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Numerical Study of the Features of Ti-Nb Alloy Crystallization during Selective Laser Sintering

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Abstract. The demand for implants with individual shape requires the development of new methods and approaches to their production. The obvious advantages of additive technologies and selective laser sintering are the capabilities to form both the external shape of the product and its internal structure. Recently appeared and attractive from the perspective of biomechanical compatibility are beta alloys of titanium-niobium that have similar mechanical properties to those of cortical bone. This paper studies the processes occurring at different stages of laser sintering using computer simulation on atomic scale. The effect of cooling rate on the resulting crystal structure of Ti-Nb alloy was analysed. Also, the dependence of tensile strength of sintered particles on heating time and cooling rate was studied. It was shown that the main parameter, which determines the adhesive properties of sintered particles, is the contact area obtained during sintering process. The simulation results can both help defining the technological parameters of the process to provide the desired mechanical properties of the resulting products and serve as a necessary basis for calculations on large scale levels in order to study the behaviour of actually used implants.

1. Introduction

Currently, the dominant materials for producing bio-implants are titanium and titanium alloys. Along with the recognized advantages of titanium as the implant material (magnetic inertia, biocompatibility, low density combined with high strength, high corrosion resistance and others), titanium has a relatively high modulus of elasticity. It was found that from attractive perspective of high biomechanical compatibility, beta alloys of titanium-niobium may be considered, which may also have the effect of pseudoelasticity bringing them closer in properties to the properties of cortical bone [1, 2]. Metallurgical methods for producing such alloys are well known but they are complicated, laborious and expensive. This is caused, in particular, by a large difference between the melting points and densities of titanium and niobium. It should be noted that titanium and niobium are significantly different in thermal properties (thermal conductivity, specific heat, coefficient of linear expansion). Manufacturing also requests complex multistep thermomechanical methods in order to generate alloys with homogeneous structure and chemical composition. Furthermore, after such treatment, up to 50% of preform volume is lost.

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The additive technologies being developed over recent years, in particular, the methods of layerwise laser synthesis, allow solving the abovementioned problems and accomplish the objectives of personalized medicine [3, 4]. Specific advantages of additive technology and selective laser sintering are the capabilities of forming not only the volume of the product, but also the internal structure. When forming structure, it is possible to simultaneously synthesize a new material (alloy) using the components of initial powder mixture in desired proportions.

Obviously, the physical properties of samples are determined primarily by processing conditions and the properties of the initial powder. In turn, the problem of determining the optimal impact parameters on the initial powder to produce samples with desired mechanical properties requires a deep understanding of mechanisms that are taking place during laser sintering at different scale levels. Picosecond duration and high power of laser beam makes the direct experimental study of the effects of a high-energy impact appreciably difficult. One of the research directions allowing us to identify the main regularities of the formation of Ti-Nb alloy by layering laser synthesis, depending on the parameters and intensive modes of heating, is the use of numerical modelling. Thus, using the numerical method of *ab initio* calculations described in [5], the optimal stoichiometry for obtaining the desired elastic modulus for Ti-Nb alloy system was found. In the present paper, a mathematical model of the process of low modulus β-Ti-Nb alloy system formation produced by laser sintering from titanium and niobium powders was developed. To do so, the method of atomic-scale particles (method of molecular dynamics) was used to model the process of alloy crystallization at different temperature gradients. Alteration of the temperature gradients was determined by the regimes of initial temperature state of the system and different intensity of heat removal determined by thermophysical properties of the substrate. Further, the adhesion between the particles of obtained Ti-Nb alloy determined by the duration of the high-energy laser exposure was estimated.

2. Calculation Results

2.1. Features of Ti-Nb alloy crystallization

To study the features of Ti-Nb alloy crystallization under different temperature gradient conditions on the scale of single atoms, the method of molecular dynamics in the form of LAMMS software [6] was used. Interatomic interaction was described using an interatomic potential calculated using the embedded atom method [7, 8], which earlier had been verified in test problems by calculating elastic and energy characteristics. The simulated system consisted of two spherical crystallites, one of which corresponding to the lattice of titanium, and the second one, to the lattice of niobium. The initial sample structure is shown in Figure 1a.

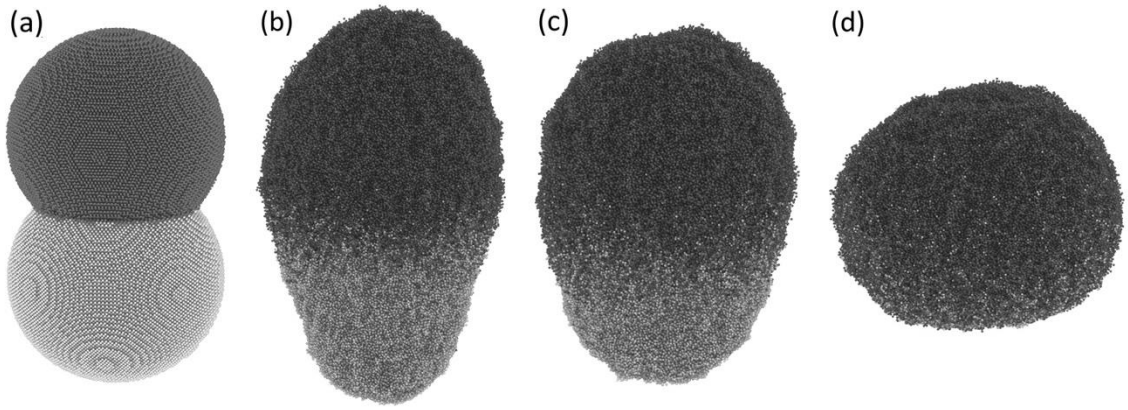

Figure 1. (a) The initial structure of the modeled particles of Ti (dark gray) and Nb (light gray) and structure corresponds to different moments of time of the high-speed heating process up to 6000K: (b) 70 ps, (c) 120 ps and (d) 220 ps.

The diameter of each sphere was 10 nm, which is 5 times less than the characteristic size of the powder particles used for laser synthesis. The total number of atoms exceeds 150000. In order to study the effect of varying duration of a laser beam exposure, the high-speed warm-up of two particles up to temperature of 6000 K, 5000 K and 3000 K in various tasks was realized. Snapshots given in Figures 1b and 1c demonstrate the structure of the modeled system at different moments of time corresponding to the heating process. Because of warm up stage, the uniform melting for both metals within one particle was achieved as shown in Figure 1d.

The future solidification procedure, during which a linear decrease of the system temperature from a high value down to ambient one (300 K) was carried out. The following cooling rates of the modeled ensemble of atoms were studied: 9.5, 5.7 and 3.1 deg./ps. The corresponding time dependencies of the temperature changing for the modeled system during cooling stage are shown in Figure 2. Note that in order to achieve the cooling rate of 3.1 deg./ps, the resulting temperature of the system after heating stage was decreased down to 5000 K. The resulting structure of the sample after cooling was analyzed using the algorithm, which allows determining the local topology of interatomic structure corresponding to bcc, fcc and hcp crystal lattices. The influence of the cooling rate on the fraction of atoms with bcc local topology of Ti-Nb alloy was studied.

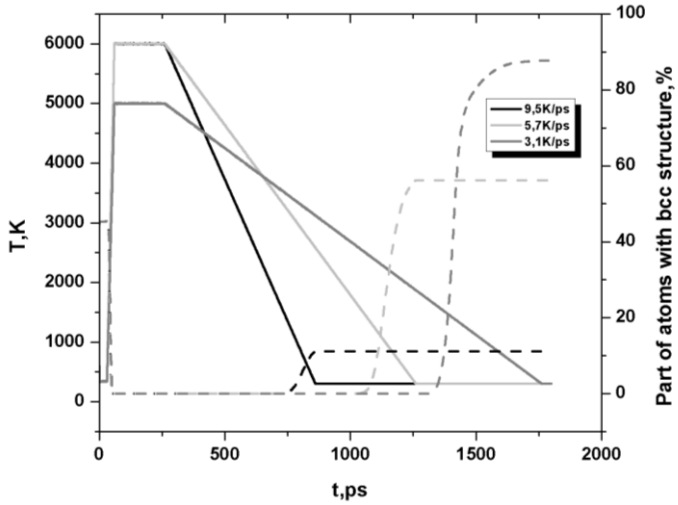

Figure 2. The results of crystallization process for Ti-Nb system. Time dependencies of the system temperature and fraction of fcc atoms for three cooling rates.

The resulting structures for considered variants of cooling rates are shown in Figures 3a-3c. The percentage of bcc atoms for the resultant state depends on the cooling rate and amounts to 11.2%, 56.2% and 87.7%, respectively. Further reduction of the system cooling rate did not result in a noticeable change in the proportion of atoms with bcc lattice in the resulting state. Thus, by trying different cooling modes of the system, we found that the cooling rate of 3.1 deg./ps or less for two-component system is sufficient to ensure the formation of the resulting polycrystalline structure of Ti-Nb beta-alloy. The remaining 12% correspond to the surface atoms, and atoms located near the formed grain boundaries.

These results allow using mechanical and physical characteristics of the formed particles of Ti-Nb alloy as the parameters needed to describe the interaction between particles for models of mesoscopic scale. It is also noteworthy that there is a qualitative conformance of modeling results with obtained experimental data on the influence of preheating of the powder mixture and usage of substrate for producing beta-titanium-niobium alloy by laser sintering.

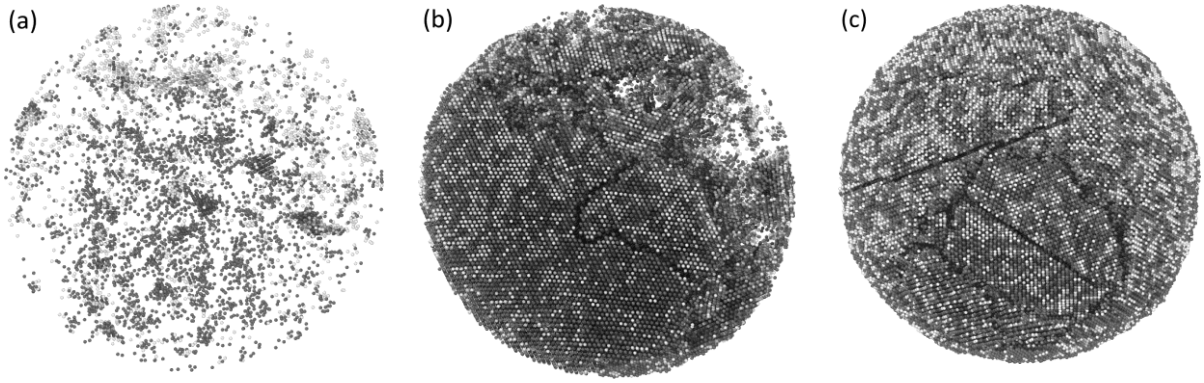

Figure 3. The final structure of the modeled sample after crystallization with different cooling rates: (a) 9.5 deg./ps, (b) 5.7 deg./ps and (c) 3.1 deg./ps.

2.2. Adhesion properties of Ti-Nb particles

Next stage of research was devoted to studying the influence of the heating duration of alloy particle system and its cooling rate on the value of the resulting adhesive force. For this purpose, two hemisphere-shaped particles with an internal structure corresponding to the structure of β-alloy Ti-Nb system obtained by crystallization were simulated. Testing was carried out as follows. Initially, the hemisphere juxtaposed for the distance between their poles of about 1 nm. The configuration of this modelled system is shown in Figure 4a. The crystallographic orientation of the particles was chosen so that in the area of convergence of the particles a grain boundary was formed.

At the next stage the heating of particles in the area of juxtaposed poles was simulated by adding kinetic energy to the surface atoms considering the ratio 1 eV/ps for the whole system. As a result, melting of the hemispheres and their subsequent sintering occurred. Depending on the duration of heating the sintering area was changing. The resulting structure, corresponding to the contact area of 8500 $Å^2$ is shown in Figure 4b. This configuration was obtained by heating the modelled system in the area of converged tops of particles up to ~3000 K within 50 ps, followed by cooling.

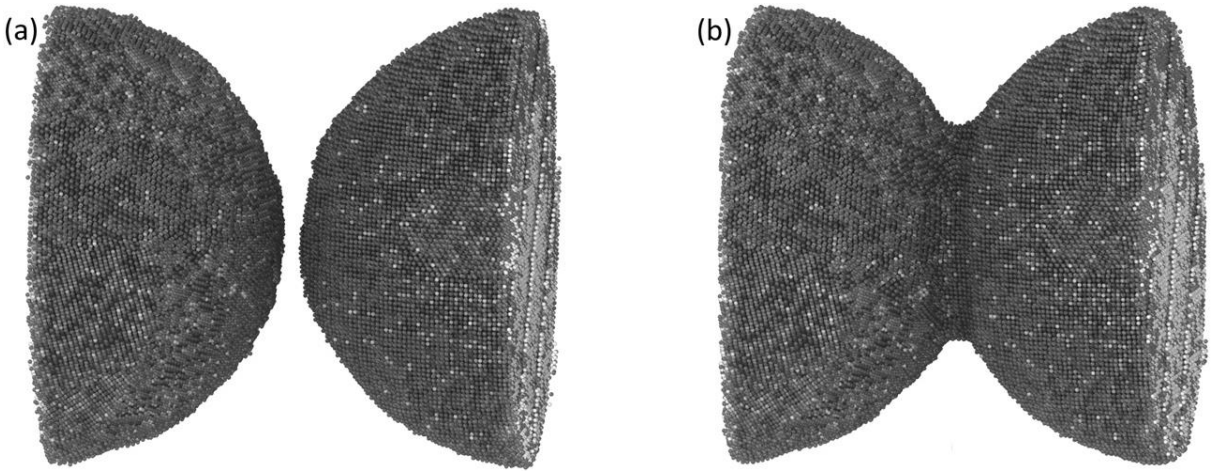

Figure 4. The structure of the modeled setup of Ti-Nb β-alloy at different stage: (a) before heating, (b) after heating.

To assess the adhesive force, the configurations, not only with different values of the contact square, but also with a different structure of resulting contact were created. The modifications in the structure were achieved by changing the cooling rate of the molten area. At low cooling rates, the crystallization of the molten contact area with formation of a grain boundary was observed. At

relatively high cooling rates the amorphization of a conjugated area was taking place. The final stage of adhesion force estimation included the simulation of the break of the formed fused region. To do this, the atoms in the base of the hemispheres were assigned constant values of speed oriented in opposite directions along X axis. Figure 5 depicts the dependence of ultimate value of force of resistance to break on the initial area of fusion region. Evidently, there is a clearly pronounced linear dependence between forces and areas for all considered cases. In these particular cases features of structure of the molten area does not have a significant impact on the resulting dependence.

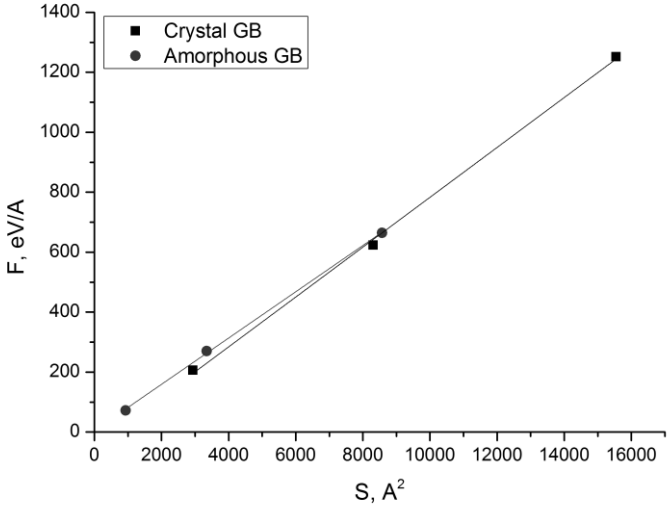

Figure 5. The dependence of adhesion strength on the area and the structure features of the molten area of two particles of Ti-Nb β-alloy.

Thus, the main factor determining the magnitude of the adhesive force is the area of the surface involved in the contact between two particles. This parameter directly depends on the duration of thermal exposure. The cooling rate and the related structure of the molten area has almost no effect on the resulting adhesion properties.

3. Conclusions

The results of computer simulation of melting process, followed by the crystallization of a mixture of particles of titanium and niobium, for different values of the temperature gradient allowed determining the conditions necessary to obtain a system with a maximum content of beta-crystal structure of the alloy Ti-Nb. It was found that the cooling rate of 3.1 deg./ps or less for considered two-component system is sufficient to ensure that the resulting polycrystalline structure will be a beta alloy with maximum content of bcc lattice. The variation of temperature gradients was determined by initial system temperature and various intensity of heat removal defined by thermophysical properties of the substrate. It should be noted that the obtained results qualitatively conform with experimental data on the effect of preheating the powder mixture and the use of substrate during the production of beta-alloy of titanium-niobium system by selective laser sintering [9, 10]. According to the simulation results, it was shown that the main factor determining the value of adhesion forces between the particles is the area of the region involved in the contact between two particles. The rate of cooling and the structure of the obtained contact region has almost no effect on the properties of the resulting adhesion. The obtained result will be used to specify the mechanical and physical characteristics of the formed powder particles of Ti-Nb alloy in the description of the interaction between the particles in the model of a mesoscopic scale.

Acknowledgments

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References

[1] Bai Y, Deng Y, Zheng Y, Li Y, Zhang R, Lv Y, Zhao Q, Wei S 2016 *Mat. Sci. Eng.* C **59** 565
[2] Andrade D P, Vasconcellos L M R, Carvalho I C S, Santos E L S, Prado R F, Santos D R, Cairo C A A, Carvalho Y R 2015 *Mat. Sci. Eng.* C **56** 538-544
[3] Fischer M, Joguet D, Robin G, Peltier L and Laheurte P 2016 Mat. Sci. Eng. C (doi://dx.doi.org/10.1016/j.msec.2016.02.033)
[4] Silva D N, Oliveira M G, Meurer E, Meurer M I, Silva J V L, Santa-Bárbara A 2008 *J. Craniomaxillofac Surg* **36** 443-449
[5] Nikonov A Yu, Zharmukhambetova A M, Skripnyak N V, Ponomareva A V, Abrikosov I A, Barannikova S A, and Dmitriev A I 2015 *AIP Conf. Proc.* **1683** 020165
[6] Plimpton S J 1995 *J. Comp. Phys.* **117** 1-19
[7] Daw M S and Baskes M I 1984 *Phys. Rev.* B **29** 6443
[8] Jones C and Farkas D 1996 *Comp. Mat. Sci.* **6** 231-239
[9] Khimich M A, Parilov E A, Kovalevskaya Zh G and Sharkeev Yu P 2015 *IOP Conf. Ser.: Mater. Sci. Eng.* **93** 012042
[10] Saprykina N A, Saprykin A A, Borovikov I F, Sharkeev Y P 2015 *IOP Conf. Ser.: Mater. Sci. Eng*. **91** 012031