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MICROSTRUCTURE-BASED COMPUTATIONAL ANALYSIS AS A TOOL FOR COMPUTER-AIDED DESIGN OF METAL-MATRIX COMPOSITE AND COATED MATERIALS

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One of the challenges for today's materials science and engineering is the development of methods and tools for computer-aided design of new materials characterized by high strength and relatively low density. An application of these materials in the key industries would result in breakthrough technologies for manufacturing engines and apparatus with high energy efficiency. Metal-matrix composites (MMCs) and materials with composite coatings are among the candidate materials. Due to their high strength-to-density ratio, composite materials in the recent decades have been gradually pushing out purely metallic compounds from aircraft, aerospace, power engineering and machine-building industries. Earlier we studied deformation and fracture in MMCs without taking into account residual stresses (RSs) [1, 2].

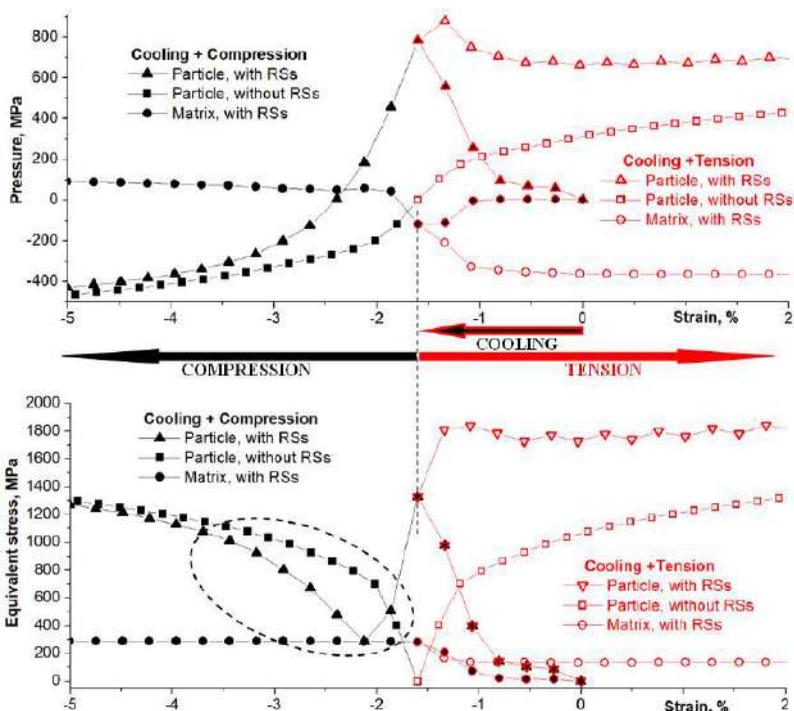


Fig. 1. Maximum residual stresses in the particle and matrix.

In this study a technique for computer simulation of three-dimensional structures of materials with reinforcing particles of complex irregular shapes observed in the experiments is proposed, which assumes scale invariance of the natural mechanical fragmentation. Two-phase structures of metal-matrix composites and coatings of different spatial scales are created, with the particles randomly distributed over the matrix and coating computational domains. Using the titanium

### Секция 3. Компьютерное моделирование и дизайн материалов с иерархически организованной структурой

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carbide reinforcing particle embedded into the aluminum as an example, plastic strain localization and residual stress formation along the matrix-particle interface are numerically investigated during cooling followed by compression or tension of the composite. A detailed analysis is performed to evaluate the residual stress concentration in local regions of bulk tension formed under all-round and uniaxial compression of the composite due to the concave and convex interfacial asperities (Fig.1).

The principal conclusions drawn from the numerical simulations are the following:

1. In the composites subjected to compression local regions of bulk tension are formed near the interfaces. In the cases of uniaxial compression such regions are observed both in the matrix and in the particles, while under all-round compression – in the matrix only. The volume fraction of tensile regions in the particles is larger and the concentration of stresses in them is lower during plastic flow in the matrix than in the case where the matrix deforms elastically. To sum up, fracture in metal-matrix composites occurs later and can be characterized by multiple cracking of the particles, while in ceramic composites it takes place earlier and is associated with propagation of isolated cracks. Stress concentration is by a factor of 1.5 times higher under all-round than under uniaxial compression.

2. Under all-round compression up to -1.6 %, which results from cooling of the composite from the melt to room temperature, local plastic strains are as large as 12 %. An inclusion of the yield point dependence on the temperature into the model qualitatively changes the plastic strain localization history during cooling, though it has little effect on the final stressed state pattern after cooling.

3. The cooling-induced residual stresses play a positive role during subsequent mechanical loading of the composite to low strain degrees and only slightly influence its strength at the strains larger than 2 %.

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