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Statistical characteristics of structural stochastic stress and strain fields in polydisperse heterogeneous solid media

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ABSTRACT

The aim of this research is to develop the mechanisms of calculation of stress and strain fields' statistical characteristics in components of heterogeneous solid media in dependence on variation of internal and external parameters in elastoplastic case.

Analytical expressions for statistical characteristics of structural fields, such as mean values and dispersions, are formed using solution of stochastic boundary value problems and structural multipoint correlation functions. The boundary value problems have been solved in elastoplastic case in the second approximation with the Green's functions method. The multipoint correlation functions up to fifth order have been built for synthesized 3D material microstructure RVE models with polydisperse spherical inclusions.

New analytical expressions and numerical results for statistical characteristics in components of elastoplastic heterogeneous solids with different types of structural parameters and properties of the phases have been obtained for simple shear state of strain. Numerical results are presented for porous composites with different inclusions volume fraction in case of simple shear state of strain.

1. Introduction

The problem of determination of heterogeneous materials' properties is highly topical [1,7,11,13]. Considerable funds and efforts can be saved by replacing experimental testing with multi-scale simulations, so that material properties are obtained by modeling at smaller scales. Many computational methods are using the homogenization approach, which is well established for linear, periodic and deterministic models [1,13]. The question which is urgent for design of advanced materials with improved properties is how to incorporate results from nonlinear micro-scale models into macro-scale ones for heterogeneous materials with random non-periodic microstructures.

One of the problems of mechanics of heterogeneous materials and composites is calculation of parameters of stress and strain fields for each phase of material in order to predict fracture processes in dependence on various microstructural parameters. Failure and elastoplastic deformations depend on specific details of the local stress fields when fluctuations are important. In this case, the first way could be to check the observable stress fields for many realizations of the microstructure. Another (and more effective) approach is to estimate the statistical moments of the stress fields and restore the probability density function for invariants of tensors [1,4]. This function will allow calculate failure probability and establish links between fracture processes at microstructural and macroscopic scales.

Multi-scale hierarchy of heterogeneous materials is typically investigated using the Representative Volume Element (RVE) concept when parameters of larger scale models are measured or calculated on a smaller scale [2,5,8]. For non-periodic randomly reinforced heterogeneous solids, stochastic methods based on random functions theory are used for determination of the statistical characteristics of microscopic fields [1,12–15]. According to such methods, characteristics of stress and strain fields in distinct phases of composite are determined from the boundary value problem solution while statistical information about the heterogeneous structure is carried by multipoint correlation functions, which can be obtained by structure modeling or from real composite specimen analysis [1,6,13,15].

2. Statistical characteristics and boundary value problem

According to stochastic approach, the indicator function $\lambda(\vec{r})$ is used in physical and phenomenological equations to define properties of each phase of two-phase heterogeneous material on a

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microscopic scale [1,4,14,15]. Value of this function depends on position of the radius-vector $\vec{r}$ inside the RVE. Thus, for two-phase materials, $\lambda(\vec{r}) = 0$ if the radius-vector indicates matrix, and $\lambda(\vec{r}) = 1$ if it is inside the inclusion.

Fields of structural parameters of deformation process are presented in the form of statistically homogeneous coordinate functions, so that they take into account randomness of the relative position of elements in the structure and statistical dispersion of the components' properties. These functions depend on the radius-vector and can be developed as a sum of a mean and a fluctuation:

$$\sigma_{ij}(\vec{r}) = \langle\sigma_{ij}(\vec{r})\rangle + \sigma'_{ij}(\vec{r}) \tag{1}$$

$$\varepsilon_{ij}(\vec{r}) = \langle\varepsilon_{ij}(\vec{r})\rangle + \varepsilon'_{ij}(\vec{r}) \tag{2}$$

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

$$u_m(\vec{r}) = \langle u_m(\vec{r})\rangle + u'_m(\vec{r}), \tag{4}$$

$$\lambda(\vec{r}) = \langle\lambda(\vec{r})\rangle + \lambda'(\vec{r}) \tag{5}$$

where angle brackets $\langle\ \rangle$ denote a volume average, Eq. (1) is stress field, Eq. (2) is strain field, Eq. (3) is field of structural elasticity modulus, Eq. (4) is field of displacements, Eq. (5) is earlier introduced indicator function.

Deformation processes can be characterized with multipoint statistical moments of stochastic stress and strain fields in the microstructural components of a composite. The first order moments (or mean values) are usually suitable only for prediction of the effective elastic properties. The higher order moments are used in elastic and elastoplastic models for the fracture processes studying and for developing recommendations for the optimal design of new materials. In this work the methodology will be illustrated on the example of obtaining of the first two moments of microstructural fields, which can be used for reconstructing the probability density function for invariants of microscopic stress tensor with assumption of normal distribution of microscopic stress.

The formulas for mean values and second order moments (dispersions) in matrix M and inclusions I in general view are expressed through the fluctuations of stochastic fields (1)–(5):

$$\langle\varepsilon_{ij}\rangle_I = e_{ij} + \frac{1}{p}\langle\lambda'(\vec{r})\varepsilon'_{ij}(\vec{r})\rangle \tag{6}$$

$$\langle\varepsilon_{ij}\rangle_M = e_{ij} - \frac{1}{1-p}\langle\lambda'(\vec{r})\varepsilon'_{ij}(\vec{r})\rangle \tag{7}$$

$$\begin{aligned}\langle\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\rangle_I = {} & \langle\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\rangle + e_{ij}e_{\alpha\beta} - \langle\varepsilon_{ij}\rangle_I\langle\varepsilon_{\alpha\beta}\rangle_I \\ & + \frac{1}{p}\Big(\langle\lambda'(\vec{r})\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\rangle + e_{ij}\langle\lambda'(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\rangle + e_{\alpha\beta}\langle\lambda'(\vec{r})\varepsilon'_{ij}(\vec{r})\rangle\Big)\end{aligned} \tag{8}$$

$$\begin{aligned}\langle\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\rangle_M = {} & \langle\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\rangle + e_{ij}e_{\alpha\beta} - \langle\varepsilon_{ij}\rangle_M\langle\varepsilon_{\alpha\beta}\rangle_M \\ & - \frac{1}{1-p}\Big(\langle\lambda'(\vec{r})\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\rangle + e_{ij}\langle\lambda'(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\rangle + e_{\alpha\beta}\langle\lambda'(\vec{r})\varepsilon'_{ij}(\vec{r})\rangle\Big),\end{aligned} \tag{9}$$

where p is inclusions volume fraction. Expressions for stress field have the same structure. The moments $\langle\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta})(\vec{r})\rangle, \langle\lambda'(\vec{r})\varepsilon'_{ij}(\vec{r})\rangle$ and $\langle\lambda'(\vec{r})\varepsilon'_{ij}(\vec{r})\varepsilon'_{\alpha\beta}(\vec{r})\rangle$, which are part of Eqs. (6)–(9), can be analytically constructed using the stochastic boundary value problem solution in fluctuations of displacements $u'_m(\vec{r})$ and multipoint correlation functions of indicator function fluctuation $\lambda'(\vec{r})$.

The stochastic boundary volume problem statement for the RVE with boundary conditions in displacements can be defined as follows:

$$\sigma_{ij,j}(\vec{r}) = 0, \tag{10}$$

$$\varepsilon_{ij}(\vec{r}) = \frac{1}{2}\big(u_{i,j}(\vec{r}) + u_{j,i}(\vec{r})\big), \tag{11}$$

$$\sigma_{ij}(\vec{r}) = C_{ijkl}(\vec{r})\varepsilon_{kl}(\vec{r}), \tag{12}$$

$$u_i(\vec{r})|_{\vec{r}\in\Gamma_V} = \varepsilon^*_{ij}r_j, \tag{13}$$

where Eq. (10) is stress equilibrium equation, j stands for the derivative $\partial/\partial x_j$, Eq. (11) is Cauchy relations, Eq. (12) is state equation, $C_{ijkl}(\vec{r})$ is tensor of structural elasticity modulus. The boundary conditions (13) on the RVE surface are set in displacements and ensure uniformity of the macroscopic deformation, ε^*_{ij} is arbitrarily assigned constant symmetric tensor of small strains, $\vec{r}$ is radius-vector with components (x_1, x_2, x_3), r_j are coordinates of points on RVE surface Γ_V.

The type of interface between two phases of the material is ideal adhesion. In mathematical terms:

$$u_i^{(M)}(\vec{r})\Big|_{\vec{r}\in\Gamma_{V_M}} = u_i^{(I)}\Big|_{\vec{r}\in\Gamma_{V_I}}(\vec{r}),$$

where Γ_{V_M} is the inner surface of the matrix, Γ_{V_I} is the outer surface of an inclusion.

With the Green's function method, the boundary value problem (10)–(13) is reduced to the integral–differential stochastic equation for fluctuations of displacements [12,15]. The equation has the following recurrent form:

$$\frac{\partial u_i'^{(\chi)}(\vec{r})}{\partial x_j} = \int_{V_1}\frac{\partial G_{im}(\vec{r},\vec{r}_1)}{\partial x_j}\left[C'_{mnkl}(\vec{r}_1)e_{kl} + C'_{mnkl}(\vec{r}_1)\frac{\partial u_k'^{(\chi-1)}(\vec{r}_1)}{\partial x_l}\right]_{,1n}dV_1 \tag{14}$$

where $G_{im}(\vec{r},\vec{r})$ is the Green's function [1,14,15], χ is approximation order. In the first approximation fluctuations of displacements in the right part of Eq. (8) are taken zero. In the second approximation, result obtained from the first approximation is substituted into the right part of the equation. In order to obtain new precise solution, the second approximation will be used in this research. The Green's function selection depends on the type of the media. This solution is used to form equations for the moments of stress and strain fields as a superposition of multidimensional integrals. For instance, the mixed moment $\langle\lambda'(\vec{r})\varepsilon'_{ij}(\vec{r})\rangle$ can be expressed through the second approximation of Eq. (14):

$$\begin{aligned}\langle\lambda'(\vec{r})\varepsilon'_{ij}(\vec{r})\rangle^{(2)} = \frac{1}{2}\Big(& e_{kl}\overline{C}_{mnkl}\int_{V_1}(G_{im,jn}(\vec{r},\vec{r}_1) + G_{jm,in}(\vec{r},\vec{r}_1))K_\lambda^{(2)}(\vec{r},\vec{r}_1)dV_1 \\ & + e_{oq}\overline{C}_{fsoq}\overline{C}_{mnkl}\int_{V_1}\int_{V_{11}}(G_{im,jn}(\vec{r},\vec{r}_1) \\ & + G_{jm,in}(\vec{r},\vec{r}_1))G_{kf,ls}(\vec{r}_1,\vec{r}_{11})K_\lambda^{(3)}(\vec{r},\vec{r}_1,\vec{r}_{11})dV_{11}dV_1\Big),\end{aligned}$$

where $K_\lambda^{(2)}(\vec{r},\vec{r}_1)$ and $K_\lambda^{(3)}(\vec{r},\vec{r}_1,\vec{r}_{11})$ are structural correlation functions of second and third order.

3. Multipoint correlation functions

The multipoint high order correlation functions $K_\lambda^{(n)}(\vec{r},\vec{r}_1,\ldots,\vec{r}_n)$ of the fluctuation of indicator function $\lambda'(\vec{r})$ represent statistical information about the structure geometry at a microscopic scale:

$$K_\lambda^{(n)}(\vec{r},\vec{r}_1,\ldots,\vec{r}_n) = \langle\lambda'(\vec{r})\lambda'(\vec{r}_1)\ldots\lambda'(\vec{r}_{n-1})\rangle,$$

where n indicates the order of the function.

Complexity of a micro-scale structure of heterogeneous materials is one of the major barriers for applications of multi-scale