $x - x' \rightarrow \infty$ . When  $x - x' \rightarrow 0$ , then the correlation will be a constant and independent of  $x$ , and when  $x - x' \rightarrow \infty$  there will be no correlation between two points. This can be proven for the case of a two-phase composite using [Equation \(18\)](#)

$$\begin{aligned} x - x' \rightarrow 0 &\implies \begin{cases} P_{11} \rightarrow v_1 \\ P_{12} \rightarrow 0 \\ P_{22} \rightarrow v_2 \end{cases} \implies \langle \tilde{c}_{ijk}(x) \tilde{c}_{pmrs}(x') \rangle \rightarrow \text{constant}, \\ x - x' \rightarrow \infty &\implies \begin{cases} P_{11} \rightarrow v_1^2 \\ P_{12} \rightarrow v_1 v_2 \\ P_{22} \rightarrow v_2^2 \end{cases} \implies \langle \tilde{c}_{ijk}(x) \tilde{c}_{pmrs}(x') \rangle \rightarrow 0. \end{aligned} \quad (22)$$

Therefore the second term in [Equation \(21\)](#) will be equal to zero, and the components of the first integral,  $I_{ijrs}^1$ , can be calculated by

$$I_{ijrs}^1 = (\tilde{c}_{ijk}^1 \tilde{c}_{pmrs}^1 v_1 + \tilde{c}_{ijk}^2 \tilde{c}_{pmrs}^2 v_2) K c_{kpum}, \quad (23)$$

where

$$K c_{kpum} = \int K_{kpu} d\hat{A}_m, \quad (24)$$

and is evaluated as

$$\begin{aligned} K c_{iiii} &= -\frac{(16/15\bar{K})}{8\bar{\mu}}, \\ K c_{ijij} &= K c_{jiji} = \frac{(4/3 - 4/5\bar{K})}{8\bar{\mu}}, \\ K c_{ijji} &= K c_{jiii} = K c_{iijj} = K c_{jjii} = -\frac{(2/3 + 2/15\bar{K})}{8\bar{\mu}}, \end{aligned} \quad (25)$$

where  $\bar{K}$  is the average property of two phases

$$\bar{K} = \frac{\bar{\lambda} + \bar{\mu}}{\bar{\lambda} + 2\bar{\mu}}. \quad (26)$$

Note that  $i$  and  $j$  can vary from 1 to 3, but there is no summation on the indices in Equation (25). Although a two-point correlation function shows up in the integral  $I_{ijrs}^1$ , this integral is the result of the contribution of one-point statistics since the only variables contributed in the calculations of Equations (25) and (26) are volume fractions of two phases.

The second term in Equation (19) can also be found using

$$I_{ijrs}^2 = - \int_V K_{kpum}(x, x') \langle \tilde{c}_{ijk}(x) \tilde{c}_{pmrs}(x') \rangle dX'. \quad (27)$$

This integral can be shown to be zero for isotropic composites. In isotropic composites the correlation term will be only a function of  $r$  ( $F(r)$ ). On the other hand, by assuming the definition of isotropic Green's function [Kröner et al. 1987],  $K_{kpum}$  is derived as

$$\begin{aligned} K_{kpum} = & \frac{1}{8\pi\bar{\mu}} \left\{ [\bar{K} \delta_{uk} \delta_{pm} + (\bar{K} - 1)(\delta_{pu} \delta_{km} + \delta_{um} \delta_{pk})] / |r|^3 \right. \\ & + [(3 - 3\bar{K})(r_m r_k \delta_{pu} + r_m r_u \delta_{kp}) \delta_{uk} \delta_{pm} - 3\bar{K}(r_m r_p \delta_{ku} + r_n r_p \delta_{km} + r_k r_p \delta_{um} + r_k r_n \delta_{pm})] / |r|^5 \\ & \left. + [15\bar{K}(r_p r_m r_u r_k)] / |r|^7 \right\}. \quad (28) \end{aligned}$$

Therefore, the integrand of the Equation (27) can be integrated with respect to  $r$ , separately. Some components of the integral of  $I_{ijrs}^2$  are evaluated here as an example:

$$\begin{aligned} I_{1111}^2 &= \frac{1}{8\pi\bar{\mu}} \int_r \int_\theta \int_\phi F(r) \left[ (3\bar{K} - 2) \sin \phi + (6 - 18\bar{K}) \cos^2 \theta \sin^3 \phi + 15\bar{K} \cos^4 \theta \sin^5 \phi \right] / r dr d\theta d\phi = 0, \\ I_{1212}^2 &= \frac{1}{8\pi\bar{\mu}} \int_r \int_\theta \int_\phi F(r) \left[ \bar{K} \sin \phi - 3\bar{K} \sin^3 \phi + 15\bar{K} \sin^2 \theta \cos^2 \theta \sin^5 \phi \right] / r dr d\theta d\phi = 0, \\ I_{1122}^2 &= \frac{1}{8\pi\bar{\mu}} \int_r \int_\theta \int_\phi F(r) \left[ (\bar{K} - 1) \sin \phi + (3 - 3\bar{K}) \sin^2 \theta \sin^3 \phi - 3\bar{K} \cos^2 \theta \sin^3 \phi \right. \\ & \quad \left. + 15\bar{K} \sin^2 \theta \cos^2 \theta \sin^5 \phi \right] / r dr d\theta d\phi = 0. \end{aligned}$$

For more details on the integration please refer to [Saheli 2006]. This can be shown in a general form

$$I_{iii}^2 = I_{ijij}^2 = I_{ijjj}^2 = 0, \quad (29)$$

where  $i$  and  $j$  vary from 1 to 3, indicating the three directions in spherical coordinates. Note that there is no summation on the indices in Equation (29). Therefore  $I_{ijrs}^2$  has been shown analytically to be zero for isotropic distributions found in [Beran 1968] and [Kröner 1977]. This is in agreement with the numerical results that Beran et al. [1996] obtained in their work. In this work, as the oxygen free electronic (OFE) alloy 101 copper plates were nearly isotropic, it was observed numerically that the contribution of the second integral is almost zero in the calculation of elastic properties. Hence the effect of spatial arrangement of the crystals was not observed.

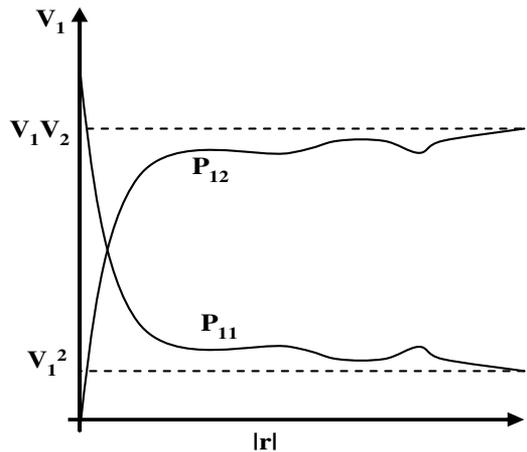
Also note that in the previous works by [Garmestani and Lin \[2000\]](#) only an isotropic composite was considered. Therefore the effect of morphology and spatial arrangement of the features in the microstructure on properties was not completely evident; however, in the following section of this research, it will be shown that the contribution of two-point statistics is very significant in anisotropic composites.

## 5. Numerical analysis

In the last section it was shown that  $I_{ijrs}^2$  is zero for isotropic composites; however, it is nonzero and should be evaluated by [Equation \(27\)](#) in anisotropic composites. The numerical integration has been done using Simpson's rule (see [mathworld.wolfram.com/SimpsonsRule.html](http://mathworld.wolfram.com/SimpsonsRule.html)). For this purpose, a sphere is divided into  $n_r \times n_\theta \times n_\varphi$  units, where  $n_r$  is the number of sections for variable  $r$  (radius) and  $n_\theta$  and  $n_\varphi$  are the number of sections for variables  $0 < \theta < 2\pi$  and  $0 < \varphi < \pi$ , respectively, in spherical coordinates. The variable  $r$  also changes between 0 and  $\infty$ . There are two issues to be taken into account to perform the integration. One is the singularity of the Green's function at  $r = 0$  and the other is the definition of  $\infty$  for  $r$  in the integration. Empirical forms of the probability density functions were introduced earlier. It can be shown that for all physically realizable forms of the probability density functions for a random media, they merge to a constant value at large  $r$  (as shown schematically in [Figure 2](#)).

The correlation function defined in [Equation \(18\)](#) becomes zero when the probabilities  $P_{11}$ ,  $P_{12}$ ,  $P_{21}$ , and  $P_{22}$  reach their limits. Therefore the coherence radius, ( $R_c$ ), is defined as the limiting value of the probability functions. This value should be used as an upper limit (or  $\infty$ ) for  $r$  in the volume integral ( $I_{ijrs}^2$ ). Since the Green's function is undefined at  $r = 0$ , the integral can be divided into two parts with respect to variable  $r$ , ( $0$  to  $r_{\min}$ ) and ( $r_{\min}$  to  $R_c$ ). For infinitesimally small values of  $r$  ( $0$  to  $r_{\min}$ ) the correlation does not change, so the correlation term can be taken out of the integral, and therefore the term

$$\int_V K_{kpum}(x, x') dX'$$



**Figure 2.** Schematic representation of two-point probability functions ( $P_{11}$  and  $P_{12}$  merge to their limiting values as the dimension of vector  $r$  increases).

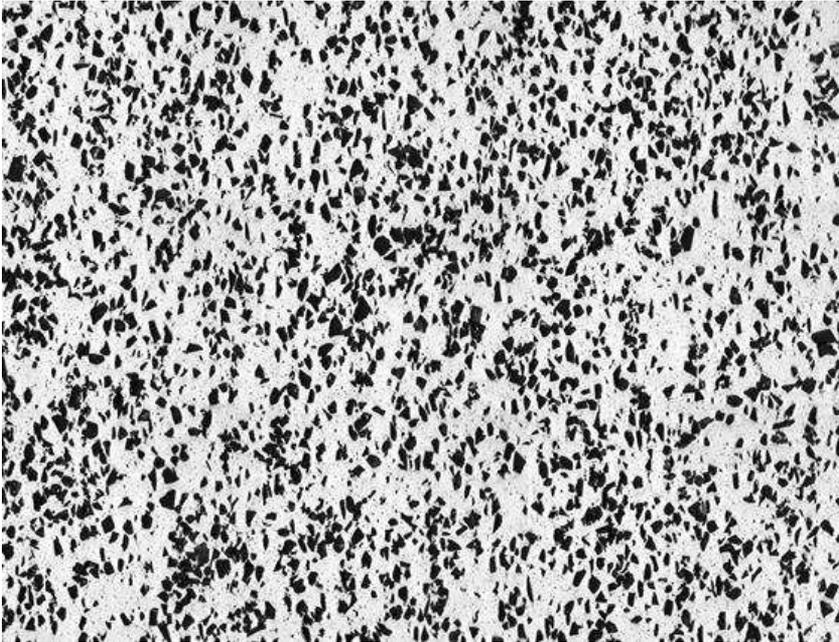
has to be calculated. Similar to the case of isotropic composites, this integral can be shown to be zero. Therefore the integral,  $I_{ijrs}^2$ , needs to be evaluated between  $r_{\min}$  and  $R_c$  for anisotropic composites. On the other hand,  $r_{\min}$  should be chosen as a small nonzero value in such a way as to be small enough to bring the contribution of two-point correlations for small radius and large enough to pass the singularity. For this purpose, a numerical procedure should be adopted that calculates a  $r_{\min}$  by reducing  $r$  until a saturation is reached for the value of the integral, not reaching infinity. Therefore the volume integral needs to be calculated from  $r_{\min}$  to  $R_c$ . Furthermore, time of operation is another aspect that has to be considered. For instance, in the case of Al-Pb composites [Saheli et al. 2004], if  $r_{\min} = 0.03$  and  $\Delta r = 0.1$  it takes about 20 minutes for the codes to calculate one elastic constant in a Pentium IV machine, 2.4 MHZ. However, if  $r_{\min}$  is chosen the same and  $\Delta r = 0.01$  then it takes about 2 hours and 35 minutes to calculate one elastic constant. The difference between the two results is about 0.04 percent. In contrast, for  $r_{\min} = 0.003$ ,  $\Delta r = 0.01$  it takes about 20 hours, where the difference in the calculation compared to the first case is less than 0.5 percent.

## 6. Applications

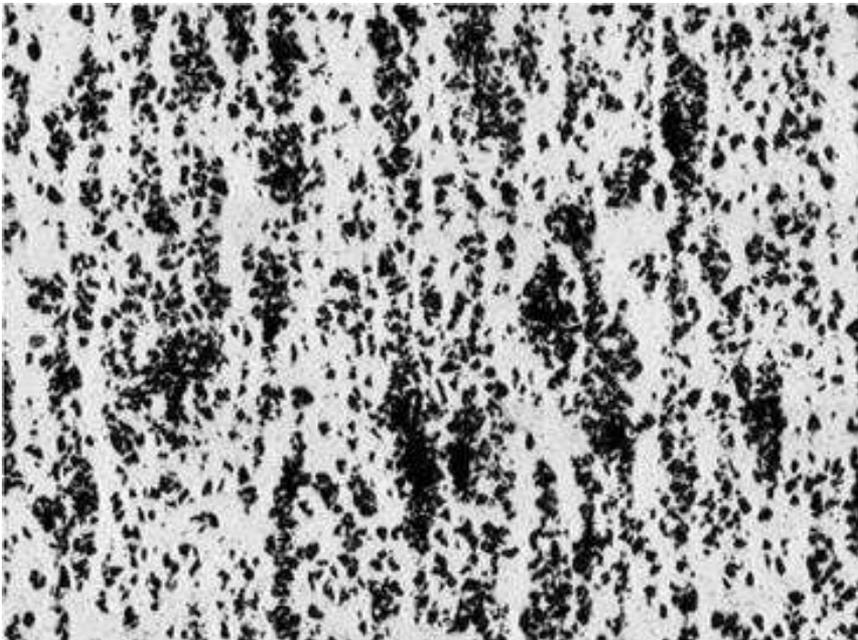
It was shown that two-point statistics does not contribute in the evaluation of elastic properties of isotropic composites. However, it has a considerable effect in the case of anisotropy. The key to this approach is the correct representation of the microstructure. In the previous works [Garmestani and Lin 2000; Saheli et al. 2004] a simplified empirical form of the two-point probability function was used for the microstructure representation, whereas in this work the statistical information has been measured directly from the microstructure and used as a database.

In this section, the statistical continuum mechanics model presented earlier as a homogenization technique will be studied in anisotropic composite materials. For this purpose, elastic properties of Al-SiC composite will be calculated by using the two-point statistical homogenization technique, and the contribution of two-point statistics will be discussed. The results of the simulation will be compared with experiments to validate the theory.

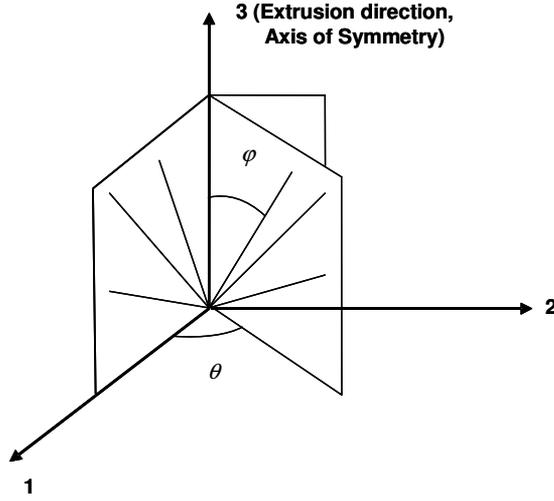
**6.1. Al-SiC samples.** An Al-SiC composite was fabricated by extrusion by varying the distribution of two different sizes of Al particles mixed with SiC particles. The difference in the initial particle sizes of SiC reinforcement phases and Al-alloy matrix results in the heterogeneity of the microstructure. The micrographs of the two samples with different PSR are shown in Figures 3 and 4. The particles of SiC are clustered in the sample with PSR = 8:1, therefore they introduce more anisotropy in the extrusion direction. However, the microstructure with PSR = 2:1 seems to have a smaller anisotropy. The validity of this interpretation will be studied by computing the elastic properties of the two samples. Note that the anisotropy of the microstructure has been considered in 1-3 or 2-3 plane (Figure 5). The distribution of the two-point correlation functions in these microstructures is symmetric with respect to the extrusion axis (Figure 5). Therefore the extrusion axis is chosen as the vertical axis. The probability distribution function changes with orientation  $\varphi$  and the magnitude of the vector  $r$  in each section. However, these probabilities are the same for all planes with different  $\theta$  which include extrusion (vertical) axis. Therefore the measurements of this composite on any section including the vertical axis provides the same statistical information within which the statistics may be anisotropic and would be sufficient for the simulation ( $\theta$



**Figure 3.** Micrograph of Al-SiC composite, PSR = 2:1.



**Figure 4.** Micrograph of Al-SiC composite, PSR = 8:1.

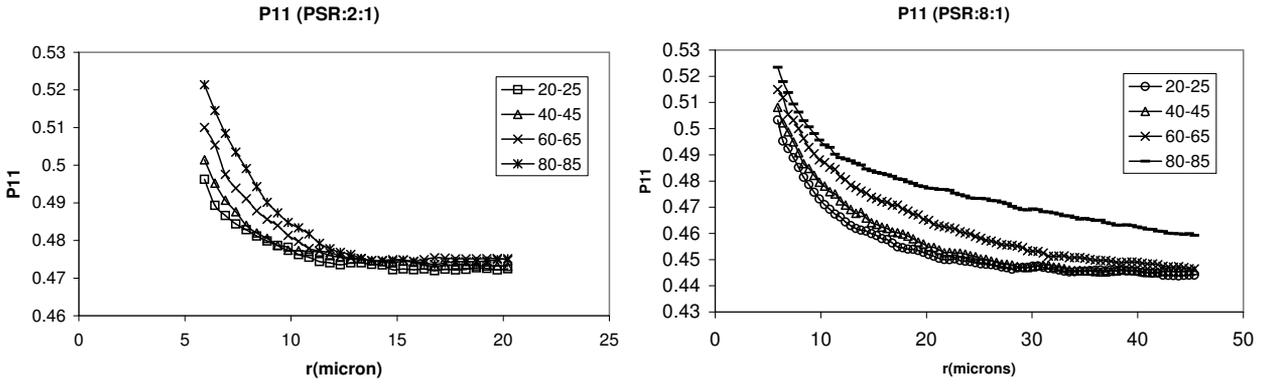


**Figure 5.** Representation of symmetry in samples of Al-SiC.

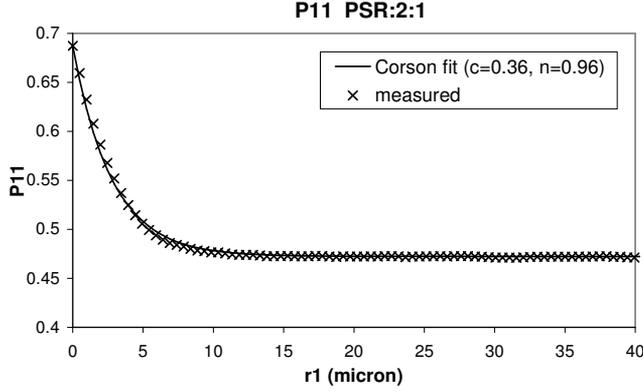
and  $\varphi$  are respectively the angles with axis 1 and axis 3 in spherical coordinates). Therefore the two-point probability functions are measured directly from the microstructure for a different range of  $\varphi$  on any plane including extrusion axis, which can be averaged as [Tewari et al. 2004]

$$\langle P_{ij}(r) \rangle = \frac{\int_{\varphi_1}^{\varphi_2} [P_{ij}(r, \varphi)] v d\varphi}{\int_0^{2\pi} d\varphi}. \tag{30}$$

As an example the measured values of  $P_{11}$  are shown in Figure 6 as a function of  $r$  and  $\varphi$  in each section containing extrusion (shown in Figure 5). In addition, Corson’s equation is used to measure values of  $P_{11}$  in Figure 7. It is observed that the measured values show an exponential trend which follows Corson’s equation (Equation (1)), and empirical factor  $n$  in Corson’s equation is calculated near 1, in agreement



**Figure 6.** Measurement of two-point statistics in a vertical section ( $P_{11}$ ) of two samples for different angles.



**Figure 7.** Fitted curve to the measured values of  $P_{11}$ .

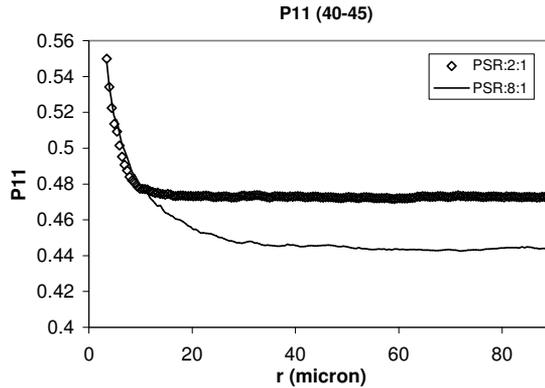
with results by [Tewari et al. \[2004\]](#).  $P_{11}$  for two samples at  $40 < \varphi < 45$  are shown in [Figure 8](#). The value of  $P_{11}$  (defined in [Equation \(1\)](#)) reaches its limit  $v_1^2 = 0.4761$  for the case of PSR = 2:1 faster than it reaches its limit  $v_1^2 = 0.4489$  for the case of PSR = 8:1.

Using the measured two-point probabilities and preparing the simulation code based on the homogenization relations described in previous sections, one can calculate elastic stiffness matrices for each sample. The mechanical properties of each phase are assumed as (based on previous experimental data)

$$E(\text{Al}) = 69 \text{ GPa}, \quad \nu(\text{Al}) = 0.33, \quad (31)$$

$$E(\text{SiC}) = 393 \text{ GPa}, \quad \nu(\text{SiC}) = 0.19. \quad (32)$$

In this simulation both integrals in [Equation \(19\)](#) are calculated, as the samples are considered anisotropic. Therefore the effect of anisotropy as introduced by clustering is studied in the estimation of elastic properties of these two samples.



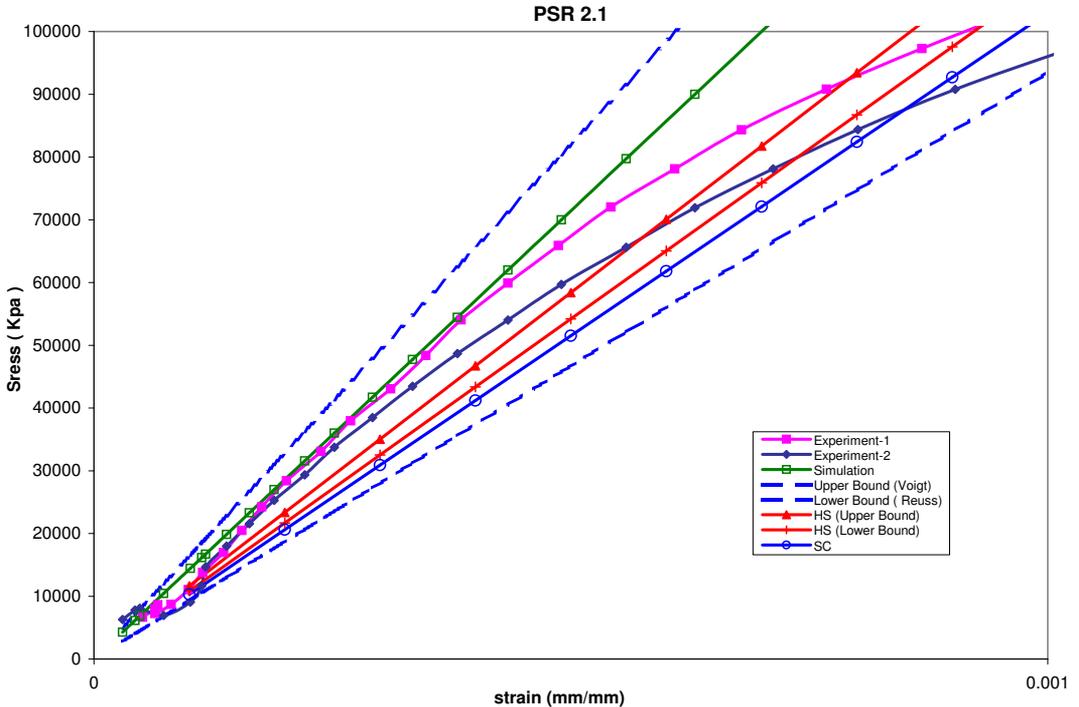
**Figure 8.** Measured  $P_{11}$  for two samples.

$C$	Upper Bound	$C$ (statistical model)	One-point	Two-point	Lower Bound
$C_{1111}$	229.86	205.08	-15.85	8.92	139.81
$C_{1313}$	72.43	71.95	-2.70	-2.23	36.18

**Table 2.** Contribution of one-point (Equation (19)) and two-point (Equation (26)) statistics in calculation (Equation (13)) of elastic constants of Al-SiC sample (PSR = 8:1).

**6.2. Results.** Calculating both integrals in Equation (19), the results show that the contribution of the second integral is about 30 and 50 percent in the calculation of  $C_{iiii}$  and  $C_{ijij}$  respectively. 1 and 3 indicate transverse and longitudinal (extrusion) directions. For example, when  $i = 1$ ,  $C_{iiii}$  refers to  $C_{1111}$ . Some of the components of effective elastic constants for an 8:1 sample are shown in Table 2.

Using the simulated values of the longitudinal elastic modulus, the linear behavior of the stress-strain curve in the elastic region is shown in Figures 9 and 10. The enlarged elastic region of stress strain curves obtained through mechanical testing is also shown in the graphs. In addition, upper bound [Voigt 1889] and lower bound [Reuss 1929], Hashin–Shtrikman upper and lower bound [Hashin and Shtrikman 1962; 1963], and self-consistent approximation [Hill 1965] are calculated and shown in the figure as well as in Table 3 for comparison to the simulation and experimental results. The linear elastic modulus calculated from the statistical simulations represented the best slope for the experimental stress-strain curves in the elastic region.



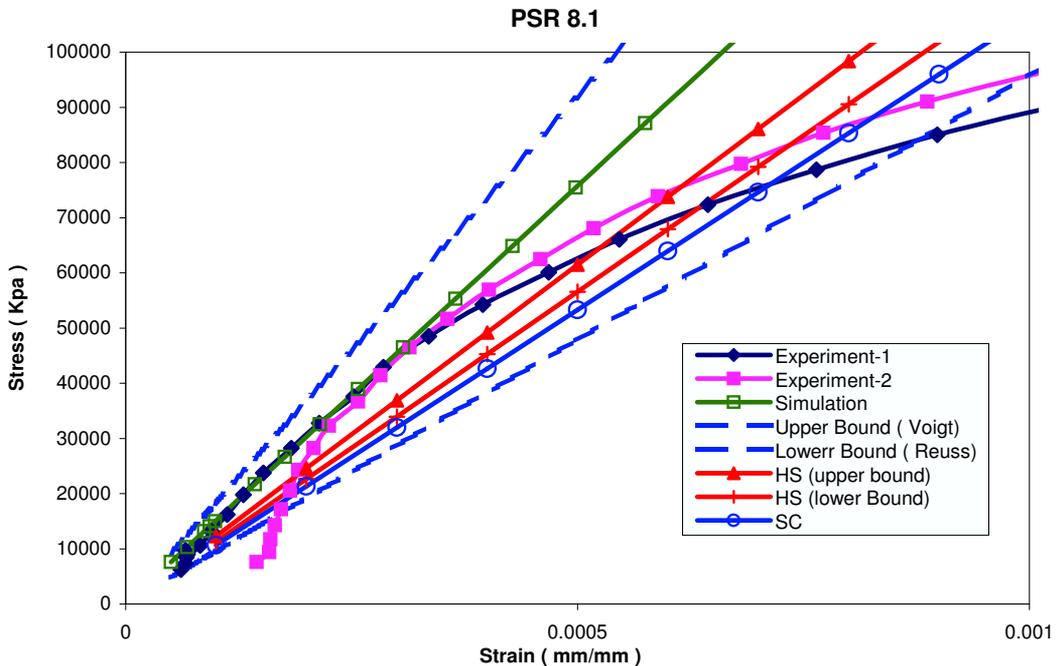
**Figure 9.** Stress-strain curve for Al-SiC PSR = 2:1.

E	REUSS	HS-LB	Statistics	Experiment	SC	HS-UB	VOIGT
PSR = 2:1	95.67	175.2	143.12	151.51	102.99	175.61	176.72
PSR = 8:1	98.43	185.65	161.29	156.82	106.63	186.04	184.07

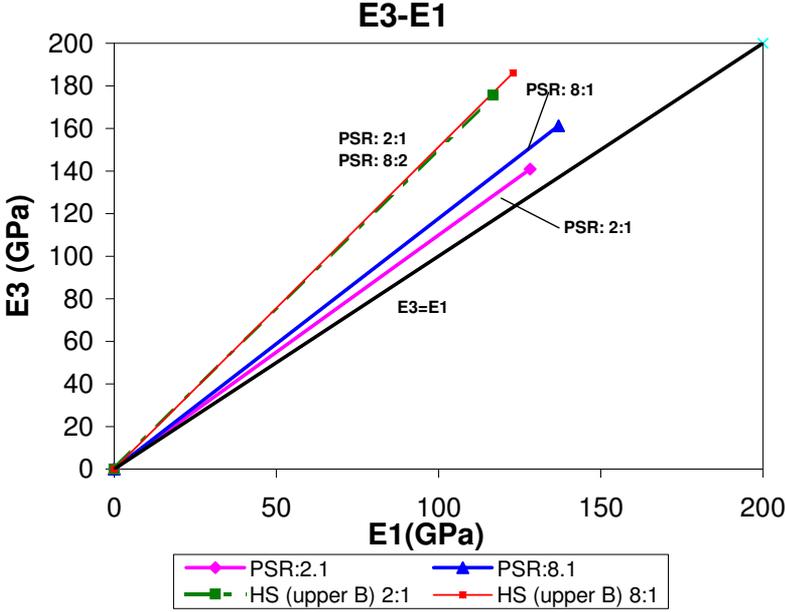
**Table 3.** Comparison of calculated longitudinal elastic modulus of two samples with different models.

The error is estimated to be between 0.07% and 20%, where 20% error relates to the points that have the largest deviation from experimental data in elastic region. The elastic moduli in two different directions (longitudinal and transverse) are shown for two samples in Figure 11. It was observed from the micrographs that clustering in the sample with PSR = 8:1 introduces more anisotropy in the elastic modulus than the other sample. This verifies the results of the simulation in Figure 11.

The volume fraction of the second phase (SiC) in two microstructures with PSR = 2:1 and PSR = 8:1 is estimated to be 31% and 33%, respectively. Although the volume fractions are very close, it shows a different degree of anisotropy (about 15% in the two samples). The upper Hashin–Shtrikman bounds for the two samples shown in this figure are not able to represent the anisotropy in the system properly. It shows an identical slope for the two cases, whereas the statistical calculations predict different elastic properties in the two directions.



**Figure 10.** Stress-strain curve for Al-SiC PSR = 8:1.



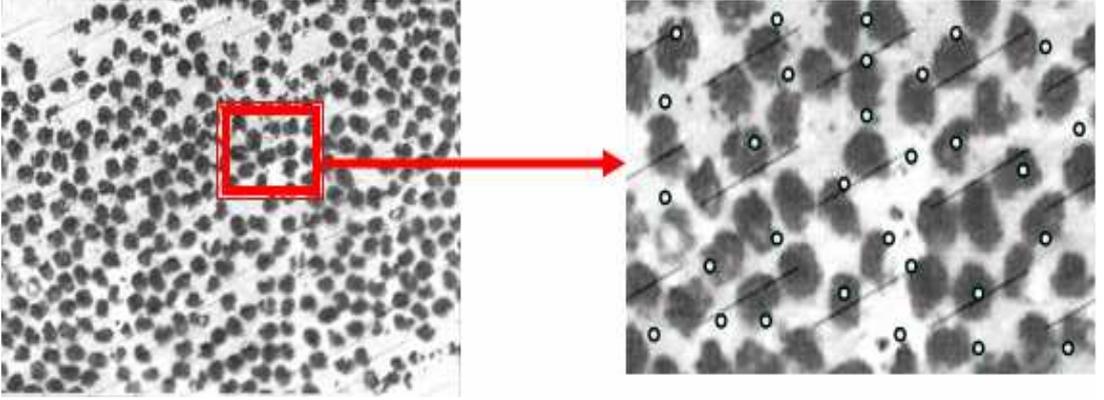
**Figure 11.** Comparison of longitudinal elastic modulus and transverse elastic modulus for two samples.

### 7. Summary

Statistical continuum mechanics modeling has been extended to include anisotropy in the calculation of elastic properties of composites. The effect of one-point and two-point statistics on the calculation of elastic properties of composites was studied in detail. It was shown analytically that two-point statistical information does not contribute in the calculation of elastic properties of isotropic composites, whereas it plays a major role for anisotropic materials. The homogenization technique was then applied to an Al-SiC composite with two different PSR’s. In this simulation two-point statistical functions were measured directly from the microstructures, and the statistical formulation uses the two-point probability functions to incorporate the effect of the microstructure distribution. Applying statistical continuum mechanics analysis, the effective properties of the two samples of Al-SiC composite were estimated and compared with the experimental data, the upper (Voigt) and lower bounds (Reuss), Hashin–Shtrikman bounds, and self-consistent approximations. Although the microstructures of the two composite samples have very similar volume fractions, this analysis results in different values of the effective elastic properties and predicts different anisotropy levels for them. Therefore the results show that the statistical analysis can provide a good estimate for the elastic effective properties, considering the spatial distribution of the phases.

### Appendix A: Definition of one-point and two-point statistics functions

**One-point probability functions.** To measure a one-point probability function, a random number of points ( $N$ ) have to be inserted in the microstructure (Figure 12). The number of points located in one



**Figure 12.** Schematic representations of one-point statistics measurement in a two-phase composite microstructure.

phase with respect to the total number of points ( $N$ ) indicates a one-point probability

$$\begin{aligned} P(\phi_1) &= P_1 = \frac{n_1}{N} = v_1 \\ P(\phi_2) &= P_2 = \frac{n_2}{N} = v_2, \end{aligned} \quad (\text{A.1})$$

where phase one and phase two have been considered as matrix and particles respectively, and the normalization relationship

$$P(\phi_1) + P(\phi_2) = 1. \quad (\text{A.2})$$

is always satisfied.

**Two-point probability functions.** A two-point probability function can be defined as a conditional probability function when the statistics of a three-dimensional vector  $r$  are investigated once attached to each set of the random points in a particular microstructure (Figure 13). Two-point statistics can be calculated by the probability of a specific phase at the head of the vector given the phase at the tail of the vector, and can be shown by  $P(r | \{1, 2\}, \{1, 2\})$ .

The following normalization relationship is valid for all the functions:

$$\begin{aligned} P_{11} + P_{12} &= v_1 \\ P_{22} + P_{21} &= v_2 \\ P_{11} + P_{12} + P_{21} + P_{22} &= 1. \end{aligned} \quad (\text{A.3})$$

As it is observed from the above normalization relationship,  $P_{11}$  is the only independent variable.

### Appendix B: Torquato probability functions

Functions  $V(r)$  and  $M(r)$  in Equation (3) are defined as

$$\begin{aligned} V(r) &= \frac{4\pi}{3} \left[ 1 + \frac{3r}{4} - \frac{r^3}{16} \right], & r < 2, \\ V(r) &= \frac{8\pi}{3}, & r > 2, \end{aligned} \quad (\text{B.1})$$

and

$$\begin{aligned} M(r) &= \left[ -\frac{16}{9} + \frac{r^3}{3} - \frac{r^4}{10} + \frac{r^6}{1260} \right] \pi^2 + \frac{16\pi^2}{9}, & 0 \leq r < 2, \\ M(r) &= \left[ \frac{256}{35r} - \frac{128}{9} + \frac{32r}{5} - \frac{5r^3}{9} + \frac{r^4}{10} - \frac{r^6}{1260} \right] \pi^2 + \frac{16\pi^2}{9}, & 2 \leq r < 4, \\ M(r) &= \frac{16\pi^2}{9}, & r \geq 4. \end{aligned} \quad (\text{B.2})$$

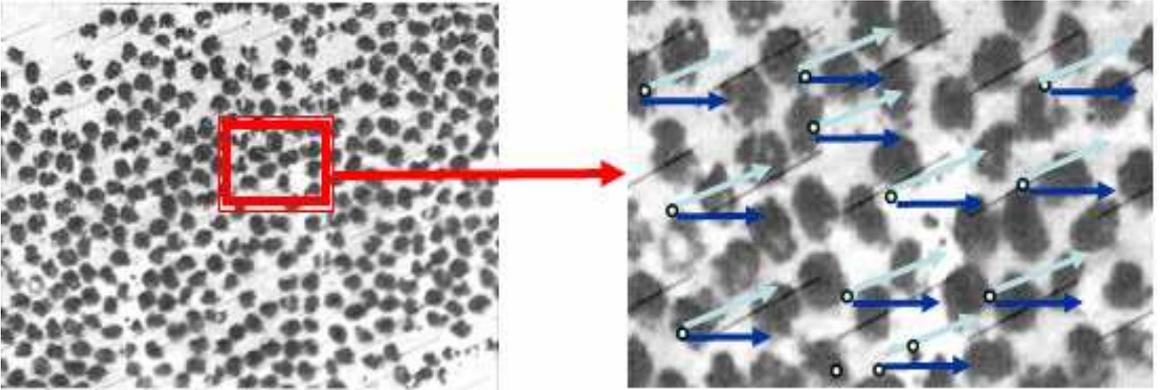
Note that  $r$  in general is a vector; however, for an isotropic two-phase composite,  $r$  is considered to be a scalar.

### Appendix C: Green's function definition

Green's function for the case of isotropic materials is defined by the closed form equation as in [Kröner et al. 1987]

$$G_{kp}(x, x') = \frac{1}{8\bar{\mu}\pi|r_{12}|} \left\{ 2\delta_{kp} - \frac{\bar{\lambda} + \bar{\mu}}{\bar{\lambda} + 2\bar{\mu}} \left( \delta_{kp} - \frac{r_{12k}r_{12p}}{|r_{12}|^2} \right) \right\}, \quad (\text{C.1})$$

where  $\bar{\lambda}$  and  $\bar{\mu}$  are the average values of Lamé's Constants in the composite.



**Figure 13.** Schematic representations of two-point statistics measurement in a two-phase composite microstructure.

However in the case of anisotropy and texture, there is no closed form equation, and it can be written in the numerical form [Bacon et al. 1980]

$$G_{ij}(x - x') = \frac{1}{8\pi^2|x - x'|} \oint_{|z|=1} (zz)_{ij}^{-1} ds, \quad (C.2)$$

where

$$(zz)_{ij} = C_{kijl}z_kz_l, \quad (C.3)$$

$$(z_{ij})^{-1} = \frac{\varepsilon_{ism}\varepsilon_{jrw}(zz)_{sr}(zz)_{mw}}{2\varepsilon_{pgn}(zz)_{1p}(zz)_{2g}(zz)_{3n}}. \quad (C.4)$$

$T$  is the unit vector in the direction of the line connecting two position  $x$  and  $x'$ . The general expression for the  $n$ -th derivative of the Green's function is given by

$$G_{ij,s_1 \dots s_n} = (x - x') = \frac{(-1)^N T_{k_1} \dots T_{k_N}}{8\pi^2|x - x'|^{N+1}} \times \oint_{|z|=1} \frac{\partial^N [(zz)_{ij}^{-1} z_{s_1} \dots z_{s_N}]}{\partial Z_{k_1} \dots \partial Z_{k_N}} ds, \quad (C.5)$$

$$G_{ij,s}(x - x') = \frac{1}{8\pi^2|x - x'|^2} \times \oint_{|z|=1} [T_s(zz)_{ij}^{-1} - z_s F_{ij}] ds, \quad (C.6)$$

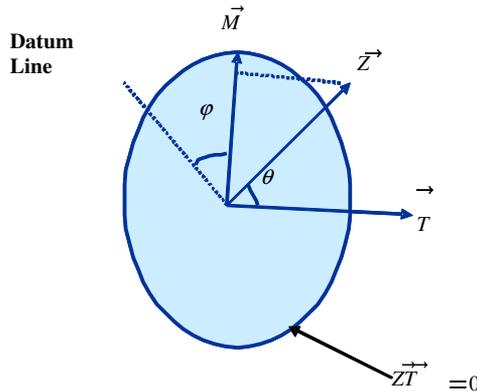
$$G_{ij,sr}(x - x') = \frac{1}{8\pi^2|x - x'|^3} \times \oint [2T_s T_r (zz)_{ij}^{-1} - 2(z_s T_r + z_r T_s) F_{ij} + z_s z_r E_{ij}] ds, \quad (C.7)$$

where

$$F_{ij} = (zz)_{im}^{-1} (zz)_{kj}^{-1} [(zT)_{mk} + (Tz)_{mk}], \quad (C.8)$$

$$E_{ij} = [(zT)_{mk} + (Tz)_{mk}] [F_{im} (zz)_{kj}^{-1} + (zz)_{im}^{-1} F_{kj}] - 2(zz)_{im}^{-1} (zz)_{kj}^{-1} (TT)_{mk}. \quad (C.9)$$

The resulting integral is a line integral on a circle defined in a perpendicular plane to  $T$  with a unit radius (Figure 14).



**Figure 14.** Schematic representation of different vectors in calculating Green's function for anisotropic case ( $\vec{T} \equiv \vec{r}$ ).

### Appendix D: Derivation of homogenization relations

Substituting the stress definition from Equation (5) into Equation (4), using the definition of local stress and strain, and finally substituting strain field by displacement field, the equilibrium equation can be solved by Equation (10). For this purpose the Green's function was used to solve the PDE. The strain field is finally obtained as

$$\tilde{u}_k(x) = \int_V G_{kp}(x, x') \frac{\partial[\tilde{c}_{plrs}(x')\varepsilon_{rs}(x')]}{\partial x'_l} dX', \quad (D.1)$$

where  $dX'$  is the volume integral on the volume element around position  $x'$ ,

By differentiating the above equation,  $\tilde{\varepsilon}_{ku}(x)$  is calculated by

$$\tilde{u}_{k,u}(x) = \int_V G_{kp,u}(x, x') \frac{\partial[\tilde{c}_{plrs}(x')\varepsilon_{rs}(x')]}{\partial x'_l} dX' + \overbrace{\int_V G_{kp}(x, x') \frac{\partial[\tilde{c}_{plrs}(x')\varepsilon_{rs}(x')]}{\partial x'_l \partial x_u}}^0 dX'. \quad (D.2)$$

It is observed that the second term is zero, since the term  $[\tilde{c}_{plrs}(x')\varepsilon_{rs}(x')]$  is just a function of  $x'$ , whereas the derivative is with respect to  $x$ . Therefore, the strain can be calculated as

$$\tilde{\varepsilon}_{ku} = \int_V \frac{1}{2} [G_{kp,u}(x, x') + G_{up,k}(x, x')] \frac{\partial[\tilde{c}_{plrs}(x')\varepsilon_{rs}(x')]}{\partial x'_l} dX'. \quad (D.3)$$

Defining the first derivative of the Green's function as

$$K_{kpu} = \frac{(G_{kp,u} + G_{up,k})}{2}, \quad (D.4)$$

multiplying the strain in Equation (D.3) by the value of the local moduli  $\tilde{c}_{ijk}(x)$ , and averaging with respect to  $x$ ,

$$\langle \tilde{c}_{ijk}(x) \tilde{\varepsilon}_{ku}(x) \rangle = \int_V \int_{V'} K_{kpu} \tilde{c}_{ijk}(x) \frac{\partial[\tilde{c}_{plrs}(x')\varepsilon_{rs}(x')]}{\partial x'_l} dX' dX, \quad (D.5)$$

is found, where  $dX$  is the volume integral on the volume element around position  $x$ . Substituting the local strain field from Equation (8), the above equation can be rewritten by

$$\begin{aligned} \langle \tilde{c}_{ijk}(x) \tilde{\varepsilon}_{ku}(x) \rangle &= \int_V \int_{V'} K_{kpu} \frac{\partial[\tilde{c}_{ijk}(x) \tilde{c}_{plrs}(x')]}{\partial x'_l} dX' dX \langle \varepsilon_{rs}(x) \rangle \\ &\quad + \int_V \int_{V'} K_{kpu} \frac{\partial[\tilde{c}_{ijk}(x) \tilde{c}_{plrs}(x') \tilde{\varepsilon}_{rs}(x')]}{\partial x'_l} dX' dX. \end{aligned} \quad (D.6)$$

Showing the integral over the variable  $x$  as an ensemble average, the above equation is reduced to

$$\begin{aligned} \langle \tilde{c}_{ijk}(x) \tilde{\varepsilon}_{ku}(x) \rangle &= \int_V K_{kpu} \frac{\partial \langle \tilde{c}_{ijk}(x) \tilde{c}_{plrs}(x') \rangle}{\partial x'_l} \langle \varepsilon_{rs} \rangle dX' \\ &\quad + \int_V K_{kpu} \frac{\partial [\langle \tilde{c}_{ijk}(x) \tilde{c}_{plrs}(x') \tilde{\varepsilon}_{rs}(x') \rangle]}{\partial x'_l} dX'. \end{aligned} \quad (D.7)$$

In the above equation  $\langle \tilde{c}_{ijku}(x)\tilde{c}_{pmrs}(x') \rangle$  is called a two-point correlation function, and can be calculated using Equation (18). It is observed that the second term is a three-point correlation function. At this time the calculation is truncated up to a two-point probability function. For this research the second term is neglected. Therefore to get the microstructural information and correlate them to properties, one needs to calculate the first integral in Equation (D.7). A fourth rank tensor  $\langle a \rangle$  was introduced as the deviation in the strain field,

$$\langle \tilde{\varepsilon}_{ku} \rangle = \langle a_{kurs} \rangle \langle \varepsilon_{rs} \rangle. \quad (\text{D.8})$$

Substituting the above equation in Equation (D.7) and omitting  $\langle \varepsilon_{ku} \rangle$  from both sides, the equation is reduced to

$$\langle \tilde{c}_{ijku}(x)a_{kurs} \rangle = \int_V K_{kpu} \frac{\partial \langle \tilde{c}_{ijku}(x)\tilde{c}_{plrs}(x') \rangle}{\partial x'_l} dX'. \quad (\text{D.9})$$

Applying integration by parts to the above equation, it can be rewritten as

$$\langle \tilde{c}_{ijku}(x)a_{kurs}(x) \rangle = \int_{V'} \frac{\partial [K_{kpu} \langle \tilde{c}_{ijku}(x)\tilde{c}_{plrs}(x') \rangle]}{\partial x'_l} dX' - \int_{V'} K_{kpul}(x, x') \langle \tilde{c}_{ijku}(x)\tilde{c}_{plrs}(x') \rangle dX'. \quad (\text{D.10})$$

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Received 17 Jan 2006. Accepted 8 May 2007.

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