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VIII ВСЕРОССИЙСКАЯ НАУЧНО-ПРАКТИЧЕСКАЯ КОНФЕРЕНЦИЯ С МЕЖДУНАРОДНЫМ УЧАСТИЕМ, ПОСВЯЩЕННАЯ 50-ЛЕТИЮ ОСНОВАНИЯ ИНСТИТУТА ХИМИИ НЕФТИ

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COMPUTER SIMULATION OF THE SYNTHESIS OF COMPOSITE MATERIALS OF MEDICAL APPLICATION WITH THE REQUIRED STRUCTURAL AND MECHANICAL CHARACTERISTICS

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The presented researches are devoted to the development of the basis for the synthesis of a promising class of biodegradable, bioactive materials with a given complex of structural and mechanical properties. The researches serve as a basis for creating modern biocomposites for personalized replacement of bone tissue defects. The relevance of the researches caused by the needs of regenerative surgery in multivariate compositions of bioresorbable materials that imitates the structural and functional state of the regenerating tissue and allows varying the actual composition depending on the characteristics of the patients. The results of investigatin are focused on the introduction of modern digital techniques in the practice of personalized regenerative medicine.

Due to this investigation, a computer modeling approach has been developed. This aproach allows to obtain technological conditions (modes) for the synthesis of composite materials for medical purposes with the required structural and mechanical characteristics. A complex physical and mathematical model of the synthesis of the structure of a low-temperature multicomponent nano-modified composite material is based on the model of mechanochemical processes in reacting powder mixtures [1] and the computer modeling approach that built for LTCC synthesis [2]. All the characteristics of the medium are considered as effective with taking into account local concentrations and state parameters in every microvolumes of the model body wich formed in the process of discretization of the computational domain. These characteristics are refined iteratively at each time point. The representative volume of the original compact includes representative parts of individual layers and interlayer interfaces. The model structure of the original compact is represented by a periodic system of such selected volumes. One-dimensional distributions over the thickness of the layer of volumetric concentrations of components (refractory, low-melting components and pores) are investigated for the considered model porous powder body. The developed approach allows to take into account the scatter of volume concentrations of dispersed components and pores, the possibility of convective heat and mass transfer, phase transitions of components, polydispersity of components (the presence in the mixture of component fractions of particles of various sizes), the anisotropy of shrinkage and effective characteristics of the synthesized material, residual stresses in the matrix of a multicomponent low-temperature material after the synthesis, the possibility of forming the inner frame of the interacting particles of refractory components, and other factors and behaviors of multicomponent composite materials.

The developed approach provides the carrying out multifactor multiparameter computational experiments to optimize the composition and structure of the original multicomponent dispersion for the synthesis of a bioresorbable nano-modified multicomponent low-temperature material with the required structural and mechanical characteristics.

The results of the research will serve as the basis for ensuring the development of technological regimes for the synthesis of a new class of bioresorbable nano-modified multicomponent materials for the replacement of bone tissue defects.

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