Multiscale modeling of deformation and damage of elastic-plastic particle reinforced composites

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Abstract. A model is proposed for the deformation of elastic-plastic particle reinforced composite materials of a periodic structure with allowance for the damage. The model is based on a variant of the deformation theory of plasticity under active loading, in which the damage parameter is introduced, taking into account the difference in the accumulation of damage in phases during shear, tension and compression. The method of asymptotic homogenization of periodic structures was used to model the effective characteristics of elastic-plastic composites. Examples of numerical calculation are carried out for particle-reinforced metal composite - aluminum matrix filled with SiC particles.

Introduction
Methods for modeling the elastic-plastic characteristics of composites began to develop quite a long time ago [1], but until now these methods are mainly based on an approximate analysis of the mechanical behavior of composites based on certain hypotheses regarding joint deformation of composite components [2, 3]. At present, the most promising method for predicting the effective properties of composites and simulating micromechanical processes in composites is the asymptotic averaging method (homogenization method) [4–11]. The purpose of this paper is to further develop the research begun in [9–11] for the case of elastic-plastic deformations of composites when taking into account the effects of detectability.

State of the problem for the mechanics of elastic-plastic composites with micro-damage

Consider a composite, to which in space $\mathbb{R}^3$ there corresponds a region $\mathcal{V}$ with a surface $\Sigma$. A composite consists of $N$ components $V_\alpha$, $\alpha = 1...N$, components with indices $\alpha = 1,...,N - 1$ are inclusions of various types, and a component with index $\alpha = N$ is a matrix. We denote $\Sigma_\alpha$ - the surfaces of the regions, $V_\alpha$ and $\Sigma_{\alpha N}$ the surfaces of the contact of the matrix and inclusions. The inclusions and the matrix are assumed to be isotropic elastic-plastic, corresponding to the deformation theory of plasticity with allowance for micro-damage [12]. Then in each area $V_\alpha, \alpha = 1...N$ we have the following problem of mechanics of elastic-plastic media with micro-damage

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\[
\begin{align*}
\nabla_j \sigma_{ij}^a &= 0, \quad e V_a \\
\sigma_{ij}^a &= \mathcal{F}_{ij}^a \left( z^a, \varepsilon_{ij}^a \right), \quad e V_a \cup \Sigma_a \\
\varepsilon_{ij}^a &= \frac{1}{2} \left( \nabla_j u_{ij}^a + \nabla_i u_{ij}^a \right), \quad e V_a \\
u_i^a &= u_i^N, \quad \left( \sigma_{ij}^a - \sigma_{ij}^N \right) n_j = 0 \\
\psi_i^a &= u_i, \quad u_i \Sigma_{ae}^1, \quad \sigma_{ij}^a n_j = S_{ie}, \quad u_i \Sigma_{ae}^2
\end{align*}
\]

(1)

here \( u_i^a, \sigma_{ij}^a, \varepsilon_{ij}^a \) - displacements, stresses and deformations in the \( \alpha \)-th component, \( \nabla_j u_{ij}^a = \partial u_{ij}^a / \partial x_j \) - are partial derivatives with respect to Cartesian coordinates \( x_j \), the last two conditions in system (1) are the conditions of ideal contact of the matrix and inclusions, and the conditions on the external surfaces, \( z^a = z^a(\sigma_{ij}^a) \) - are micro-damage parameters that depend on stress \( \sigma_{ij}^a \), and \( \mathcal{F}_{ij}^a \left( z^a, \varepsilon_{ij}^a \right) \) - nonlinear tensor function of the defining relations of elastic-plasticity with active loading.

**Model of the of elastic-plasticity for media with damage**

Let us choose the tensor functions \( \mathcal{F}_{ij}^a \left( z^a, \varepsilon_{ij}^a \right) \) corresponding to an isotropic medium obeying the modified A.Il'yushin theory of small elastoplastic deformations for active loading [12], which is modified by introducing the dependence of the elastic constants on the micro-damage parameter \( z^a = z^a(\sigma_{ij}^a) \). In this case, the function \( \mathcal{F}_{ij} \left( z^a, \varepsilon_{ij}^a \right) \) (index \( \alpha \) is omitted) has the following form

\[
\sigma_{ij} = \mathcal{F}_{ij} \left( z^a, \varepsilon_{ij}^a \right) = (K(z) - \frac{2}{3} G(z)(1-\omega))\varepsilon_{ij} \delta_{ij} + 2G(z)(1-\omega)\varepsilon_{ij},
\]

(2)

where \( \phi(\varepsilon_u) \) is the plasticity function of A.A. Il'yushin, which we choose in power form [23]

\[
\phi(\varepsilon_u) = \begin{cases} 
0, & \varepsilon_u \leq \varepsilon_T \\
1 - (\varepsilon_T / \varepsilon_u)^{-n}, & \varepsilon_u > \varepsilon_T
\end{cases}
\]

(3)

where \( n \) - is the hardening rate, \( \varepsilon_T \) - is the strain on the beginning of the material's fluidity, \( \varepsilon_u \) - is the second invariant (intensity) of the strain tensor [24], \( K(z) \) - is the bulk modulus of the material, \( G(z) \) - is the shear modulus depending on the micro-damage parameter \( z \): \( K(z) = K_0 a(z) \), \( G(z) = G_0 a(z) \), where \( K_0 \) and \( G_0 \) are elastic constants, \( a(z) \) - the function describing the micro-damage of the material, choose it as follows:

\[
a(z) = \frac{1}{2} \left( |1 - (1 - a_z)z^m| + 1 - (1 - a_z)z^m + \frac{a_m}{2} (1 - z - |1 - z|) \right),
\]

(4)

where \( m \) is a constant. For the damage parameter \( z \), we take the following dependence on the stress tensor invariants
\[
z = \frac{\sigma_u^2}{3\sigma_s^2(1 + BV(\sigma))} + \left(\frac{1}{\sigma_i^2} - \frac{1}{3\sigma_s^2}\right)\sigma_i^2
\]  
(5)

Here are the invariants of the stress tensor: \(\sigma\) - the first, \(\sigma_u\) - the second and \(\sigma_s = (|\sigma| \pm \sigma) / 2\) - the sign-constant, \(\sigma_t\), \(\sigma_c\), \(\sigma_s\) - strength in tension, in compression and in shear. The constant \(B_t\) is expressed through the limits of static strength under compression and shear \(B = (\sigma_s^2 / 3\sigma_s^2 - 1) / \sigma_c\). The function \(V(\sigma)\) in (7) describes a smooth transition of the accumulation of micro-damage between areas of tension and compression:

\[
V(\sigma) = \begin{cases} 
0, & \text{if } \sigma > 0 \\
-\sigma, & \text{if } -\sigma_c < \sigma < 0 \\
\sigma_c, & \text{if } \sigma < -\sigma_c 
\end{cases}
\]  
(6)

Model (5) with regard to (6) allows to take into account the effect of the difference in the accumulation of micro-damages in the area of tension and compression, which is characteristic of most materials.

**Application of the asymptotic averaging method for elastic-plastic composites with damage**

Let the composite material have a periodic structure, introduce a small parameter \(\kappa = l / L << 1\) for it, as the ratio of the characteristic size of the periodicity cell (PC) to the characteristic size of the entire composite, and also introduce dimensionless global \(x^k = \bar{x}^k / L\) and local \(\xi^k = x^k / \kappa\) coordinates. Then we solve the solution of the problem (1),(2) in the form of asymptotic expansions of the form:

\[
u_i^\alpha = u_i^{(0)}(x^k) + \kappa u_i^{\alpha(1)}(x^k, \xi^k) + \kappa^2 \ldots ,
\]  
(7)

Substituting asymptotic expansions (7) into system (1), and collecting terms at the same powers of \(k\), we obtain the so-called local problem \(L_{pq}\) of the zero approximation over PC \(V_{\xi}\):

\[
\sigma_{ij}^{(0)}(x^k) = 0, \quad \text{in } V_{\xi}
\]
\[
\sigma_i^{\alpha(0)} = \mathcal{F}_{ij}^\alpha \left(\varepsilon_i^{\alpha(0)}, \varepsilon_{kl}^{(0)}\right), \quad \text{in } V_{\xi} \cup \Sigma_s
\]
\[
\varepsilon_{ij}^{\alpha(0)} = \delta_{ij} \delta_{kl} \tilde{e}_{pq} + \tilde{e}_{ij}^{\alpha(0)}, \quad \varepsilon_{ij}^{\alpha(0)} = \frac{1}{2} \left(u_i^{\alpha(1)} + u_j^{\alpha(1)}\right) \quad \text{in } V_{\xi}
\]
\[
u_i^{\alpha(1)} = u_i^{N(1)}
\]
\[
\left(\sigma_i^{\alpha(0)} - \sigma_i^{N(1)}\right) n_j = 0 \quad \text{at } \Sigma_{\xi}^{\alpha N}
\]
\[
\left\{u_i^{\alpha(1)}\right\} = 0, \left\{\tilde{u}_i^{\alpha(1)}\right\} = 0.
\]

Here are denoted \(\sigma_{ij}^{\alpha(0)} = \partial \sigma_{ij}^{\alpha(0)} / \partial x_j\) , \(\sigma_{ij}^{\alpha(0)} = \partial \sigma_{ij}^{\alpha(0)} / \partial x_i\) , \(\left\{u_i^{\alpha}\right\}\) - is the averaging operator over \(V_{\xi}\), \(\left\{u_i^{\alpha}\right\} = 0\) - is the condition of periodicity on the boundary of the PC. Due to the periodicity of the functions \(u_i^{\alpha(1)}\), the following relationship holds: \(\tilde{e}_{ij}^{\alpha(0)} = \frac{1}{2} \left(u_i^{(0)} + u_j^{(0)}\right)\).
A numerical method for solving the local problem of deforming an elastic-plastic material with damage is described in [8, 9]. The software implementation of the developed numerical method was carried out using the SMCM software environment developed in the Scientific and Educational Center "Supercomputer engineering modeling and development of software systems" ("SIMPLEX") of the Bauman Moscow State Technical University and designed to solve the problems of mechanics of a deformable solid body by finite element methods.

Calculation of the effective elastic-plastic characteristics of the composite

After solving a series of problems \( L_{pq} (8) \) for all \( pq \), we integrate the resulting stresses \( \sigma^{(a)}_{\rho r(pq)} \) over the areas occupied by the fillings and the matrix

\[
\bar{\sigma}_{ij} = \left\{ \sigma^{(a)}_{ij} \right\} = \left( F^{a}_{ij} \left( z^{(a)}_{ij}, \delta_{ij} \bar{E}_{pq} + \bar{E}^{(0)}_{pq} \right) \right) = F^{a}_{ij} \left( \bar{E}_{pq} \right)
\]

as a result, we obtain the averaged stresses in the composite, which, with active loading, are functions of the averaged deformations \( \bar{E}_{pq} \). Relations (9) are non-linear defining relations of a composite. To find these constitutive relations, we apply the method of tensor-invariant approximation, according to which for the geometrically-isotropic structure of the PL, relations (9) are also non-linear-isotropic and can be represented as tensor-nonlinear isotropic functions [12]

\[
\bar{\sigma}_{ij} = (K(\bar{E}) - \frac{2}{3} G(\bar{E})(1 - \bar{\omega})) \bar{E}_{kk} \delta_{ij} + 2G(\bar{E})(1 - \bar{\omega}) \bar{E}_{ij}
\]

where \( \bar{\omega} (\bar{E}_{u}, \bar{E}) \) is the averaged plasticity function for a composite, generally speaking, depending on the 1st and 2nd invariant of the averaged strain tensor \( \bar{E} = \bar{E}_{kk}, \bar{E}_{u} \), and \( \bar{E} \) is a measure of the composite damageability, for which, due to the isotropy of the composite, it is also possible to adopt model (4) - (6). Relations (10) can be written as the ratio between the first and second invariants of the averaged stress tensor \( \bar{\sigma} = \bar{\sigma}_{kk}, \bar{\sigma}_{u} \) and the averaged strain tensor \( \bar{E}_{u}, \bar{E} \)

\[
\bar{\sigma} = K(\bar{E}) \bar{E}, \quad \bar{\sigma}_{u} = 2G(\bar{E})(1 - \bar{\omega}) \bar{E}_{u}
\]

Modeling the processes of deformation and damage of composite materials based on the aluminum matrix and SiC particles

As an example, we performed numerical calculations of micromechanical stress and strain fields in PL in a composite material based on an aluminum alloy filled with SiC particles (Fig. 1). Figure 2 shows the deformation diagrams of the Al + SiC composite under tension along the axis direction up to separation into parts.

Figure 3 shows the dependences of the first invariant of the averaged stress tensor \( \bar{\sigma} = \bar{\sigma}(\bar{E}_{u}, \bar{E}) \) on the first invariant of the averaged strain tensor \( \bar{E} \) for fixed values of the 2nd invariant \( \bar{E}_{u} \). Calculations show that this dependence can indeed be considered linear, in accordance with (12). Figure 4 shows the dependences of the 2nd invariant of the averaged stress tensor \( \bar{\sigma}_{u} = \bar{\sigma}_{u}(\bar{E}_{u}, \bar{E}) \) on the 2nd invariant of the averaged strain tensor \( \bar{E}_{u} \) for fixed values of the 1st invariant \( \bar{E} \). Calculations show that this dependence is indeed non-linear, but can be approximated with sufficient accuracy as a function of one variable (12), since the influence of the 1st invariant is not significant.
Figure 1. PC of particle reinforced Al + SiC composite with a high concentration of particles (a) and calculated diagrams of the deformation of the Al matrix /m/, SiC particle /f/ and composite /c/ (b).

Figure 2. (a) Calculated effective relation $\bar{\sigma} = \bar{\sigma}(\bar{\varepsilon}_u, \bar{\varepsilon})$ for fixed values $\bar{\varepsilon}_u: 0$ (1), 0.6% (2); (b) effective relation $\bar{\sigma}_u = \bar{\sigma}_u(\bar{\varepsilon}_u, \bar{\varepsilon})$ for fixed values $\bar{\varepsilon}: 0$ (1), 0.6% (2) for particle reinforced Al-SiC composite.

Conclusion

A model of multiscale deformation of elastic-plastic composite materials with regard to micro-damage damage is proposed. The model is based on a variant of the deformation theory of plasticity under active loading, taking into account micro-damage, which differs in tension and compression. The method of asymptotic homogenization of periodic structures is used to simulate the deformation of elastic-plastic composites. An example of numerical simulation of the process of deformation and damage for a dispersion-reinforced composite based on an aluminum matrix filled with SiC particles.
is given. It is shown that the averaged defining relations of the composite are also quite well described by the same deformation theory of plasticity as the elastic-plastic matrix.

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