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Study of Effect of Damage Accumulation on Stress Distribution Parameters in Mesovolume of Biocomposite and Its Performance Characteristics

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Abstract—A numerical study of mechanical properties of zirconium ceramic—cortical bone tissue biocomposite has been fulfilled using a multiple-scale approach. Evolution of mesoscopic stress distribution in the components of biocomposite during its deformation has been studied with the assumption of damage accumulation until the macrostrength criterion is fulfilled. It has been shown that the parameters of the laws of distribution change with damage accumulation.

Keywords: porous ceramic, damage accumulation, effective mechanical properties, numerical modeling, multiple-scale approach
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INTRODUCTION

Recently, new materials and medical equipment that could increase human life expectancy, have been extensively developed. Modern medicine uses these new materials for the fabrication of higher quality products of medical equipment and development of new technologies. One example is that the products from ceramic materials can be used in surgical medicine for the design of "substituents" of damaged or destroyed tissues of the human body. In order to design bone prostheses, ceramic materials based on zirconia, which is characterized by high strength, as well as high biocompatibility with living tissues of human body, are of great interest [1–4]. Success of these materials in medicine is mainly determined by knowledge of their mechanical and biological properties. At present, computer modeling is widely used to obtain this information, the validity of which depends on the quality of the computer models of biomaterials. To evaluate the mechanical properties of ceramic materials, various approaches and numerical methods are used [5–10]. At present, one of the most promising and extensively developed approaches is a multiple-scale approach [11–14]. This approach considers various structural features and their effect on the effective mechanical properties of composites.

After the incorporation of an implant in the body, its pores are gradually filled with a living bone tissue. A strong bond is gradually formed between the pore surface and living bone tissue, which indicates the formation of a specific material, namely, biocomposite. Experimental study of mechanical characteristics of biocomposites is a complex, expensive, and long-term process. For this reason, the development of numerical methods for the study of mechanical behavior of structurally heterogeneous systems, which include biocomposites, is a relevant problem.

The aim of this work is a numerical simulation of the mechanical behavior of zirconium ceramic—cortical bone tissue biocomposite at the mesoscale with the assumption of damage accumulation using a multiple-scale approach.

PROCEDURE OF STUDY

To achieve the stated aim, a two-dimensional geometrical model of biocomposite was generated (Fig. 1). The biocomposite represents a porous ceramic based on zirconia filled with a cortical bone tissue. The porous structure of the ceramic implant is described in explicit form. The pores in the geometrical model are represented in the form of circular inclusions and chaotically located in the modeled volume with a polydisperse size distribution. It is considered that the pores are filled with bone tissue. The volume whose dimensions are 15 times larger than the largest pore size was considered as a representative volume. This size fulfills the usual requirements on the procedures of study of the structural parameters of material in the mechanics of composites.

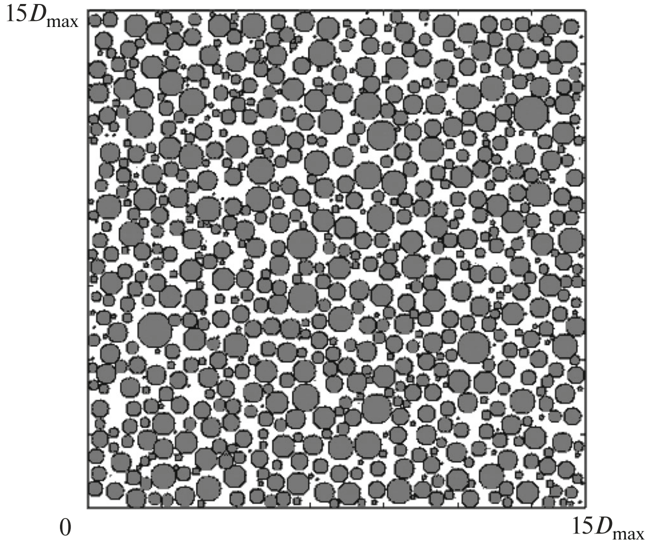

Fig. 1. Schematic depiction of the model structure of biocomposite.

The studies were carried out within a multiple-scale approach to the description of mechanical properties of materials. According to this approach, three levels of modeling of material can be emphasized: microscopic, mesoscopic, and macroscopic. At the microscopic level, the volumes fully belong to a particular component of the material; the mesoscopic level consists of locally representative volumes of the material, which sizes are chosen having regard to local structural features of the material; the macroscopic level contains representative (effectively homogeneous) volumes of the composite.

The parameters of stress–strain state of the biocomposite bulk at the mesoscopic level were calculated using the finite element method [15] in a two-dimensional formulation. The case of quasistatic uniaxial loading using an isotropic elastobrittle model of the material was considered. When the local criterion of fracture was fulfilled, the parameter of damage was calculated for each component of the composite k in elementary volumes according to the formula (1)

$$\Pi_k = \frac{V_k^*}{V_k}, \quad (1)$$

where V_k is the full volume of the kth component in the mesovolume and V_k^* is the damaged fraction of the volume of the kth component in the same volume. The elastic modulus is calculated with consideration of damage for each kth component of the composite according to the formula

$$E_k = E_k^0(1 - \Pi_k), \quad (2)$$

where E_k^0 is the elastic modulus of the undamaged material. It is considered that the mesovolume retains its carrying ability until the following condition is fulfilled for each structural component:

$$\Pi_k < \Pi_k^{max}, \quad (3)$$

where Π_k^{max} is the maximum allowable specific volume of damage in the kth component of the composite. This value is specified with consideration of both physical considerations and the requirements on the stability of the computational method and was assumed to be 0.75 according to the studies from [12].

During the evaluation of the strength of the material at the macroscale, an approach based on percolation theory was used [16]. Percolation theory predicts the transition of systems from one state to another. During the evaluation of strength, these states can be represented by the initial (undamaged) state and final (damaged) state. According to the considerations of cluster analysis, the points in the identical state can be combined into a cluster. It is considered that the formation of joint cluster of damage is a criterion of transition of the system into a new state (condition of macroscopic fracture) (Fig. 2).

Assuming a nonlinear character of the problem of determining the parameters of the stress–strain state at the mesoscale, it was solved using a stepwise loading, which allows for reducing the solution of the nonlinear problem to a sequence of linear problems. An increment of macroscopic deformation corresponding to 0.003% was specified at each stage. It was considered that the problem could be solved in a linear form at such an increment. The fields of mesoscale stresses and strains, as well as the parameters of damage of ceramic and bone, were calculated in each volume at each loading stage.

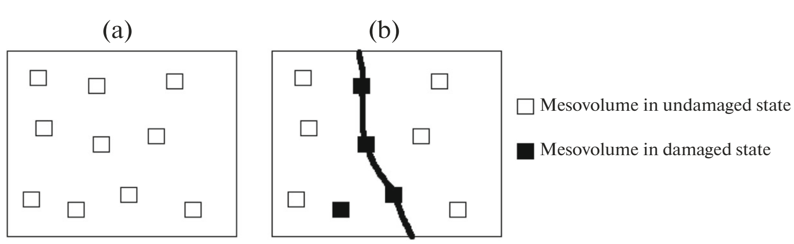

Fig. 2. Diagram of the employment of the percolation criterion at the macroscale: (a) set of mesovolumes in “initial state” (undamaged) and (b) formation of a joint cluster of damage.

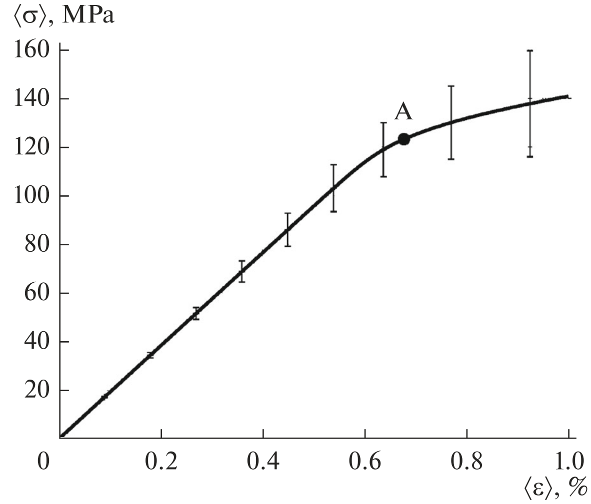

Fig. 3. Stress-strain diagram of zirconium ceramic—cortical bone tissue biocomposite.

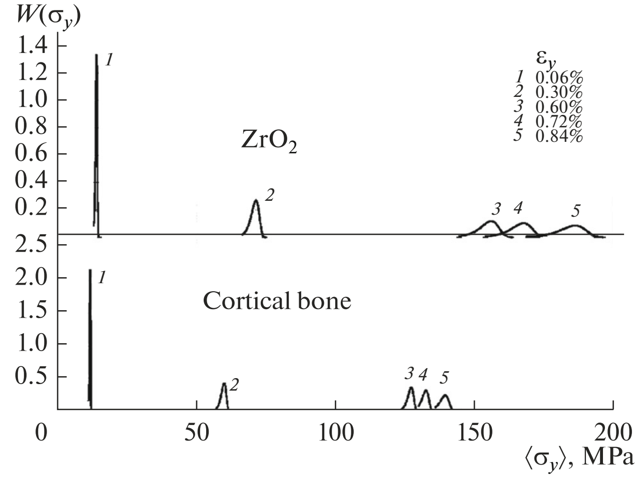

Fig. 4. Weibull density distribution functions of stresses σ_y of the ceramic and cortical bone at various effective strain values.

RESULTS AND DISCUSSION

In Fig. 3, the calculated stress-strain diagram of zirconium ceramic—cortical bone tissue biocomposite is given, which was plotted according to the effective stress and strain values averaged over the mesovolume. Vertical sections show the variation ranges of local stresses. Their increase with the growth of strain is explained below in the discussion of stress distribution.

As follows from Fig. 3, there is a linear correlation between effective stress and strain values in the initial section of the diagram. Starting from the strain of 0.6%, this linear correlation is violated. This is caused by the fact that local damage conditions are fulfilled in individual volumes at the mesoscopic scale at this strain value. Damage is accumulated with the growth of deformation; for this reason, the slope of the strain curve decreases, which implies a decrease in the effective elastic modulus.

Point A on the deformation curve corresponds to the effective stresses and strains at which the percolation criterion of macrostrength is fulfilled. The percolation criterion is fulfilled for the chosen parameters of the model at following effective stresses and strains: $\sigma_{\mathrm{eff}} = 124$ MPa and $\varepsilon_{\mathrm{eff}} = 0.68\%$.

The evolution of distribution of stress tensor components along the loading axis σ_y was studied in the mesovolume. The results of the study showed that there is no damage in the material at the macrostrains of less than 0.66%, while a joint cluster of damage was indicated at the deformation of 0.72%. The following intrinsic strain values were chosen: 0.06 and 0.3% are elastic strains, 0.66% is the onset of damage accumulation, 0.72% is the formation of a joint cluster of damage, and 0.84% corresponds to the developed damage over all mesovolumes. At given strain values, the Weibull density distribution functions of the stress tensor component σ_y of ceramic and cortical bone are given in Fig. 4.

As follows from the plots in Fig. 4, the Weibull distributions shift to higher stresses with an increase in the strain. It is clear from Fig. 4 that the dispersion of the distribution is extremely low at the initial loading stage and indicates a uniform stress field. With the growth of loading, the dispersion increases, which indicates an increase in the nonuniform character of stress field, and this is caused by the damage accumulation and different local elastic moduli. Such an increase in the dispersion of stresses for the entire composite also manifests itself in the increase in the dispersion of stresses as indicated by vertical sections in Fig. 3. Similarity of stress distribution functions is observed for each component of the composite before damage accumulation. Similarity of the distribution functions may be caused by the fact that the elastic moduli of the components remain constant without damage accumulation and all stresses increase proportionally with the growth of deformation. After a significant damage accumulation, nonzero threshold values appear in the distribution functions. This is particularly clear on the stress distribution plots in bone tissue indicated by *4* and *5* in Fig. 4, because damage accumulates faster in a weaker bone tissue.

CONCLUSIONS

The described approach to the modeling of biocomposite based on the considerations of a multiple-scale character of the formation of its mechanical properties allows one to evaluate the effective characteristics of the composite on the basis of the data on mechanical characteristics of its components and on the structural parameters of the composite. The results of this study state that damage accumulation affects the form of stress distribution functions at the mesoscopic level, which is displayed in the appearance of a threshold value of stress distribution, as well as in a significant increase in the dispersion of the distribution. Limiting values of effective stress and strain are also found corresponding to the percolation criterion of strength: $\sigma_{eff} = 124$ MPa and $\varepsilon_{eff} = 0.68\%$.

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