Modeling of Bone Tissue Structure and Porous Ceramics

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Abstract. The results of computer modeling of the structure and mechanical behavior of porous ceramics, microvolumes of compact bone tissue and mesovolumes of bone containing compact and spongy bone tissue are presented. The structure and mineral content of bone tissue fragments are determined in which the most uniform distribution of deformations is realized under axial tension and compression. It was found that the geometry of the porous space of ceramic samples significantly influences the character of the distribution of the regions in which microfractures are possible.

1. Introduction

The long-term experience of the synthetic materials’ use to repair the bone elements by means of endoprosthesis replacement points out that the biochemical compatibility of the implant with the body is an essential, although insufficient, condition for functioning of the implant - bone system as a whole. Their biomechanical compatibility is an important condition. It is known that a difference in the mechanical behaviour of the bone and implant can result in the loss of the latter due to the subsequent resorption of the bone tissue, which is in contact with the implant.

As regards the biochemical compatibility with the body, the preferred materials for the endoprosthesis replacement of the bone tissue are those referred to the ceramics class. Ceramics are identical to the inorganic bone matrix in the type of chemical bond. The strong interest in the use of ceramics for biomedical engineering applications has been developed from the end of the 20th century. New ceramics [1-4], with very improved properties, contribute to increasing the possibilities of using ceramics as osteoimplants.

Using the computer modeling methods creates the preconditions for better understanding of the laws of the human bone functioning and promotes to the development and selection of an appropriate prosthesis for a specific individual.

The results of computer modeling of the structure and mechanical behavior of porous ceramics, microvolumes of compact bone tissue and mesovolumes of bone containing compact and spongy bone tissue are presented.

2. Models of bone fragments and ceramic samples

The computer simulation of the mechanics of compact bone microvolumes, bone mesovolumes and ceramic samples was performed in the software package ANSYS.

The geometrical model of the compact bone tissue microvolume (Figure 1) was based on a real image of the natural bone microstructure.
The microvolume was simulated as a reinforced composite material comprising the reinforcing structural elements, i.e. the osteons with the Haversian canals inside, the matrix and the cement streak separating the osteons and the matrix (Fig. 2). The total porosity of the simulative fragment of the compact bone P was derived by Haversian canals being explicitly simulated (Fig. 2), and Volkmann's canals being implicitly considered in the calculation of the effective mechanical characteristics of the structural elements of the simulative microvolume.

The material of the structural elements of the simulative microvolume of the compact bone was considered transversely isotropic. The effective mechanical properties of the matrix material and the reinforcing elements, osteons, were calculated subject to the volume ratio of the collagen and mineral components, the porosity due to the presence of Volkmann's canals, the direction of the collagen-mineral fibers [5] (I type - transverse fibers, I±45º type - fibers are arranged at an angle of ±45º in the neighboring osteon lamellas, II type – the fibers change their direction from perpendicular on parallel to a bone axis in the osteon lamellas, III type - longitudinal fibers).

Bone fragments (mesovolumes) were simulated as layered composite materials. Structural layers were associated with compact and spongy bone tissues and intermediate layer interfacing those tissues. The ratio of compact (c) and spongy (s) bone tissues volumes $V_c / V_s$ varied from 0.25 to 4.0 (Fig. 3).

Modulus of elasticity of compact (Ec) and spongy (Es) components of the modeled sample was set up depending on their density $\rho$ (g/cm$^3$) and mass fraction of minerals $\alpha$ in accordance with Hernandez model [6]. The density of compact bone $\rho_c$ varied from 1.6 to 1.9 g/cm$^3$, and the density of spongy bone $\rho_s$ varied from 0.3 g/cm$^3$ to 1.0 g/cm$^3$ [7]. The mineral content in the compact bone tissue varied from 0.3 to 0.6, and for the spongy bone tissue it was from 0.25 to 0.53 [8]. Poisson’s ratios of the compact and spongy layers were considered to be 0.32 and 0.2 respectively. Modulus of elasticity and Poisson’s ratio of the intermediate layer were defined as arithmetical mean between corresponding values of the compact and spongy layers.
The geometric models of zirconium ceramic samples with porosity 7% were constructed based on the histogram of pore size distribution of ceramics obtained experimentally. Figure 4 shows the geometric models of ceramic samples with different geometry of pore space.

![Figure 4. The geometric models of zirconium ceramic samples with different geometry of pore space](image)

The material was considered homogeneous and isotropic. The modulus of elasticity of the material was assumed equal to 200 GPa, Poisson’s ratio 0.3. The accepted characteristics correspond to the non-porous ceramic ZrO$_2$ (Y$_2$O$_3$).

The stress-strain state of the model samples of the bone fragments and ceramics at a compressive or tensile stress was calculated using the method of the finite elements. The tasks were solved within the context of the linear elasticity theory.

3. Results of calculation

The structure and mineral content mesovolumes and microvolumes of compact bone tissue, at which the most uniform distribution of strain components is realized in the case of axial compression or stretching, was determined. The ratio of the maximum value of the strain components to the minimum value, $\max \epsilon_x / \min \epsilon_x$, is considered as a quantity that determines the uniformity of the distribution of deformation components. The maximum value of the strain components in bone meso volumes belongs to the compact layer, and the minimal belongs to the spongy layer. For microvolumes of compact bone tissue, the maximum value of the strain components belongs to the matrix, the minimum belongs to osteons.

It was found that the most uniform distribution of deformation components in axial compression is realized in the meso-volume of bone with a ratio of the volumes of compact and spongy layer 0.5 at a ratio of the densities of these layers of 2.75 and the ratio of their mass fractions of minerals 1.2. The most uniform distribution of strain components at axial compression is realized in a microvolume of compact bone tissue with a porosity of 3%, a mass fraction of 35% of minerals and the direction of the collagen-mineral fibers perpendicular to the axis of the osteons (bone axis) (Fig. 5, a). The most uniform distribution of strain components at axial tension is realized in a microvolume of compact bone tissue with a porosity of 15%, a mineral mass fraction of 60%, and the parallel to the osteon axis direction of the collagen-mineral fibers (Fig. 5, b).

The stress-strain state of model samples of porous zirconium ceramics is calculated at a compressive stress of 1300 MPa. Figure 6 presents the calculation results of the regions of model samples of zirconium ceramics (light gray color) in which the compressive normal stresses $\sigma_y$ exceed the ultimate compression strength of non-porous ceramic 2000 MPa. It is believed that the micro fractures of the material are possible in these regions.

Regions in which micro-fractures of a material are possible can be concentrated both near individual pores and also connect several pores with each other.
4. Conclusion
The structure and mineral content of bone tissue fragments are determined in which the most uniform distribution of deformations is realized under axial tension and compression. It was found that the geometry of the porous space of ceramic samples significantly influences the character of the distribution of the regions in which micro-fractures are possible. Regions in which micro-fractures of a material are possible can be concentrated both near individual pores and also connect several pores with each other.

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