Numerical modeling and prediction of mechanical properties of ceramic composite

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Abstract. The paper is devoted to the numerical simulation of the composite consisting of ZrO₂-based ceramics and cortical bone performed with making use of a multi-scale approach. The specificity of the approach considered is the using of a geometrical model of the composites representative volume that must be generated with taking into account the composite reinforcement structure. It is shown that such approach can be used to predict the value of composite macroscopic ultimate strength. The evolution of mesoscopic stress distributions in the composite components during its deformation was investigated with taking into account damage accumulation up to the fulfillment of the macroscopic strength criterion. It is shown that damage accumulation has an impact on the stress distribution laws at the mesoscopic level, which is manifested in the appearance of a threshold for the stress distribution, as well as in a significant decrease in distribution amplitude.

1. Introduction
Currently, modern medicine uses new materials for the production of high-quality medical equipment and development of new technologies. For example, products from ceramic materials can be used to produce a “substitute” of destroyed or damaged human tissues in surgical medicine. Ceramic materials have unique properties. These are high hardness, wear resistance, low density, high compressive strength, etc. For bone prostheses, the great interest is expressed in ceramic materials based on zirconia. These materials are characterized by high strength and excellent biocompatibility with living tissues of the human body [1–6]. A successful application of such materials in medicine, as in other applications, is largely determined by the completeness of information on their mechanical and physical properties. Computer simulation is widely used currently to obtain such information. The correctness of these simulations directly depends on the quality of computer models of the materials. Different numerical techniques and approaches can be used to evaluate the mechanical properties of ceramic materials. The authors of studies [7–11] used the movable cellular automaton method in modeling brittle porous ceramics. The advantage of this method is the successful modeling of multiple cracking and fracture of materials that was shown in the above mentioned papers. Here we are going to use the conventional finite element method like in [12–14]. Regarding the influence of the structure on the mechanical properties of composite materials, we follow one of the most promising approaches as in papers [7–18] and many others. It is a multi-scale approach. This approach allows taking into account the type of structure and its influence on the properties of composites.
The aim of the paper is to study the features of changes in the stress, strain and damage distributions at the mesoscale level in ceramic composite materials under mechanical loading. To achieve this goal numerical simulation of the mechanical behavior of the composite was performed with taking into account damage accumulation.

2. Numerical Model and Method
The composite material consists of matrix and filler. The matrix is porous ZrO₂-based ceramics. The filler material is bone tissue. So, it is a kind of biocomposite when the pores of ceramics are filled with bone tissue. The porous structure of the ceramic implant is described explicitly. We suggest that the pores have a circular shape. Their radius and position within the mesovolume geometrical model are determined in a random manner. The size of the square comprising the representative geometric model is 15 times larger than the greatest pore size, which was shown to be quite enough [19].

The study was conducted within the multi-scale approach to the description of mechanical properties of materials discussed in [12]. A composite material is considered at several scale levels: macro-, meso- and microlevels. On the macro level, a material is treated as an quasihomogeneous one. The properties of the composite material at this level may vary with space coordinates but quite smoothly. So, the properties at this level are characterized by some effective values representing the result of compilation of information about the behavior of the material obtained at the mesolevel. Mesovolume is a fragment of a piecewise-homogeneous medium for which the distribution of the components and loading conditions are clearly defined [20, 21]. For the mesovolume there is a concept of locally-effective properties, which are defined as the average (effective) ones for the selected limited fragment of a heterogeneous medium. On the micro level we consider the volumes which dimensions are much larger than the interatomic distances but at the same time are smaller than the characteristic dimensions of the composite structural components. It is believed that for such a volume the postulates of continuum mechanics are acceptable, i.e. the hypothesis of continuity and homogeneity hypothesis are accomplished for it, and mathematical apparatus of integral and differential calculus can be used for its description. The properties of the material at this level are described by constitutive relations of anisotropic media (e.g., crystalline or bone tissue components).

Mechanical behavior of the composite on all scale levels is governed by equations of solid mechanics which include equilibrium equations, Cauchy (geometric) equations and constitutive relations [22]. When the local failure criterion is fulfilled the parameters of mesovolume damage for each component of the composite are calculated according to the formula [23]:

$$\Pi_k = \frac{V_k^*}{V_k},$$

where $V_k$ is the total volume of the $k$-th component in the mesovolume, $V_k^*$ is the damaged fraction of the volume of the $k$-th component in the same mesovolume. The modulus of elasticity is calculated taking into account the damage for each $k$-th component of the composite by the equation:

$$E_k = E_k^0(1 - \Pi_k),$$

where $E_k^0$ is the value of the modulus of elasticity of the undamaged material. It is believed that the mesovolume retains its carrying capacity until the following condition is fulfilled for each of its structural components:

$$\Pi_k > \Pi_k^{\text{max}},$$

where $\Pi_k^{\text{max}}$ is the maximum permissible value of damage in the $k$-th component of the composite. This value was chosen taking into account both physical considerations and the stability requirements.
of the computational method and according to the studies in [23] was considered equal to 0.75. To estimate the strength of material at the macro-scale we used a percolation criterion discussed in [23].

The calculation of stress and strain for the composite at the meso level was performed using the finite element method [24] in the two-dimensional formulation. Various examples of the investigated finite element models of mesovolumes are represented in figure 1. The case of quasi-static uniaxial loading along the vertical axis and elastic-brittle constitutive model of material were adopted.

![Figure 1](image)

**Figure 1.** Typical finite-element representations of characteristic fragments of the model structure.

### 3. The Results of Computer Modeling

As a result of the calculations, the parameters of the distribution laws of effective values of strain and stress at the mesolevel in the course of the material loading were determined. The evolution of the distributions of the mesoscopic stress in the components of the composite during its uniaxial compression with taking into account damage accumulation up to the fulfillment of the macro strength criterion was investigated and presented in figure 2.

![Figure 2](image)

**Figure 2.** The Weibull probability density functions of the stress components along the axis of compression $\sigma_y$ for ceramics and cortical bone at different values of effective strain.
The following values of strain were selected as characteristic ones for the analysis of evolution of stress distributions: 0.06 % and 0.3 % for the elastic stage of deformation; 0.66 % for the onset of damage accumulation; 0.72 % for the formation of a connective cluster of damages, 0.84 % for the stage of extensive damage in the mesovolume. The Weibull distributions are shifted to higher stresses with an increase in strain for ceramics and bone tissue. The scatter of the distributions at the initial stage of loading is extremely small as can be seen in figure 2 that points to the uniformity of stress fields in this case. The scatter increases with the growth of load implying the increase of stress field irregularity that is explained by damage accumulation and different local values of the modulus of elasticity according to equation (2).

The stress distribution functions are similar for each component of the composite before damage accumulation starts as one can see in figure 3a. The similarity of distribution laws can be explained by the fact that in the absence of damage the modulus of elasticity of each component keeps its value and all the stresses increase proportionally with increasing strain.

![Figure 3](image_url)

**Figure 3.** The Weibull probability density functions of the stress components $\sigma_y$ for ceramics and cortical bone at the following values of effective strain 0.06 % (a) and 0.72 % (b).

In the presence of damage, the stress distributions for ceramics remain similar to the stress distributions in the absence of damage though the scatter increases (figure 3b). For the bone tissue, the scatter of stress distributions is smaller as compared to the ceramics but the parameters of stress distribution laws change as compared to the intact condition, in particular, a lower threshold of distributions is observed as in figure 3b. The reason of this is more active damage accumulation in the bone tissue in comparison with the ceramic matrix.

4. **Summary**

The study of the evolution of the mesoscopic stress distribution laws in the composite components with taking into account damage accumulation showed that stress distributions for different values of strains are similar to each other in the absence of damage, but the scatter of the distributions increases and its amplitude reduces with the increase in strain. It is shown that damage accumulation has an impact on the stress distribution laws at mesoscopic level, which is manifested in the appearance of a threshold for the stress distribution, as well as in a significant decrease in distribution amplitude.

The value of the effective Young’s modulus of the studied composite materials was obtained to be $E = 18.7$ GPa which is quite close to the Young’s modulus of bone tissue $E = 16$ GPa. The limit values of effective stress and strain corresponding to percolation criterion of strength are found to be $\sigma_{\text{eff}} = 124$ MPa, $\varepsilon_{\text{eff}} = 0.68 \%$. 
Acknowledgments
The research was supported by “The Tomsk State University competitiveness improvement programme”, grant 8.2.12.2017 and the Program of basic scientific research of the Russian Academy of Sciences in 2013–2020, project 23.2.3.

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