Effective Elastic Properties of an Al-SiC Composite Using Two-point Statistical Mechanics Approach

G. Saheli, H. Garmestani, A. Gokhale

School of Materials Science and Engineering Georgia Institute of Technology Atlanta, GA

Abstract. In this paper, statistical continuum mechanics modeling is applied to predict the elastic mechanical properties of an anisotropic Al-SiC composite. Two-point statistics are measured on vertical metallographic planes in three-dimensional microstructures. As a result of anisotropy the correlation functions are orientation dependent. Longitudinal and transverse elastic moduli are calculated for two samples with different PSR and clustering, and the results are compared with upper and lower bound and experimental data. It's observed that the theoretical results are in good agreement with experimental data and two-point statistics significantly contribute to the estimation of the elastic modulus.

Introduction

The prediction of mechanical property from the details of the microstructure such as phase, crystalline grain distribution and morphology has received a special attention in the mechanics and materials community [1, 2]. Two-point statistical modeling has been used for microstructure quantitative characterization and mechanical properties prediction in the last few decades. The use of two-point statistics allows the composite designer to include the morphology and distribution in addition to the properties of the individual phases and components.

The mathematical description of heterogeneity in microstructures has received some breakthroughs in the last three decades with the works of Kröner and Beran [3, 4, and 5]. More progress has been achieved to calculate 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…). Statistical distribution functions are commonly used for the representation of microstructures and also for homogenization of materials properties. Orientation Distribution Function (ODF) is an example of a one-point statistical distribution function that only considers volume fractions (or number fractions) of crystallites with the same orientation. Two-point statistical function can be used as a first order correction to the average representation. Two point correlation functions [1, 2, 6, 7, 8, and 9] provide information about near neighbor and far field effects and allow the defect sensitive properties to be incorporated in the analysis. The extension to higher order statistics adds a higher order of dimensionality in the Materials Hull. It also presents two major improvements in the analysis for the calculation of effective properties and the evolution of microstructures [6, 8].

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 [10]. Measurements of local orientation and misorientation of polycrystalline materials are now possible. For the composite, if the orientation of each phase is ignored, the correlation functions can be measured using imaging techniques (optical, SEM...). The use of OIM for the measurement of orientation for a multiphase composite can introduce a large amount of detail and higher order statistical formulations will be needed to incorporate such information for Material Science Design (a Methodology defined by Adams[11]) and microstructure analysis.

The composite formulation will be markedly enhanced by the use of two point correlations [1, 12, and 13]. The use of two-point statistics allows the materials designer to include the morphology and distribution in addition to the properties of the individual phases and components. Statistical continuum mechanics provides a direct link between the microstructure and properties (elastic and plastic) in terms of these two point statistical functions.

In this paper, two-point correlation functions are used for the description of a composite. The two-point correlations are measured for two samples of Al-SiC with different PSR. The elastic moduli of the composite are calculated in two longitudinal and transverse directions and the effect of anisotropy resulted from clustering is observed in the results. In this work the contribution of two-point in calculation of effective elastic properties will be observed. Finally the simulation results will be compared with experimental value of elastic modulus that is obtained through mechanical testing, and upper and lower bound for verification.

Two-Point Distribution Function

The statistical details of a microstructure can be represented by an n-point probability distribution function. The volume fractions, v_1 and v_2 define the one-point probability distribution function that can be 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 can only be realized by using higher order distribution functions [1, 12]. 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 the random points in a particular microstructure. The exponential form of the distribution function as proposed by Corson has been shown to be appropriate for random microstructures [12]. It is represented as

$$P_{ij}(r) = v_i v_j + (-1)^{i+j} v_i v_j \exp\left[-c_{ij} r^{n_{ij}}\right], \quad (1)$$

where **r** is a vector in this equation, however in isotropic case, the probability doesn't depend on the direction and r is assumed to be a scalar.

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_{21}(**r**). The empirical coefficients c_{ij} and n_{ij} are also microstructure parameters: n_{ij} is usually very close to 1 and c_{ij} is a scaling parameter representing the correlation distance.

These coefficients can be reformulated into an anisotropic form

$$n_{ij}(\theta, a) = n_{ij}^{0}\left(1 - (1 - A)\sin\theta\right) \qquad (2)$$

$$c_{ij}(\theta, a) = c_{ij}^{0}\left(1 + (1 - A)\sin\theta\right), \qquad (3)$$

where A is a material parameter that represents the degree of anisotropy in a microstructure such that A=1 corresponds to an isotropic microstructure.

Effective Elastic Constants

Statistical continuum mechanics analysis is used to predict the elastic properties of a composite. The theoretical framework has been developed for isotropic distributions in composites by Garmestani, et. al. [6,7] and for a textured polycrystalline material by Adams et.al [14, 15]. Here, a brief discussion is provided for the calculation of the effective elastic constants for isotropic distribution and will be extended to anisotropic distributions.

Effective Elastic constants "C" of a composite are defined by the equation:

$$\bar{\sigma} = C\bar{\varepsilon}, \qquad (4)$$

where $\bar{\sigma}$ and $\bar{\varepsilon}$ are the average stress and strain respectively, and C is the effective elastic constant of the composite. Applying Hill's criteria the effective elastic constants can be written as (for details see paper by Garmestani, et. al. [6, 7]):

$$C = \langle c \rangle + \langle ca \rangle, \qquad (5)$$

where $\langle c \rangle$ is the average elastic tensor and $\langle ca \rangle$ is the average deviation of the elastic constants from the mean value. The fourth rank tensor a = (a_{ijkl}) is introduced here to represent the local inhomogeneity. Therefore the effective property can now be defined by:

$$C_{ijkl} = \langle c_{ijkl} \rangle + \langle \tilde{c}_{ijmn}(x) a_{mnkl}(x) \rangle, \qquad (6)$$

where $\tilde{c}_{ijmn}(x)$ is the deviation from the local stiffness and can be defined by:

$$\tilde{c}_{ijmn}(x) = c_{ijmn}(x) - \langle c_{ijmn} \rangle, \qquad (7)$$

where $c_{ijmn}(x)$ is the local stiffness.

To calculate the effective stiffness of the composite, the second term in Eq. (6) has to be calculated and added to the mean value of stiffness.

The equilibrium equation is written as:

$$\sigma_{ij,j} = 0, \qquad (8)$$

where the stress-starin relationship are defined by:

$$\begin{aligned} \sigma_{ij}(x) &= c_{ijkl}(x)e_{kl}(x) \\ \langle \sigma_{ij} \rangle &= C_{ijkl}\langle e_{kl} \rangle \quad , \qquad (9) \\ e_{ij} &= (1/2)(\partial u_i / \partial x_j + \partial u_j / \partial x_i) \end{aligned}$$

where $e_{kl}(x)$ and $\langle e_{kl} \rangle$ are local strain and average stain respectively. Also u_i shows the local displacement. By substituting local stress in equilibrium Equations (8), an equation for displacement is obtained. Differentiating the equation of displacement and multiplying the result by c_{ijkl}, the second term in Eq. (6) will be calculated by:

$$\begin{aligned} &\langle \tilde{c}_{ijku}(x) a_{kurs}(x) \rangle = \\ &\int_V \partial \left[K_{kpu}(x,x') \langle \tilde{c}_{ijku}(x) \tilde{c}_{pmrs}(x') \rangle \right] / \partial x'_m dX' \quad (10) \\ &- \int_V K_{kpum}(x,x') \langle \tilde{c}_{ijku}(x) \tilde{c}_{pmrs}(x') \rangle dX' \end{aligned}$$

Note x and x′ are two different position in the media, and dX′ shows the volume integral on the volume element around the position x′.

In which the correlation function is defined by:

$$\begin{aligned} &\langle \tilde{c}_{ijku}(x) \tilde{c}_{pmrs}(x') \rangle = \\ &\tilde{c}_{1ijku} \tilde{c}_{1pmrs} p_{11} + \tilde{c}_{1ijku} \tilde{c}_{2pmrs} p_{21} \quad , \qquad (11) \\ &+ \tilde{c}_{1ijku} \tilde{c}_{2pmrs} p_{12} + \tilde{c}_{2ijku} \tilde{c}_{2pmrs} p_{22} \end{aligned}$$

and:

$$\begin{aligned} K_{kpu} &= \left(G_{kp,u} + G_{up,k} \right)/2 \\ K_{kpum} &= \left(G_{kp,um} + G_{up,km} \right)/2 \end{aligned} , \qquad (12)$$

where G is the Green's function used for solving the equilibrium equations. For definition of Green's function for isotropic and anisotropic refer to [7, 16].

Simulation and Results

In this section the elastic properties are calculated for two samples of Al-SiC composite. The composite was produced by extrusion with distribution of different sizes of Al particles in SiC. So the difference in initial particle sizes of SiC reinforcement phases and Al-alloy matrix results in the heterogeneity of the microstructure. The micrographs of two samples are shown in Fig.1 and Fig.2.

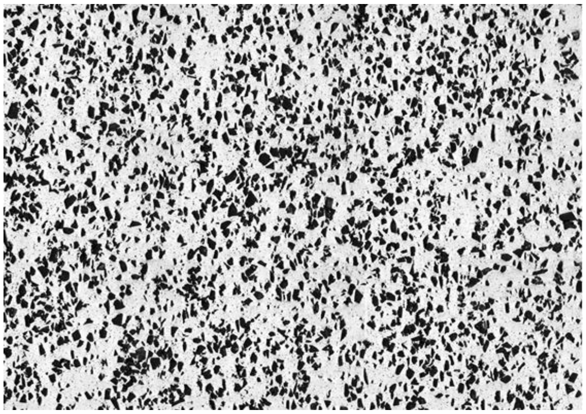

Figure.1. Micrograph of Al-SiC Composite, PSR=2:1

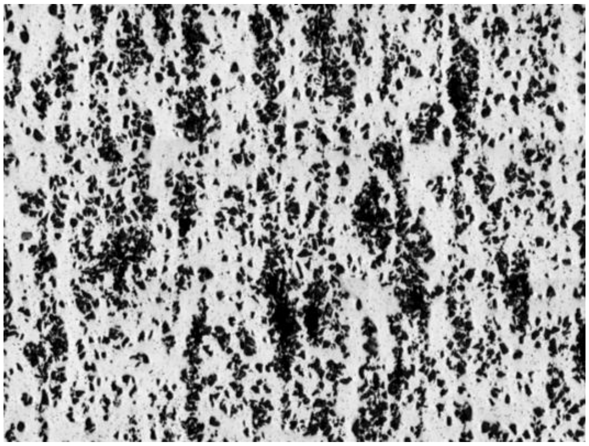

Figure.2. Micrograph of Al-SiC Composite, PSR=8:1

In the simulation of these microstructures, the distribution of two point correlation functions is symmetric respect to the extrusion axis. Therefore the extrusion axis is chosen as the vertical axis. Each section, that contains the extrusion axis, displays similar statistical distributions.

The probability distribution function changes with orientation and magnitude of the vector "**r**" on each section. The measurements of this composite on any section including the vertical axis provides the same statistical information within which the statistics maybe anisotropic. Therefore measurement of two-point correlations on just one section is sufficient for simulation.

In this simulation the probability is measured directly from the microstructure. As an example the measured values of p_{11} are shown in Fig.3 as a function of r and

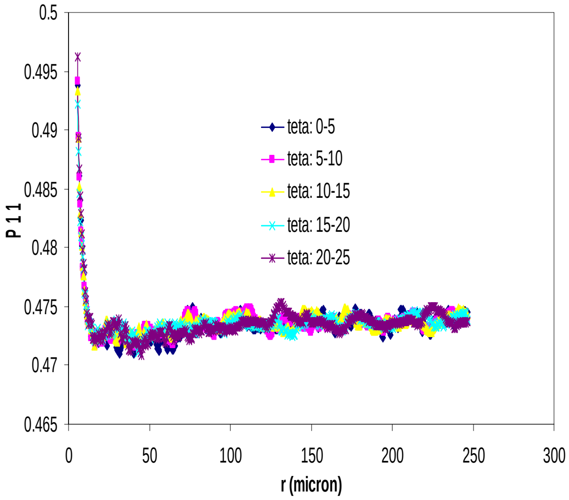

Figure.3. Measurement of two-point statistics in one section (P_{11})

θ in each section including extrusion axis. It's seen that the measured values show the same trend as the Corson's equation (Eq.1).

Using the measured two-point probabilities and preparing the simulation code based on the theory described in previous section calculate elastic stiffness matrices for each sample. In this simulation both Integrals in Eq(10) are calculated, as the samples are considered anisotropic. The second Integral includes the two-point statistics information and goes to zero for isotropic microstructures [17]; however it has a major role in the calculation of effective properties for anisotropic cases.

It's observed that the contribution of the second integral is about 30 percent in the calculation of C_{iiii} and about 50 percent in the calculation of C_{ijij}. Note that i and j can vary from 1 to 3 and they don't show summation on the indices. Direction 1 shows transverse direction and direction 3 is parallel to the extrusion axis. For example when i equal to 1, C_{iiii} shows C_{1111}. Longitudinal (parallel to the extrusion axis) and transverse (perpendicular to the extrusion axis) elastic modulus is calculated for two samples from the simulation values of elastic stiffness matrices.

Using the simulated values of longitudinal elastic modulus, the linear behavior of stress-strain curve in elastic region is shown in Fig.4 and Fig.5. The stress strain curves obtained through mechanical testing are also shown in the graphs. Also, upper bound (Voigt) and lower bound (Reuss) are calculated and shown in the graphs for a comparison with simulation and experimental results. Voigt assumes a uniform strain, and Reuss assumes uniform stress in both phases [18, 19]. It's observed that the linear part of the experimental stress-strain curve is in a good agreement with the line calculated by simulated elastic modulus. The error is estimated to be less than 20%. Therefore it's concluded that the statistical model provides a good estimate for the elastic properties.

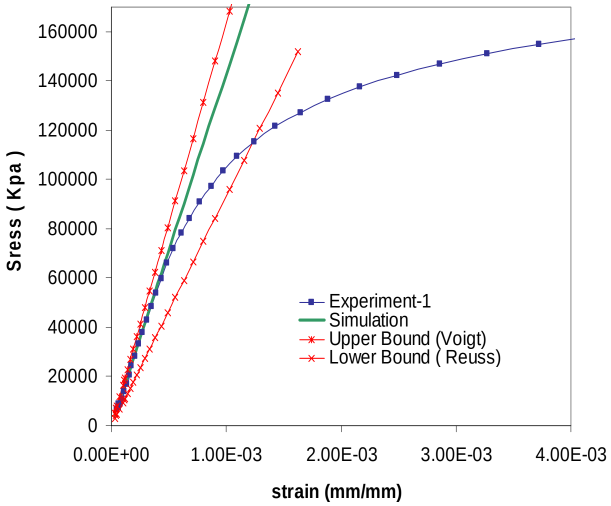

Figure.4. Stress-strain curve of Al-SiC for PSR=2:1

It's observed from the micrographs that the particles of SiC are clustered in the case of PSR: 8.1, therefore they introduce anisotropy in the microstructure in one direction, whereas in the case of 2.1 the microstructure doesn't show a significant anisotropy.

The elastic moduli in two different directions

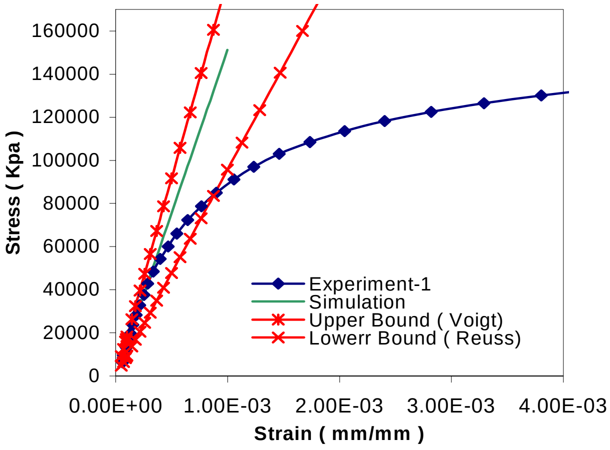

Figure.5. Stress-strain curve of Al-SiC for PSR=8:1

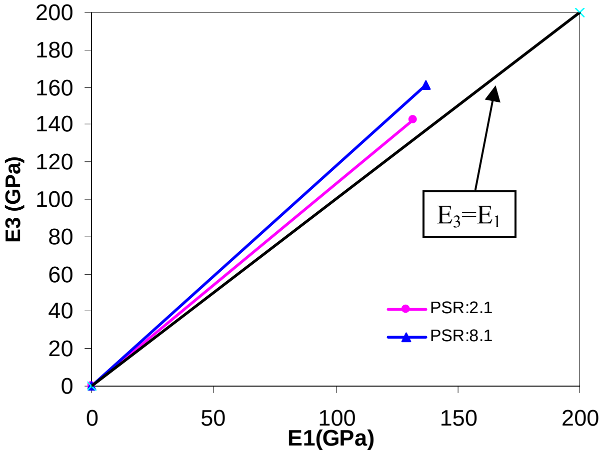

Figure.6. Longitudinal elastic modulus (E_3) vs. transverse elastic modulus (E_1)

(longitudinal and transverse) are shown in Fig.6. The clustering in the sample with 8 PSR introduces more anisotropy than the other sample. This verifies with the results of simulation. Figure.6 illustrates that the sample with 8 PSR has a larger anisotropy.

The volume fraction of the second phase (SiC) in two microstructures with 2:1 and 8:1 PSR is estimated to be 31% and 33% respectively. Although the volume fractions are very close, it's observed different degree of anisotropy in two samples. Therefore it can be concluded that the two point statistics considerably contributes in the calculation of elastic properties, whereas it doesn't contribute in isotropic composites.

Summary

Statistical continuum mechanics modeling has been applied to a two-phase composite. Al-SiC composite with two different PSR is considered in this simulation. Two-point statistical functions are measured directly from the microstructures. The statistical formulation uses the two point functions to incorporate the effect of the microstructure distribution. By applying statistical continuum mechanics analysis the effective properties of the composite is estimated and compared with the experimental data and upper and lower bounds. The results show that the statistical analysis can provide a good estimate for the elastic effective properties.

Although the microstructures of two composite samples have very close volume fraction this analysis results in different effective properties and predict different anisotropy degree for them. Therefore the two-point statistics has a significant contribution in the calculation of the elastic properties in anisotropic composites.

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