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Statistical continuum mechanics analysis of an elastic two-isotropic-phase composite material

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Abstract

A statistical mechanics theory is formulated to capture the effect of microstructure distribution on the effective elastic moduli of a composite material. Two point probability functions are used as a major component of the statistical theory. The statistical correlation functions represent the morphology and the distribution (random, periodic,…) of phases. The theory can benefit from simple mathematical representation of distribution or the shape of the second phase (circular, elliptical,…). A two-point probability function is used to approximate the correlation functions for a general class of geometries with isotropic and random distributions. The simulations are also provided and compared to other (periodic) distributions. The results show that the theory is capable of capturing the microstructural featuring in addition to the statistical distributions. © 2000 Elsevier Science Ltd. All rights reserved.

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1. Introduction

The mathematical description of heterogeneity has received some breakthroughs in the last two decades with the works of Kröner [1,2] and Beran [3]. 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,…). Kröner [1,4] proposed a statistical continuum approach to find an approximation for the elastic moduli of a heterogeneous random medium. 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 geometry characteristics of the microstructure. It was realized that in order to use the measured materials' heterogeneity, it is necessary to incorporate the 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 to measure individual crystalline orientation in polycrystalline materials [5,6]. Extension of this effort to non-random microstructures requires proper definition of *n*th degree statistical correlation functions. A statistical continuum mechanics approach for an inelastically deforming composite was introduced earlier by Garmestani et al. [7]. In the present paper, such an effort is extended to an elastically deforming composite structure. The present effort is different from other statistical mechanics formulations since it includes second order correlation functions to calculate effective properties. In this paper, the technique is applied to a periodic and randomly distributed microstructure.

Some of the early works in the area of elastic moduli prediction are due to Voigt [8] and Reuss [9] which produce the upper and lower bounds to the true effective elastic moduli [10]. Hashin and Shrikman [11] found narrower bounds for the effective elastic moduli based on elasticity solutions using energy methods and by developing solutions to the spherical and cylindrical inclusion problems. Such efforts resulted in exact solutions for mechanical properties of specific types of composites [12,13].

Many attempts have been made in the past few decades to develop new formulations to improve the bounds for the effective elastic moduli in composite materials. Methods based on the self consistent approach have been shown to provide better bounds for the prediction of the mechanical behavior of heterogeneous materials. Some of the original work in this area by Hershey [14], Kröner [15] and Eshelby [16] were performed on single crystal and polycrystalline materials. The model is based on the assumption that the

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effective elastic moduli should be equal to the moduli obtained by averaging the stress and strain in a spherical or ellipsoidal grain over all orientations. Eshelby developed a tensor that provided a mechanism to relate such efforts to multi phase materials [16]. Eshelby's tensor relates the strain of an inclusion inside an infinite elastic matrix to the strain of the same inclusion, when placed outside the matrix free of the stresses imposed by the matrix. Such an analogy ignores the effect of inclusions on each other. This analysis can only be applied to dilute composites and those that the second phase reinforcements are located far from each other. Budiansky [17] utilized this analogy to derive the effective elastic moduli of a composite material for higher concentration of the second reinforcing phases. Hill [18], Budiansky [17] and Nemat-Nasser et al. [19] provided different solutions of the self consistent scheme. Other efforts are due to Kneer [20], Morris [21], Mori-Tanaka [22], and Christian and Lo [23]. Walker et al. [24,25] used a non-dilute self consistent scheme to obtain a better and more simplified solution for the elastic and inelastic bound. Such efforts provide corrections to the first order bounds of Voigt and Reuss and are classified as second order bounds. Following the method of Hashin and Shrikman, Avellaneda used the energy method to provide better bounds for composites materials with specific symmetries [26].

Statistical continuum theory for the effective elastic moduli was initiated by Volkov and Klinskikh [27], Lomakin [28,29], Beran and Molyneux [30] and Kröner [4]. Kröner [1,2,31] applied the continuum theory to calculate the effective elastic moduli for a randomly distributed microstructure. Torquato [32–35] extended the formulation to include the *n*-point correlation functions in the calculation of the effective properties of random heterogeneous media for specific second phase shapes and microstructures. The application to anisotropic materials was studied by Zeller and Dederichs [36]. McCoy [37] provided a review of the statistical modeling effort for a randomly distributed microstructure.

The application of these theories to composite materials provides better bound for the moduli for any distribution of phases. Second phase interactions (fiber to fiber) are usually ignored in other models and at best, it is assumed that they are periodically distributed. The real microstructure deviates from such an ideal condition for the fact that there may exist a range of size distributions for the fibers and the shape of the constituents may not be represented by exact mathematical formulations. As an alternative to such approaches, the statistical continuum theory uses probability functions to represent such details in the microstructure. Statistical continuum theory can only be applied to cases where a complete statistical information is available about the morphology and the distribution of the constituents in composite materials. Such information is represented in the form of correlation functions. Depending on the complexity of the microstructure, more information in the form of higher order correlation functions can be incorporated in the statistical formulation for a better representation of the material. It will be shown that in reality, good approximation can be obtained by using only correlation functions of lower orders. In this paper, a two-point correlation function is formulated using a two-point probability function in the statistical model to calculate the elastic moduli. Correlation functions have been studied in detail by Torquato [32–34] and exact forms have been offered for different well-known microstructures. The functional form of the two-point probability functions used here is a general one and is suitable for any isotropic microstructure distribution as long as it satisfies global statistical homogeneity. The formulation presented here can use any form of the probability function and is not limited to one form or another. As a matter of fact one may choose not to use a mathematical form for the probability function and the probability function can be stored as a set of data acquired from the microstructure. The statistical formulation presented here would then simulate the probability data as an input to calculate the effective properties. In the following paragraphs it will be shown that the statistical formulations based on one point correlation functions may not distinguish two microstructures with the same volume fraction of the second phase once the shape of the second phase is kept the same. In the present formulation, such a difference is recognized as a result of the inclusion of the second order correlation functions.

The statistical continuum theory also plays an equally important role with the self-consistent model in the plasticity of large deformation as it did in elasticity. Adams et al. [38], presented a statistical formulation of viscoplastic behavior in heterogeneous polycrystals by taking the approach, which parallels the constructs in the statistical continuum theory of linear-elastic polycrystals [2,4,31,37]. A secant modulus formulation of the single crystal constitutive law was used. The interaction law from equilibrium conditions and incompressibility condition was obtained by using Green's function method. The statistical formulation was formed from the interaction law by incorporating the two-point probability density function of lattice orientations, that can also be called the crystallite orientation correlation function (OCF) [39]. The statistical theory of Adams et al. [38] was first applied to the prediction of initial texture evolution in FCC polycrystals under uniaxial creep [40].

In the following sections, the general statistical formulation to calculate the effective moduli is introduced for an elastic material first, then the two-point correlation functions are incorporated in the general theory using the two-point probability functions. Finally, a numerical method for the simulation of the effective modulus for a two-isotropic-phase composite material is presented. A simple form for the two-point probability function is used to simulate a randomly distributed structure originally suggested by Corson [41,42]. A randomly distributed microstructure is then compared to a periodic microstructure, which did not require a mathematical form for its probability function.

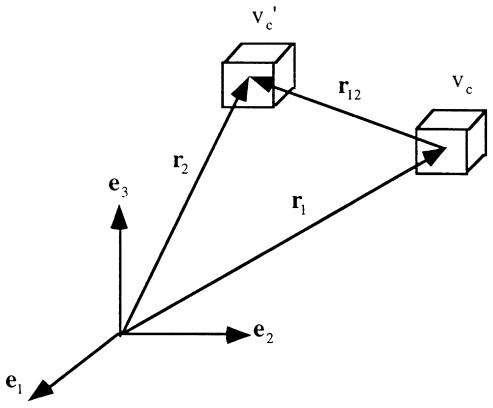

Fig. 1. Two elements geometry of the convolution integral problem $\mathbf{G} \times \mathbf{F}$.

These results are compared to the Voigt's and Reuss's upper and lower limits.

2. Effective elastic moduli

Let us assume that a macroscopic elastic moduli exists in specific regions of a composite material. This implies that the scale of fluctuation (and the range of inhomogeneity) is very small compared to the dimensions of the specimen under investigation. The local elastic moduli $\mathbf{c}(\mathbf{r}) = c_{ijkl}$ tensor is a function of position and changes from point to point depending on the property of each individual constituent. Globally, the distribution of the elastic moduli in this domain is statistically homogeneous. We also assume that Ergotic Hypothesis is valid within a representative coherent volume of the microstructure. It is further assumed that this scale of microstructure is much smaller than the material under investigation. In such a situation the macroscopic or effective elastic moduli tensor $\mathbf{C} = (C_{ijkl})$ may be calculated from the local moduli $\mathbf{c}$. Let us assume further that the complete statistical information in the form of correlation functions is available.

In the following paragraphs the averages are denoted over the representative volume V using brackets $\langle\ \rangle$. The average for the elastic moduli $\mathbf{c}$ is then represented as:

$$\langle c_{ijkl} \rangle = \langle c_{ijkl}(\mathbf{r}) \rangle = \frac{1}{V} \int_V c_{ijkl}(\mathbf{r})\, \mathrm{d}V \tag{1}$$

where $\mathbf{r}$ is the position vector. Because the specimen considered contains a sufficiently large number of grains of the second phase and is macroscopically homogeneous, Hill's condition [10] is valid. Then

$$\langle \boldsymbol{\varepsilon}\boldsymbol{\sigma} \rangle = \langle \boldsymbol{\varepsilon}\mathbf{c}\boldsymbol{\varepsilon} \rangle = \langle \boldsymbol{\varepsilon} \rangle \langle \mathbf{c}\boldsymbol{\varepsilon} \rangle \tag{2}$$

This condition was originally proposed by Hill and later used by Kröner [2] to derive the effective elastic law for a linearly elastic heterogeneous material. Here $\boldsymbol{\varepsilon} = \varepsilon_{ij}$ is the local strain tensor which varies on a microscopic scale. So the two definitions of the effective elastic moduli tensor $\mathbf{C}$ are simultaneously satisfied,

$$\langle \boldsymbol{\varepsilon} \rangle \mathbf{C} \langle \boldsymbol{\varepsilon} \rangle = \langle \boldsymbol{\varepsilon}\mathbf{c}\boldsymbol{\varepsilon} \rangle, \qquad \mathbf{C} \langle \boldsymbol{\varepsilon} \rangle = \langle \mathbf{c}\boldsymbol{\varepsilon} \rangle \tag{3}$$

The latter will be used in this formulation.

A fourth rank tensor $\mathbf{a} = (a_{ijkl})$ is introduced here to represent the local inhomogeneity. If the local deviation from the macroscopic strain is denoted by ε', then

$$\boldsymbol{\varepsilon}' = \boldsymbol{\varepsilon} - \langle \boldsymbol{\varepsilon} \rangle = \mathbf{a} \langle \boldsymbol{\varepsilon} \rangle \tag{4}$$

From Eqs. (3) and (4), a new equation for $\mathbf{C}$ can be written.

$$\mathbf{C} = \langle \mathbf{c} \rangle + \langle \mathbf{c}'\mathbf{a} \rangle \tag{5}$$

where $\mathbf{c}' = \mathbf{c} - \langle \mathbf{c} \rangle$ represents the deviation from the average. For effective elastic moduli $\mathbf{C}$, $\langle \mathbf{c}'\mathbf{a} \rangle$ can be considered as a correction term to $\langle \mathbf{c} \rangle$. Eq. (5) shows that all specimens which satisfy $\langle \mathbf{c} \rangle$ and $\langle \mathbf{c}'\mathbf{a} \rangle$ will result in the same effective elastic moduli, though the distribution of the local moduli c_{ijkl} may be different. This implies that a complete spatial distribution of c_{ijkl} is not necessary for the calculation of $\mathbf{C}$ and the full statistical information is enough. In order to represent $\mathbf{C}$ as a function of $\mathbf{c}$, the correlation between $\langle \mathbf{c}'\mathbf{a} \rangle$ and $\mathbf{c}$ is needed.

Locally, equilibrium is required throughout the specimen,

$$(c_{ijkl}\varepsilon_{kl})_{,j} = [(\langle c_{ijkl} \rangle + c'_{ijkl})(\langle \varepsilon_{kl} \rangle + \varepsilon'_{kl})]_{,j} = 0 \tag{6}$$

Commas represent partial differentiation with respect to position. Performing the differentiation and rearranging terms,

$$\langle c_{ijkl} \rangle \varepsilon'_{kl,j} = -(c'_{ijkl})_{,j} \langle \varepsilon_{kl} \rangle - (c'_{ijkl}\varepsilon'_{kl})_{,j} \tag{7}$$

This set of partial differential equations can be solved by the use of the elastic Green's function tensor $G_{lm}(\mathbf{r}_{12})$ through

$$\langle c_{ijkl} \rangle G_{lm,ik}(\mathbf{r}_{12}) + \delta(\mathbf{r}_{12})\delta_{jm} = 0 \tag{8}$$

where $\delta(\boldsymbol{r}_{12})$ is the Dirac's delta function for the vector relating any two points in the microstructure $\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$. G_{lm} can be written as a Fourier integral over the infinite $\mathbf{k}$-space:

$$G_{lm}(\mathbf{r}_{12}) = \frac{1}{8\pi^3} \int_{\mathbf{k} \in k^3} \tilde{G}_{lm}(\mathbf{k})\, \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_{12}}\, \mathrm{d}k^3 \tag{9}$$

where $\tilde{G}_{lm}(\mathbf{k})$ can be obtained from the Fourier transforms of Eq. (8):

$$-\langle c_{ijkl} \rangle k_i k_k \tilde{G}_{lm}(\mathbf{k}) + \delta_{jm} = 0 \tag{10}$$

For an isotropic tensor $\langle \mathbf{c} \rangle$ with Lamé constants $\bar{\lambda}$ and $\bar{\mu}$

$$\tilde{G}_{lm}(\mathbf{k}) = \frac{-(\bar{\lambda} + \bar{\mu})k_1 k_m + (\bar{\lambda} + 2\bar{\mu})k^2 \delta_{lm}}{\bar{\mu}(\bar{\lambda} + 2\bar{\mu})k^4} \tag{11}$$

and then

$$G_{lm}(\mathbf{r}_{12}) = \frac{1}{8\pi\bar{\mu}|\mathbf{r}_{12}|} \left\{ 2\delta_{lm} - \frac{\bar{\lambda} + \bar{\mu}}{\bar{\lambda} + 2\bar{\mu}} \left(\delta_{lm} - \frac{r_l r_m}{|\mathbf{r}_{12}|^2} \right) \right\} \tag{12}$$

where r_i and r_j are the components of the vector $\mathbf{r}_{12}$ (see Fig. 1).

The solution of Eq. (6) can be written as

$$\varepsilon'_{kl}(\mathbf{r}_1) = \int_V \mathrm{d}\mathbf{r}_2 G_{ik,l}(\mathbf{r}_{12})[c'_{ijmn}(\mathbf{r}_2)_{,j}\langle\varepsilon_{mn}\rangle + (c'_{ijmn}(\mathbf{r}_2)\varepsilon'_{mn}(\mathbf{r}_2))_{,j}] \tag{13}$$

Replacing $\boldsymbol{\varepsilon}'$ by $\mathbf{a}$ according to Eq. (4), the fourth rank tensor $\mathbf{a}$ is obtained.

$$a_{klmn}(\mathbf{r}_1) = \int_V \mathrm{d}\mathbf{r}_2 G_{ik,l}(\mathbf{r}_{12})[c'_{ijmn}(\mathbf{r}_2)_{,j} + (c'_{ijpq}(\mathbf{r}_2)a_{pqmn}(\mathbf{r}_2))_{,j}] \tag{14}$$

Integrating by parts, and noting that $\int_V \mathrm{d}\mathbf{r}_2\{G_{ik,l}(\mathbf{r}_{12})\times [c'_{ijmn}(\mathbf{r}_2) + c'_{ijpq}(\mathbf{r}_2)a_{pqmn}(\mathbf{r}_2)]\}_{,j}$ equals zero, we get

$$a_{klmn}(\mathbf{r}_1) = -\int_V \mathrm{d}\mathbf{r}_2 G_{ik,l}(\mathbf{r}_{12})[c'_{ijmn}(\mathbf{r}_2) + (c'_{ijpq}(\mathbf{r}_2)a_{pqmn}(\mathbf{r}_2))] \tag{15}$$

This equation can be solved by iteration (either numerically or analytically). An analytical representation can be produced by introducing a_{klmn} back into Eq. (15). $\mathbf{a}$ can be written as

$$a_{klmn} = a^{(1)}_{klmn} + a^{(2)}_{klmn} + a^{(3)}_{klmn} + \cdots \tag{16}$$

where

$$\begin{aligned} a_{klmn}(\mathbf{r}_1) &= -\int_V \mathrm{d}\mathbf{r}_2 G_{ik,jl}(\mathbf{r}_{12})c'_{ijmn}(\mathbf{r}_2) \\ a^{(2)}_{klmn}(\mathbf{r}_1) &= \int_V \mathrm{d}\mathbf{r}_2 G_{ik,jl}(\mathbf{r}_{12})[c'_{ijpq}(\mathbf{r}_2)\int_V \mathrm{d}\mathbf{r}_3 G_{rp,sq}(\mathbf{r}_{23})c'_{rsmn}(\mathbf{r}_3)] \\ &\vdots \end{aligned} \tag{17}$$

From Eq. (17), $\langle\mathbf{c}'\mathbf{a}\rangle$ can be obtained

$$\begin{aligned} \langle c'_{abkl}(\mathbf{r}_1)a^{(1)}_{klmn}(\mathbf{r}_1)\rangle &= -\int_V \mathrm{d}\mathbf{r}_{12} G_{ik,jl}(\mathbf{r}_{12})\langle c'_{abkl}(\mathbf{r}_1)c'_{ijmn}(\mathbf{r}_2)\rangle \\ \langle c'_{abkl}(\mathbf{r}_1)a^{(2)}_{klmn}(\mathbf{r}_1)\rangle &= \int_V \mathrm{d}\mathbf{r}_{12} G_{ik,jl}(\mathbf{r}_{12})\int_V \mathrm{d}\mathbf{r}_{23} G_{rp,sq}(\mathbf{r}_{23})\langle c'_{abkl}(\mathbf{r}_1)c'_{ijpq}(\mathbf{r}_2)c'_{rsmn}(\mathbf{r}_3)\rangle \\ &\vdots \end{aligned} \tag{18}$$

Here $\langle c'_{abkl}(\mathbf{r}_1)c'_{ijmn}(\mathbf{r}_2)\rangle$ and $\langle c'_{abkl}(\mathbf{r}_1)c'_{ijpq}(\mathbf{r}_2)c'_{rsmn}(\mathbf{r}_3)\rangle$ represent two-point and three-point correlation functions, respectively.

3. Correlation functions

In this section, the correlation functions that provide the statistical information are formulated using the polarized tensor c'_{ijkl}. Correlation functions are equivalent to the moments of the probability density function defined in the probability theory [2]. For instance, two-dimensional moments of the two-dimensional density $P_2(\mu_1, \mu_2)$ are defined as

$$\overline{\mu_1^j \mu_2^k} \equiv E(\mu_1^j \mu_2^k) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \mu_1^j \mu_2^k P_2(\mu_1, \mu_2)\,\mathrm{d}\mu_1\,\mathrm{d}\mu_2 \tag{19}$$

They describe a certain relationship or correlation between the results of measurements μ_1 at point x_1 and time t_1 and the results of measurements μ_2 at point x_2 and time t_2.

Correlation functions in Eq. (18) are represented as $\langle c'_{abkl}(\mathbf{r}_1)c'_{ijmn}(\mathbf{r}_2)\rangle$ and $\langle c'_{abkl}(\mathbf{r}_1)c'_{ijpq}(\mathbf{r}_2)c'_{rsmn}(\mathbf{r}_3)\rangle$. The former is a two-point correlation function and the latter is a three-point correlation function. They are defined as

$$\begin{aligned} \langle c'_{abkl}(\mathbf{r}_1)c'_{ijmn}(\mathbf{r}_2)\rangle &= \frac{1}{V}\int_V c'_{abkl}(\mathbf{r}_1)c'_{ijmn}(\mathbf{r}_2)\,\mathrm{d}V\Big|_{\mathbf{r}_{12}} \\ &= \frac{1}{V}\int_V c'_{abkl}(\mathbf{r}_1)c'_{ijmn}(\mathbf{r}_1+\mathbf{r}_{12})\,\mathrm{d}\mathbf{r}_1\Big|_{\mathbf{r}_{12}} \end{aligned} \tag{20}$$

$$\begin{aligned} &\langle c'_{abkl}(\mathbf{r}_1)c'_{ijpq}(\mathbf{r}_2)c'_{rsmn}(\mathbf{r}_3)\rangle \\ &= \frac{1}{V}\int_V c'_{abkl}(\mathbf{r}_1)c'_{ijpq}(\mathbf{r}_2)c'_{rsmn}(\mathbf{r}_3)\,\mathrm{d}V\Big|_{\mathbf{r}_{12},\mathbf{r}_{23}} \\ &= \frac{1}{V}\int_V c'_{abkl}(\mathbf{r}_1)c'_{ijpq}(\mathbf{r}_1+\mathbf{r}_{12})c'_{rsmn}(\mathbf{r}_1+\mathbf{r}_{12}+\mathbf{r}_{23}) \\ &\quad\times \mathrm{d}\mathbf{r}_1\Big|_{\mathbf{r}_{12},\mathbf{r}_{23}} \end{aligned} \tag{21}$$

where $|_{\mathbf{r}_{12}}$, $|_{\mathbf{r}_{12},\mathbf{r}_{23}}$ represent integration for fixed $\mathbf{r}_{12}$, $\mathbf{r}_{12}$ and $\mathbf{r}_{23}$, respectively. Assume the validity of the ergodic hypothesis, which permits the interchange of volume averages with ensemble averages. Eqs. (20) and (21) for two-point, three-point correlations can be rewritten as

$$\begin{aligned} \langle c'_{abkl}(\mathbf{r}_1)c'_{ijmn}(\mathbf{r}_2)\rangle &= \int_{\mathbf{h}_1\in\mathbf{c}'}\int_{\mathbf{h}_2\in\mathbf{c}'} c'_{abkl}(\mathbf{r}_1)c'_{ijmn}(\mathbf{r}_2) \\ &\quad\times P_2(\mathbf{r}_1|\mathbf{h}_1,\mathbf{r}_2|\mathbf{h}_2)\,\mathrm{d}\mathbf{h}_1\,\mathrm{d}\mathbf{h}_2 \end{aligned} \tag{22}$$

$$\begin{aligned} \langle c'_{abkl}(\mathbf{r}_1)c'_{ijpq}(\mathbf{r}_2)c'_{rsmn}(\mathbf{r}_3)\rangle &= \int_{\mathbf{h}_1\in\mathbf{c}'}\int_{\mathbf{h}_2\in\mathbf{c}'}\int_{\mathbf{h}_3\in\mathbf{c}'} \\ &\quad\times c'_{abkl}(\mathbf{r}_1)c'_{ijpq}(\mathbf{r}_2)c'_{rsmn}(\mathbf{r}_3)P_3(\mathbf{r}_1|\mathbf{h}_1,\mathbf{r}_2|\mathbf{h}_2,\mathbf{r}_3|\mathbf{h}_3)\,\mathrm{d}\mathbf{h}_1\,\mathrm{d}\mathbf{h}_2\,\mathrm{d}\mathbf{h}_3 \end{aligned} \tag{23}$$

Table 1
Limiting conditions for the two-point probability function

P_{ij}	Boundary conditions		Result coefficients	
	$r=0$	$r\to\infty$	$\alpha_{ij}=$	$\beta_{ij}=$
P_{11}	V_1	V_1^2	V_1^2	V_1V_2
P_{12}	0	V_1V_2	V_1V_2	$-V_1V_2$
P_{21}	0	V_1V_2	V_1V_2	$-V_1V_2$
P_{22}	V_2	V_2^2	V_2^2	V_1V_2

where P_2 and P_3 are the two-point and three-point probability density functions and $\mathbf{r}_1|\mathbf{h}_1$, $\mathbf{r}_2|\mathbf{h}_2$, $\mathbf{r}_3|\mathbf{h}_3$ refer to the states $\mathbf{h}_1$, $\mathbf{h}_2$ and $\mathbf{h}_3$ for $\mathbf{c}'$ to occur at positions $\mathbf{r}_1$, $\mathbf{r}_2$ and $\mathbf{r}_3$, respectively. P_2 is a function of $\mathbf{r}_2-\mathbf{r}_1$, $\mathbf{h}_1$ and $\mathbf{h}_2$, and P_3 is a function of $\mathbf{r}_2-\mathbf{r}_1$, $\mathbf{r}_3-\mathbf{r}_2$, $\mathbf{h}_1$, $\mathbf{h}_2$ and $\mathbf{h}_3$.

In order to solve Eqs. (22) and (23), which are critical to the final evaluation of $\mathbf{C}$, we need to know the probability functions P_2 and P_3. In this paper, the focus is on the two-point correlation function and its limitation in predicting the effective properties for a two-isotropic phase composite material, and consequently the contribution from the three-point probability function is ignored.

Different forms of probability functions have been already been introduced by others [35,42,43]. The formulation introduced here is independent of the mathematical form chosen for the probability function. The probability data can be calculated from the microstructure and saved as a data file used later by the present formulation. The existence of a mathematical form would allow one to perform a statistical study on the parameters in the formulation to compare various types of microstructures. For the purpose of this paper a mathematical form for the two-point probability function is used here [41,42]:

$$P_{ij}(r)=\alpha_{ij}+\beta_{ij}\,\mathrm{e}^{-m_{ij}r^{n_{ij}}} \tag{24}$$

where $i=1,2$, $j=1,2$ for a two-phase material; $P_{ij}(r)$ represents the probability occurrence of one point in phase i and the other point which is located at a distance r away in phase j. α_{ij} and β_{ij} depend on the volume fractions V_1, and V_2 of the two phases (Table 1). m_{ij} and n_{ij} are empirical constants determined by a least squares fit for the measured data and the functional form chosen for P_{ij}. m_{ij} and n_{ij} describe the statistical information of the distribution and morphology of materials. In Eq. (24) the distance r between two points is the main parameter used in the analysis. This equation represents a material, which is orientationally random. This does not mean that the material is necessarily isotropic in property, but that the probability distribution function, which is used to represent the distribution of two phases, is orientation independent. The form of the probability functions presented here imposes the assumption that orientation of vectors connecting any two related points has no influence on the properties. Accordingly, only the magnitude of vectors plays a role here. For the two-isotropic-phase materials considered here, such an assumption is valid only if the second phase particles are statistically equiaxed and distributed randomly inside the first phase.

Assume that the elastic moduli tensor $\mathbf{c}$ for two phases are $\mathbf{c1}$ and $\mathbf{c2}$. The corresponsding polarized modulus tensor $\mathbf{c}'$ for either states $\mathbf{h}_1$ and $\mathbf{h}_2$ are $\mathbf{c1}'$ and $\mathbf{c2}'$. Now Eq. (22) can take the following form:

$$\begin{aligned}\langle c'_{abkl}(\mathbf{r}_1)c'_{ijmn}(\mathbf{r}_2)\rangle = {} & c1'_{abkl}c1'_{ijmn}P_2(\mathbf{r}_1|\mathbf{c1}',\mathbf{r}_2|\mathbf{c1}')\\ & + c1'_{abkl}c2'_{ijmn}P_2(\mathbf{r}_1|\mathbf{c1}',\mathbf{r}_2|\mathbf{c2}')\\ & + c2'_{abkl}c1'_{ijmn}P_2(\mathbf{r}_1|\mathbf{c2}',\mathbf{r}_2|\mathbf{c1}')\\ & + c2'_{abkl}c2'_{ijmn}P_2(\mathbf{r}_1|\mathbf{c2}',\mathbf{r}_2|\mathbf{c2}')\end{aligned} \tag{25}$$

where Eq. (24) is used to represent $P_2(\mathbf{r}_1|\mathbf{c1}',\mathbf{r}_2|\mathbf{c1}')$, $P_2(\mathbf{r}_1|\mathbf{c1}',\mathbf{r}_2|\mathbf{c2}')$, $P_2(\mathbf{r}_1|\mathbf{c2}',\mathbf{r}_2|\mathbf{c1}')$ and $P_2(\mathbf{r}_1|\mathbf{c2}',\mathbf{r}_2|\mathbf{c2}')$ in the form of P_{11}, P_{22}, P_{33} and P_{44} as described by the following equations:

$$P_2(\mathbf{r}_1|\mathbf{c1}',\mathbf{r}_2|\mathbf{c1}')=P_{11}=V_1^2+V_1V_2\exp(-m_{11}|\mathbf{r}_2-\mathbf{r}_1|^{n_{11}}) \tag{26}$$

$$P_2(\mathbf{r}_1|\mathbf{c1}',\mathbf{r}_2|\mathbf{c2}')=P_{21}=V_1V_2-V_1V_2\times\exp(-m_{21}|\mathbf{r}_2-\mathbf{r}_1|^{n_{21}}) \tag{27}$$

$$P_2(\mathbf{r}_1|\mathbf{c2}',\mathbf{r}_2|\mathbf{c1}')=P_{12}=V_2V_1-V_2V_1\times\exp(-m_{12}|\mathbf{r}_2-\mathbf{r}_1|^{n_{12}}) \tag{28}$$

$$P_2(\mathbf{r}_1|\mathbf{c2}',\mathbf{r}_2|\mathbf{c2}')=P_{22}=V_2^2+V_2V_1\exp(-m_{22}|\mathbf{r}_2-\mathbf{r}_1|^{n_{22}}) \tag{29}$$

4. Numerical simulation

From the iterative analytical series expansion defined in Eq. (18), the second term of Eq. (5), $\langle\mathbf{c}'\mathbf{a}\rangle$, can be formulated in the following way. Here we only take the first equation, which uses a two-point correlation function, neglecting all others. Then Eqs. (5), (18) and (26) are combined and the equation for the effective elastic moduli of the two-isotropic-phase composite material is obtained:

$$\begin{aligned}C_{abmn}=\langle c_{abmn}\rangle-\int_V \mathrm{d}\mathbf{r}_{12}G_{ik,\,jl}(\mathbf{r}_{12})\{ & c1'_{abkl}c1'_{ijmn}P_{11}\\ & + c1'_{abkl}c2'_{ijmn}P_{21}+c2'_{abkl}c1'_{ijmn}P_{12}\\ & + c2'_{abkl}c2'_{ijmn}P_{22}\}\end{aligned} \tag{30}$$

or in the short form,

$$\mathbf{C}=\langle\mathbf{c}\rangle-\mathbf{G}\times\mathbf{F} \tag{31}$$

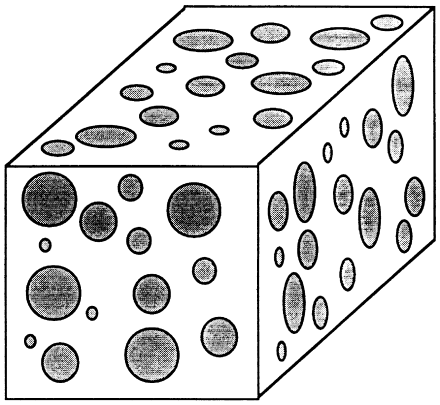

Fig. 2. Pseudo-random microstructure generated by computer.

where **F** is an 8th rank tensor of the form

$$F_{abklijmn} = c1'_{abkl}c1'_{ijmn}P_{11} + c1'_{abkl}c2'_{ijmn}P_{21} + c2'_{abkl}c1'_{ijmn}P_{12} + c2'_{abkl}c2'_{ijmn}P_{22} \quad (32)$$

For a representative two-phase material's microstructure where each phase is assumed to be isotropic (with elastic moduli tensor **c1**, **c2**), the distribution and morphology of the two phases can be represented by the volume fractions V_1, V_2 and the statistical constants m_{ij} and n_{ij} by proper experimental measurements.

In this paper a numerical routine is used to calculate the integral in Eq. (31). First, the specimen is divided in a number of cellular cubic regions appropriate for numerical integration. The cube is further divided into a number of cubes, the size of which is assumed to be small enough, to represent the complete microstructure. There are three rules for this numerical construction. First, the cubic region must contain sufficient number of grains of the two phases so that it can be taken as a statistical representation of the entire specimen. Second, the number of unit cubes is calculated based on a representative grain or size scale within the microstructure (such that the average size of such grains, are much greater than the unit cube size). Third, the cubic region is chosen large enough so that the corresponding Green's function for the maximum $\mathbf{r}_{12}$ falls within the expected error according to the higher order terms in Eq. (6). Fig. 1 shows the geometry of two cubes in the numerical model.

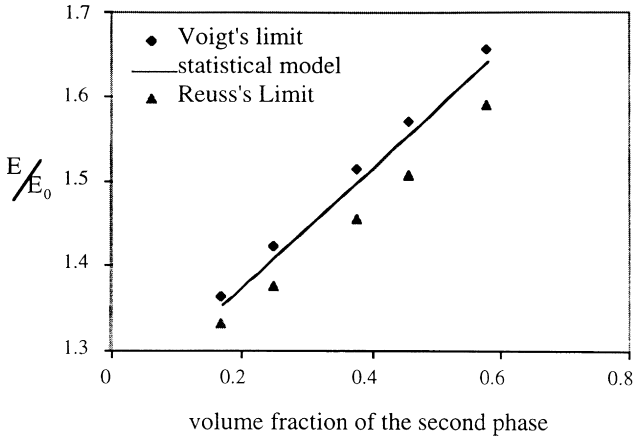

Fig. 3. The comparison of the effective Young's modulus E calculated by statistical model, Voigt's lower and Reuss's upper limits (E_0 is a reference modulus).

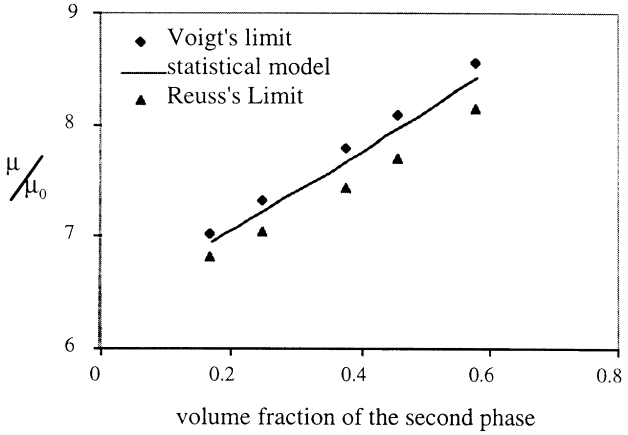

Fig. 4. The comparison of the effective shear modulus μ calculated by statistical model, Voigt's lower and Reuss's upper limits (μ_0 is a reference modulus).

Assume each cube comprises only of one phase. For each pair of cubes (shown by Fig. 1), **F** is taken to be constant over the two V_cs. Then, the numerical form for the calculation of $\mathbf{G}\times\mathbf{F}$ can be presented as

$$\mathbf{G}\times\mathbf{F} = \sum_{\substack{V'_c\in V \\ V_c\in V}} F_{abklijmn} \int_{\substack{\mathbf{r}_2\in V'_c \\ \mathbf{r}_1\in V_c}} \mathrm{d}\mathbf{r}_{12} G_{ik,jl}(\mathbf{r}_{12}) \quad (33)$$

5. Results and comparison

The simulation of the statistical theory was applied to a set of samples of composite materials with varying familiar geometries and distribution. A computer generated pseudo-random microstructure (see Fig. 2) was used to calculate the proper statistics for the analysis. In this microstructure, the spheres with varying radius represent randomly distributed second phase inclusions. The centers of these spheres were chosen at random and their radii were also varied at random. The corresponding statistical parameters m_{ij} and n_{ij} were measured also by a computer program. The numerical scheme measures the two-point probabilities (appearing on the left side of Eq. (24)) directly from the microstructure for all values of r. The constants m_{ij} and n_{ij} are then obtained by a least squares fit to the probabilities data and the functional form represented by Eq. (24). The values for r are incremented in steps of unity, the size of which is much less than the average size of grains of the second phase. A numerical model is constructed following the three rules

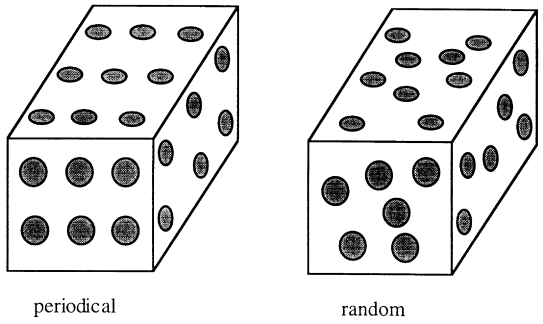

Fig. 5. Two microstructures generated by computer.

described earlier. A cubic region is chosen and divided into a number of smaller cubes with size unity. This unit size is equivalent with increments of r used in the measurement of m_{ij} and n_{ij}. For the examples which follow a $15 \times 15 \times 15 = 3375$ small cubes are used for the numerical simulation. This number was chosen based on a convergence analysis by repeating the simulation for cubic regions consisting of $8 \times 8 \times 8 = 512$ and $12 \times 12 \times 12 = 1728$ smaller cubes. The results show that the error was reduced from 1.9 to 0.5% as compared for the simulation of the results for a region consisting of $15 \times 15 \times 15 = 3375$ cubes.

Five samples were generated which contained the same two isotropic phases with varying volume fractions of the reinforcement phase (0.17, 0.25, 0.38, 0.46 and 0.58, respectively). Lamé constants λ and μ are known for both phases. Figs. 3 and 4 present the results of the simulation for the calculated effective constants of samples together with the two bounds of the Voigt and Reuss theories. The statistical theory predicts the effective modulus to be closer to the Voigt's limit (22% for Young's modulus E, and 25% for Lamé constant μ or shear modulus) than Reuss.

The following additional example is chosen to show the effectiveness of the model in distinguishing different microstructures with random or periodic distributions. In these examples, the size of the second phase is kept constant. The mathematical form (Eq. (24)) introduced earlier for a randomly distributed microstructure cannot be used for a periodic composite as in this example. Because of the simple form of periodic distribution, a mathematical form was not needed. The simulations are performed for five different volume fractions (0.17, 0.25, 0.38, 0.46 and 0.58) for the two composites in Fig. 5. The results of the simulations for these samples are shown in Figs. 6 and 7. A lower elastic modulus is observed for the microstructure with periodic arrangement than that of the random one because of the presence of more correlations.

Other models based on one point probability functions (volume fractions) cannot distinguish between the two microstructures shown in the example above. Composites are developed with a variety of second phase size distributions which deviate from a periodic microstructure or a randomly distributed one. For some well-known interwoven composites with periodic distributions, closed form solutions may not be available either. The statistical formulation presented here can deal with any distribution.

The main purpose for the present paper was the incorporation of the two point probability functions in the statistical continuum theory, and therefore, a simple form of the probability functions is used for this paper. The statistical mechanics model can be applied to any microstructure with any distribution or shape of the second phase. Any form of probability function can be used to calculate the effective properties. In the absence of such forms, the data from real microstructures can be deduced in the form of probability data. The statistical formulation can then use these data instead of the closed form presented here to simulate the effective properties. The example chosen here covers a wide range of particulate reinforced composites with varying size distribution of the second phase. It was important to find effective properties for this example and some well-known composites (random, periodic, spherical inclusion,…) to show the effectiveness of the model. The present examples are very realistic and many particulate composites of much lower volume fractions can be included in this category. The result of the analysis for the computer-generated

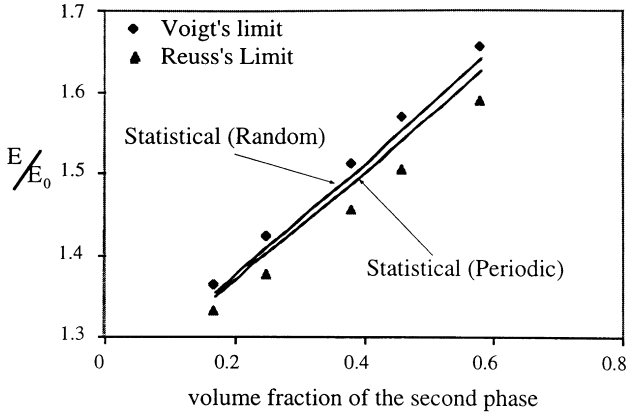

Fig. 6. The comparison of the effective Young's modulus E for two microstructures.

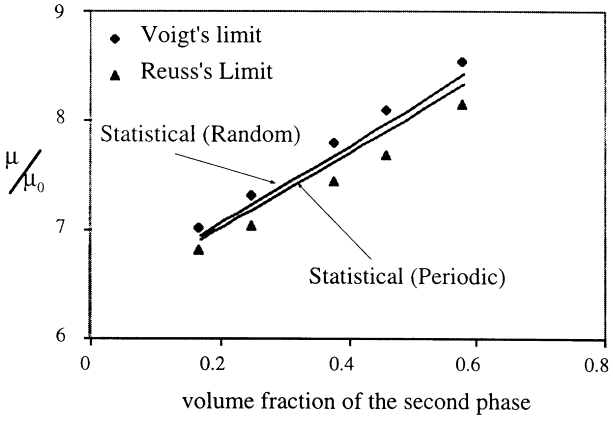

Fig. 7. The comparison of the effective shear modulus μ for two microstructures.

microstructure presented here shows the strength of the model and its capability for a wide range of applications and microstructures. A more general mathematical form of the probability functions can simplify the numerical scheme and speed up the simulation. In the absence of such forms, a large number of probability data is needed to produce reliable data. With the production of other forms of the probability functions suitable for anisotropic microstructures, the application of the present model can be extended. The closed form can also provide information about the microstructure in the form of a number of parameters (volume fraction, aspect ratio,…) that can be interpreted and compared to some ideal microstructures.

6. Summary

This paper focuses on the application of the statistical continuum theory to an elastic composite material consisting of two isotropic phases. First, the statistical theory for the effective elastic moduli of composite materials is formulated. A two-point probability function is used for calculating the two-point correlations that are the key to the statistical model. The calculated results fall within the well known upper and lower bounds due to Voigt and Reuss. The results are however closer to Voigt. The two-point correlation functions discussed here and used in the simulation are the first order corrections to the Voigt's limit. Better approximations may be obtained for more complex geometries and distributions by considering third order corrections and higher. These higher order terms require the use of higher order probability functions (third,…).

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