Computational Materials Science 116 (2016) 113–121

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Micro-scale modeling of phase-level elastic fields of SiC reinforced metal matrix multiphase composites using statistical approach

Mikhail Tashkinov

Laboratory of Mechanics of Perspective Structural and Functional Materials, Perm National Research Polytechnic University, Komsomolsky Ave. 29, 614990 Perm, Russia

ARTICLE INFO

Article history:
Received 30 June 2015
Received in revised form 28 October 2015
Accepted 30 October 2015
Available online 17 November 2015

Keywords:
Correlation functions
Random microstructure
Statistics
Metal matrix composites
High order moments
Multiphase RVE

ABSTRACT

This work is devoted to development of instruments of the statistical mechanics as well as to their application in studying microstructural behavior of the metal matrix composites reinforced with randomly positioned silicon carbide (SiC) particles. The micro-scale representative volume element (RVE) models of the materials were studied. Their microstructure was described with the correlation functions of different orders. Analytical expressions for the local stress and strain fields' statistics were obtained using the solution of the boundary value problem in statistical formulation. The developed analytical model allows to take into account both geometrical parameters of microstructure and physical–mechanical properties of constituents. The case studies of multiphase Ti + SiC and Al + SiC metal matrix composites were investigated. Analysis of influence of the microstructural parameters on behavior of each of the phases was performed with obtaining of the numerical results for the statistics of stress and strain fields.
© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Extensive interest in developing of new composite materials is supported by highly demanding tasks formulated by aerospace, automotive, electronics and other industries. The distinct class of the composites represents metal matrix, reinforced by particles of different geometrical and mechanical properties. Compared to the traditional materials and polymer matrix composites, for a number of applications metal matrix composites (MMCs) reveal better behavior under high temperatures, greater strength, improved resistance to wear and high cycle fatigue, higher stiffness-to-weight ratio, significant electrical and thermal conductivity.

Creation of analytical instruments, which can deliver recommendations for the optimal design of composite materials, appropriate to particular applications, is an important task. It was proved that the effect of constituents' distribution plays crucial role on the macro-scale behavior of composites [1–5]. Such studies were also performed for MMCs, which reinforcement types range from fibers to particles [6–8]. Precise microstructural mechanical modeling of such materials gives an opportunity for prediction of their effective behavior, taking into account micro-scale peculiarities, such as size of particles, their volume fraction, orientation, dispersion and clustering.

The approach, which this work is devoted to, is based on methods of the statistics and the theory of random functions. It presumes that the microstructural behavior of materials can be evaluated by local fields' statistics, such as first and second order moments [9–11].

The aim of this work is to develop methodology of obtaining of high order statistical descriptors for RVEs of multiphase metal matrix composites with embedded silicon carbide (SiC) randomly distributed inclusions. The derived analytical model, in general, is suitable to any multiphase composite. As the numerical case studies, the most common MMC composites with aluminum (Al) and titanium (Ti) matrix, reinforced by SiC inclusions, were analyzed.

2. Methodology description

2.1. Characterization of random microstructure

The microstructure of particle-reinforced composites often represents random heterogeneous multiphase media. According to the statistical approach, the indicator functions $\lambda_C(\vec{r})$ can be introduced to define morphology of such materials on a microscopic scale [11–13]. Values of these functions depend on position of the radius-vector $\vec{r}$ in the RVE. Particularly, $\lambda_C(\vec{r}) = 1$ if the radius-vector indicates phase C and $\lambda_C(\vec{r}) = 0$ otherwise.

Taking that into account, the stiffness tensor for such RVE is statistically homogenous and is defined as a sum of products of a stiffness tensor $C^{(z)}_{ijkl}$ and respective indicator function $\lambda_C(\vec{r})$ for each

http://dx.doi.org/10.1016/j.commatsci.2015.10.047
0927-0256/© 2015 Elsevier B.V. All rights reserved.

constituent. As a result, it takes a form of the piecewise constant coordinate function:

$$C_{ijkl}(\vec{r}) = \sum_{z=1}^{n} \lambda_C(\vec{r}) C_{ijkl}^{(z)} \tag{1}$$

Averaging Eq. (1) gives a constant isotropic tensor, which depends on the volume fractions of phases:

$$\langle C_{ijkl}(\vec{r}) \rangle = \sum_{z=1}^{n} p_{(z)} C_{ijkl}^{(z)} \tag{2}$$

where $p_{(z)} = \langle \lambda_{(z)}(\vec{r}) \rangle$ is the volume fraction of the phase z.

The hypothesis of ergodicity of the random functions $\lambda_C(\vec{r})$ allows to consider ensemble averaging of RVE's realizations equal to the averaging by a single volume [14]. In other words, it is possible to state that $\langle \lambda_{(z)}(\vec{r}) \rangle = \langle \lambda_{(z)}(\vec{r}_1) \rangle$ for every $\vec{r}$ and $\vec{r}_1$. Taking this into account, the stiffness tensors $C_{ijkl}(\vec{r})$ and the indicator functions $\lambda_C(\vec{r})$ for the RVE can be decomposed into two summands – an averaged value and a fluctuation:

$$C_{mnkl}(\vec{r}) = \langle C_{mnkl}(\vec{r}) \rangle + C'_{mnkl}(\vec{r}), \tag{3}$$

$$\lambda_C(\vec{r}) = \langle \lambda_C(\vec{r}) \rangle + \lambda'_C(\vec{r}), \tag{4}$$

where fluctuations define at which extent the value of the function differs from the averaged one. In other terms, it shows how the random structure would be different from the periodical one with the same geometrical parameters [15].

Besides the constants that quantitatively describe the structural geometrical basics, the instruments of statistical approach offer descriptors for assessing the spatial interaction between micro-scale structural components [11]. The most widely used one is the correlation functions, which describe how microscopic particles at different positions inside RVE are related [12,16]. Thus, the n-order correlation function can be defined as the average of the scalar product of n random variables at different positions of radius-vectors $\vec{r}, \vec{r}_1, \ldots, \vec{r}_n$. For the fluctuation of random indicator function, expression for the correlation function in general can be written as:

$$\begin{aligned} K_{\lambda_C}^{(n)}(\vec{r}, \vec{r}_1, \ldots, \vec{r}_n) &= \langle \lambda'_C(\vec{r}_1) \lambda'_C(\vec{r}_2) \ldots \lambda'_C(\vec{r}_n) \rangle \\ &= \langle (\lambda_C(\vec{r}_1) - p_C)(\lambda_C(\vec{r}_2) - p_C) \ldots (\lambda_C(\vec{r}_n) - p_C) \rangle, \end{aligned} \tag{5}$$

The correlation functions are sensitive to such parameters as arrangement, orientation and shape of microstructural constituents. Theoretically, the infinite number of the correlation functions can uniquely determine the microstructural morphology of composites. These functions are used as the geometrical descriptors in the problems of obtaining high order statistics for micro-stress and strain fields [11,12,17].

The methodology of correlation functions requires initial experimental data regarding the internal structure of composites RVE. The imaging techniques, such as micro-CT, are commonly used for microstructural characterization [14,18]. Another way is modeling using some predetermined geometrical parameters. In order to obtain the values of the correlation functions (5) for the microstructure, it is necessary to know the fields of indicator functions (4) values. They can be obtained by implementing algorithm, which maps a RVE with a fixed step grid and checks the presence of phases in its every node (see Fig. 1). Precision of the functions depends then on the step of the grid.

2.2. Micro-scale stress and strain fields statistics

In the terms of statistical mechanics approach, the local fields, such as displacements u_m, strain ε_{ij} and stress σ_{ij} inside RVE with random microstructure are usually considered random functions. They depend on the radius-vector and can be represented similarly to Eqs. (3) and (4):

$$u_m(\vec{r}) = \langle u_m(\vec{r}) \rangle + u'_m(\vec{r}), \tag{6}$$

$$\varepsilon_{ij}(\vec{r}) = \langle \varepsilon_{ij}(\vec{r}) \rangle + \varepsilon'_{ij}(\vec{r}), \tag{7}$$

$$\sigma_{ij}(\vec{r}) = \langle \sigma_{ij}(\vec{r}) \rangle + \sigma'_{ij}(\vec{r}). \tag{8}$$

The multipoint statistics, calculated for stress and strain fields in RVE as well as in each phase separately, can be used for analysis of microstructural parameters' influence on behavior of heterogeneous materials. The mean values in Eqs. (6)–(8) are constants, therefore the statistics are constructed for the fluctuations. The widespread models for calculating effective material's characteristics usually operate the first and the second order moments of the local fields [10,11]. The first-order moments represents average values, while the second-order moments are also referred as dispersions.

The average values of stress and strain in RVE depend on loading and on the effective stiffness tensor C^*_{ijkl}. The formulas for the second-order moment for strain fields $\langle \varepsilon'_{ij}(\vec{r}) \varepsilon'_{\alpha\beta}(\vec{r}) \rangle$ in the whole RVE can be constructed using the fluctuations of displacements $u'_m(\vec{r})$ and the Cauchy relations $\varepsilon'_{ij}(\vec{r}) = \frac{1}{2}(u'_{i,j}(\vec{r}) + u'_{j,i}(\vec{r}))$. The second-order moment for stress can be defined by taking into account the state equation $\sigma_{ij}(\vec{r}) = C_{ijkl}(\vec{r}) \varepsilon_{kl}(\vec{r})$, Eq. (8) and stress fluctuations, which are expressed as following:

$$\begin{aligned} \sigma'_{ij}(\vec{r}) &= \sigma_{ij}(\vec{r}) - \langle \sigma_{ij} \rangle \\ &= C'_{ijkl}(\vec{r}) \langle \varepsilon_{kl}(\vec{r}) \rangle - \langle C'_{ijkl}(\vec{r}) \varepsilon'_{kl}(\vec{r}) \rangle + \langle C_{ijkl}(\vec{r}) \rangle \varepsilon'_{kl}(\vec{r}). \end{aligned} \tag{9}$$

Formulas for the first- and second-order strain and stress moments for a phase C were for the first time obtained by Volkov [19] and contain mixed moments, combining fluctuations of the indicator function and local fields:

$$\langle \varepsilon_{ij} \rangle_C = e_{ij} + \frac{1}{\langle \lambda_C(\vec{r}) \rangle} \langle \lambda'_C(\vec{r}) \varepsilon'_{ij}(\vec{r}) \rangle, \tag{10}$$

$$\langle \sigma_{ij} \rangle_C = \langle \sigma_{ij} \rangle + \frac{1}{\langle \lambda_C(\vec{r}) \rangle} \langle \lambda'_C(\vec{r}) \sigma'_{ij}(\vec{r}) \rangle, \tag{11}$$

$$\begin{aligned} \langle \varepsilon'_{ij}(\vec{r}) \varepsilon'_{\alpha\beta}(\vec{r}) \rangle_C &= \langle \varepsilon'_{ij}(\vec{r}) \varepsilon'_{\alpha\beta}(\vec{r}) \rangle + e_{ij} e_{\alpha\beta} - \langle \varepsilon_{ij} \rangle_C \langle \varepsilon_{\alpha\beta} \rangle_C \\ &+ \frac{1}{\langle \lambda_C(\vec{r}) \rangle} \Big(\langle \lambda'_C(\vec{r}) \varepsilon'_{ij}(\vec{r}) \varepsilon'_{\alpha\beta}(\vec{r}) \rangle + e_{ij} \langle \lambda'_C(\vec{r}) \varepsilon'_{\alpha\beta}(\vec{r}) \rangle \\ &+ e_{\alpha\beta} \langle \lambda'_C(\vec{r}) \varepsilon'_{ij}(\vec{r}) \rangle \Big), \end{aligned} \tag{12}$$

$$\begin{aligned} \langle \sigma'_{ij}(\vec{r}) \sigma'_{\alpha\beta}(\vec{r}) \rangle_C &= \langle \sigma'_{ij}(\vec{r}) \sigma'_{\alpha\beta}(\vec{r}) \rangle + \langle \sigma_{ij} \rangle \langle \sigma_{\alpha\beta} \rangle - \langle \sigma_{ij} \rangle_C \langle \sigma_{\alpha\beta} \rangle_C \\ &+ \frac{1}{\langle \lambda_C(\vec{r}) \rangle} \Big(\langle \lambda'_C(\vec{r}) \sigma'_{ij}(\vec{r}) \sigma'_{\alpha\beta}(\vec{r}) \rangle + \langle \sigma_{ij} \rangle \langle \lambda'_C(\vec{r}) \sigma'_{\alpha\beta}(\vec{r}) \rangle \\ &+ \Big\langle \sigma_{\alpha\beta} \rangle \langle \lambda'_C(\vec{r}) \sigma'_{ij}(\vec{r}) \rangle \Big\rangle \Big). \end{aligned} \tag{13}$$

The numerical calculation of the local fields' statistics is connected with finding the fluctuations of displacements, which can be obtained from solution of the boundary value problem in the stochastic formulation.

3. Boundary value problem

The stochastic boundary value problem (SBVP) contains the following equations:

$$\sigma_{ij,j}(\vec{r}) = 0, \tag{14}$$

$$\varepsilon_{ij}(\vec{r}) = 1/2(u_{i,j}(\vec{r}) + u_{j,i}(\vec{r})), \tag{15}$$

Download English Version:

https://daneshyari.com/en/article/1559991

Download Persian Version:

https://daneshyari.com/article/1559991

Daneshyari.com