Hierarchical modeling of deformation and damage of metal matrix composite under uniaxial loading conditions

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Abstract. A three-dimensional model for deformation of metal matrix composite with aluminum matrix and silicon carbide reinforcement particles is developed. The model accounts for an internal structure of the composite, as well as rheology of its constituents. The model is further used in numerical simulations in order to study the evolution of stress-strain state parameters in a randomly-chosen composite microstructure fragment under uniaxial tension and compression loading on micro- and macroscale. The parameters include the stress stiffness coefficient, the Lode-Nadai coefficient and equivalent (von Mises) strain. It is found that local deformation regions and internal tensile stress concentration regions appear in the material of composite matrix. Adhering to a phenomenological damage theory, a damage development is computed in the matrix metal. We present damage fields and damage distributions for uniaxial tension and compression.

1. Introduction
Studies of mechanical behavior of composites under loading are crucial for the assessment of reliability, durability and usability of machine parts and structural elements produced from composites. Due to a hierarchical composite structure, these studies need to cover multiple scale levels. The established modern paradigm for such studies is the multilevel approach for describing structurally inhomogeneous materials [1–4]. Multilevel models of plastic deformation and damage are advantageous over the classical approach adopted in mechanics in a way that they allow one to observe stress concentration phenomenon leading to microcrack emergence at early deformation stages.

It is known that under conditions of a complexly changing stress-strain state, the microscopic crack stage (also known as the hidden or scattered damage accumulation stage) is described phenomenologically by damage criteria (e.g. Kolmogorov criterion, Lemaitre criterion, etc.) and it indirectly characterizes damage evolution in a microscopic volume of continuous medium [5–8]. The damage level is associated with local plastic strain and assessed by effective plastic strain before failure which is in its turn dependent on the evolution of dimensionless stress-strain state parameters: the stress stiffness coefficient and the Lode-Nadai stress state coefficient. Thus, in order to adequately describe damage process, one needs to acquire the data on stress-strain state history under severe plastic deformation conditions. To achieve this goal, numerical simulations
employing different software are widely used [2, 3, 9–12]. Simulation results allow one to obtain sufficient data for further computations.

This paper presents a numerical simulation of damage accumulation in a randomly-chosen microstructure fragment of an aluminum matrix composite under uniaxial loading conditions. The simulation is based on the multilevel approach for describing a material, a damage mechanics criterion and considers the rheology of composite constituents.

2. Material and Methodology

A specific metal matrix composite is considered to be a model material. The constituents of the composite are 99.8% commercially pure aluminum and silicon carbide reinforcement particles. The dominant particle shape is considered to be irregularly prismatic; particle sizes are in ranges of $1 \ldots 5 \mu m$ and $15 \ldots 20 \mu m$.

Particles make up 50 vol% of the composite. The composite microstructure is depicted in Fig. 1, which is obtained by means of scanning electron microscope. Experimental studies observe strong adhesive bonding between the matrix and reinforcement particles [13, 14].

The computational model has been implemented adhering to the two-level structural-phenomenological approach, which connects problem solutions on micro- and macroscale [15, 16]. According to the approach, the composite volume on microlevel is modeled by three-dimensional continuum which represents the aluminum matrix with embedded silicon carbide particles. The microstructural properties of the metal matrix composite have been chosen according to metallographic investigation [13, 14]. The composite microvolume has the shape of a cube with the edge size of $30 \mu m$. The structurally inhomogeneous microvolume is surrounded with a buffer layer. The layer has smeared macroscopic mechanical properties of the composite and dilates evenly from microvolume borders. The volume thickness is equal to the microvolume linear size. Thus, the whole microvolume is a cube with edge size of $90 \mu m$. This problem statement allows us to connect solutions on micro- and macroscale and properly meet a challenge of atypical boundary behavior. An in-house software was developed by authors in previous work [17]. The software is capable of three-dimensional model generation for structurally inhomogeneous materials with a complex internal structure. It is compatible with ANSYS finite element suite input format. The three-dimensional metal matrix composite computational model is depicted in Fig. 2. Detailed information is published in [18, 19].
Rheological properties of commercially pure aluminum were set as strain-hardening curves according to compression tests with cylindrical specimens on macro-level. Tests were conducted with a strain rate of 1 s\(^{-1}\) at 300 °C\(^1\). The materials of the matrix and the buffer layer have been considered to be isotropic plastically incompressible elasto-plastic medium. The silicon carbide particle material has been considered to be isotropic linear plastic. The elastic proprieties have been set as follows: Young's modulus \(E = 70\) GPa and the Poisson coefficient \(\nu = 0.34\) for pure aluminum \([20]\); \(E = 380\) GPa and \(\nu = 0.19\) for silicon carbide \([21]\). The elastic proprieties of the buffer layer have been obtained by the rule of mixtures \([22]\) using composite constituent volume fractions as follows: \(E = 225\) GPa and \(\nu = 0.265\).

The numerical simulation of metal matrix composite deformation has been conducted in the quasi-static statement with ANSYS finite element suite installed on a URAN GPU cluster of IMM UB RAS. Boundary conditions have been set in displacements of buffer layer facets in such a way that metal matrix composite could be considered to be 1/8 part of a body being subjected to uniaxial tension or compression along \(y\)-axis. Some facets have been placed on symmetry planes. The displacements have been set in such a way that equivalent macroscopic strain of tension or compression could reach \(\varepsilon = 0.2\) on the final load step.

The simulation allowed us to obtain stress tensor \(\sigma_{ij}\) and strain increment \(\Delta\varepsilon_{ij}\) tensor data in each node of the metal matrix composite computational model. The data have been further used to determine the stress stiffness coefficient \(k_n\) and the Lode-Nadai coefficient \(\mu_{\sigma n}\) on each computation step:

\[
k_n = \frac{\sigma}{T},
\]

where \(\sigma\) denotes mean normal (hydrostatic) stress and \(T\) denotes tangential stress intensity equal to shear yield stress in the plastic region.

\[
\mu_{\sigma n} = \frac{2(\sigma_2 - \sigma_3)}{\sigma_1 - \sigma_3} - 1,
\]

\(^1\) Experimental research was conducted in Collective centre “Plastometria” of IES UB RAS
where $\sigma_1$, $\sigma_2$, $\sigma_3$ denote principal stresses on $n$-th computational step.

The equivalent (von Mises) strain increment on $n$-th computation step has been expressed in terms of strain tensor component increments $\Delta \varepsilon_{ij}$ obtained on this step:

$$\Delta \varepsilon_n = \sqrt{\frac{2}{3}} \Delta \varepsilon_{ij} \Delta \varepsilon_{ij}$$

(3)

Thereafter, the whole accumulated equivalent deformation $\varepsilon$ in every node is computed as follows:

$$\varepsilon = \sum_{n=1}^{N} \Delta \varepsilon_n,$$

(4)

where $N$ denotes total computational step number for deformation.

In [13, 14] it is determined experimentally that in metal matrix composite specimen loading process, first cracks appear in the matrix. Considering this failure behavior, the matrix damage accumulation has been studied in scope of this work. The phenomenological theory authored by Kolmogorov V L [6, 7] has been used. This theory assumes that material damage $\omega$ lies in range $0 \ldots 1$, where 0 means undeformed material and 1 implies material failure and crack emergence. The material damage on computational step of deformation is equal to the ratio of equivalent strain increment to equivalent plastic strain to fracture and damage accumulation considered to be linear. The fracture locus of commercially pure aluminum for 300 °C has been taken from the experimental investigation [23]. A fracture locus determine the dependence of ultimate shear strain $\Lambda_f$ at fracture on stress state parameters $k$ and $\mu_\sigma$: $\Lambda_f = \Lambda_f(k, \mu_\sigma)$. Ultimate strain at fracture was calculated as follows: $\varepsilon_f = \Lambda_f/\sqrt{3}$

The damage model has been further used to compute damage and damage accumulation in every finite element node representing the metal matrix. A node has been considered to be destroyed if an accumulated damage in this node reached 1. Thus the condition of failure after $N$ computational steps has the following notion in every finite element mesh node:

$$\omega = \sum_{n=1}^{N} \frac{\Delta \varepsilon_n}{\varepsilon_f(k_n, \mu_{\sigma n})} = 1$$

(5)

For considered loading scenarios, damage distribution fields have been visualized for each computational step in whole volume of the metal matrix.

3. Result and Discussion

Finite element method simulations show that the stress-strain state in the matrix on microscale is significantly inhomogeneous on every computation step. Even on initial loading stages, the matrix material appears to have tensile stress concentration regions (characterized by $k > 0$), as well as substantial local plastic deformation regions. These peculiarities emerge in close proximity of reinforcement particles. This holds true both for tension and compression simulations. Volume fraction of such regions increases with equivalent macroscopic strain. For further information on the microvolume stress-strain state peculiarities and stress-strain state evolution during the deformation process, we refer to [18, 19].

It is known that severe tensile stresses contribute to intensive plastic dilatancy and accelerate fracture process [5, 6, 24]. This conclusion is also confirmed by numerical simulations of damage $\omega$ accumulation in the matrix metal within microvolume. It is found that the most possible regions of failure initiation (i.e. regions, where equation (5) holds true) are strain localization regions where adverse tensile stresses prevail. As an example, figures 3 and 4 depict accumulated damage distribution in central cross section $xy$ of the metal matrix within the microvolume depending on equivalent macroscopic strain $\varepsilon$ for uniaxial tension and compression.
Figure 3: Damage $\omega$ distribution in matrix. Central $xy$ cross-section of metal matrix microvolume, tension simulation at equivalent macroscopic strain $\varepsilon = 0.04$ (a) and $\varepsilon = 0.2$ (b).

Figure 4: Damage $\omega$ distribution in matrix. Central $xy$ cross-section of metal matrix microvolume, compression simulation at equivalent macroscopic strain $\varepsilon = 0.04$ (a) and $\varepsilon = 0.2$ (b).

Obviously, a damaged region grows with increase of equivalent macroscopic strain. On the tension simulation step with equivalent macroscopic strain $\varepsilon = 0.04$ the failure criterion (5) holds true for order of 30% nodes, whereas the step with $\varepsilon = 0.2$ shows that more than 70% of nodes would experience failure. Compression loading scenario is less adverse in terms of internal damage. In case of compression for analogous equivalent macroscopic strain, the failure criterion (5) holds true for less than 3% and 10% of matrix nodes within the microvolume.

4. Conclusion
Adhering to the multilevel material description approach, the three dimensional computational model of metal matrix composite deformation has been developed. The model takes into account internal structure of the composite material, as well as the rheology of its constituents. The numerical simulations with randomly-chosen microvolume of Al/SiC composite have been conducted for uniaxial tension and compression.
Adhering to the phenomenological theory of damage, a simulation of damage accumulation in composite matrix has been conducted. The evolution of stress-strain state parameters (the stress stiffness coefficient and the Lode-Nadai coefficient) has been taken into account. It is found that for considered loading scenarios the most probable failure initiation regions are regions with plastic strain localization and adverse stress state with prevalence of tensile stresses. Initial cracks can emerge in these regions, spreading through the volume of the composite with deformation increase.

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