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Multiscale modelling of BCC Ti-Nb alloy sintered under conditions similar to additive manufacturing

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The need for production of implants with an individual form leads to the necessity of developing new methods and approaches for their manufacture. The obvious advantages of using additive manufacturing and selective laser sintering are the possibility to create not only the external form of the product, but also its internal structure. Recently attractive in terms of biomechanical compatibility enhanced materials are alloys of titanium-niobium, which have similar properties to the elastic properties of cortical bone. In this paper, with use of multiscale approach a numerical study of the physical-mechanical properties of bcc titanium based alloys and their behaviour under conditions identical to the selective laser sintering was made. In the framework of first-principles method of exact muffin-tin orbital [1] the elastic properties of the bcc Ti-Nb alloy are calculated. An algorithm for optimizing of calculations has been proposed and approved. Using the molecular dynamics modelling [2], the changes of the structure of titanium and niobium nano-sized particles during melting process were studied. We also investigated the dependence of the adhesion properties of sintered nano-particles on the heating time of the system and its rate of cooling. It is shown that the main parameter, which determines the adhesive properties of sintered particles, is the contact area obtained during sintering process. Further step involves using the resulting information as input parameters for the computer model of the higher scale level. A numerical model on the basis of movable cellular automata method [3] is used to simulate the mechanical behaviour of the bcc Ti-Nb alloy specimen made under conditions similar to additive manufacturing. Various conventional tests like tension, bending and scratching are carried out in order to get new information about the material properties. Results of computer simulation are in good correlation with known experimental data.

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