Molecular dynamics study of the influence of the parameters of the crystallization process during selective laser sintering of alloy Ti-Nb

Anton Yu. Nikonov, Andrey I. Dmitriev, Yuriy P. Sharkeev
anickonoff@ispms.ru

Abstract

In the paper the study of the processes occurring at different stages of the process of laser sintering is performed using the method of computer simulation on the atomic scale. The initial configuration of the system is two spherical crystallites with properties of titanium and niobium, with the interface. Interatomic interaction was described by the embedded atom method. We analyzed the effect of cooling rate on the resulting crystal structure of the alloy Ti-Nb. We also investigated the dependence of the resistance forces to break of sintered 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. The simulation results can not only define the technological parameters of the process to provide the desired mechanical properties of the resulting products, but also are a necessary basis for calculations on large scale levels in order to study the behavior of implants in actual use.

1 Introduction

Currently, one of the dominant material for the production of bio-implants is titanium and titanium alloys. Along with the recognized advantages of titanium as the implant material (magnetic inertia, bio-compatibility, 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 high biomechanical compatibility point of view beta alloys of titanium-niobium, which may also have the effect of pseudoelasticity, bringing them closer in properties to the properties of cortical bone may be considered. [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 the titanium and niobium have a very 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, during such treatments the preform lost to half volume.
Recently use of the additive technology, in particular, methods of synthesis of layered laser solves the above problems and achieves the objectives of personalized medicine [3, 4]. Advantages of additive technology and selective laser sintering are especially the possibility of forming not only the volume of the product, but also the internal structure. When forming structure it is possible simultaneously to synthesize a new material (alloy), using as the starting powder mixture components in the desired proportions.
Obviously, the physical properties of samples are determined primarily by processing conditions and the properties of the starting powder. In turn, the problem of determining the optimal impact parameters on the starting 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. A short time duration and high power laser beam makes particularly difficult to direct experimental study the effects of high-energy impact. 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 using of methods of numerical modeling. Thus using the numerical method of *ab initial* calculations described in [5] the optimal stoichiometry to obtain the desired elastic modulus for Ti-Nb alloy system was found. In the present paper, 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. For this aim, the particle based method of atomic-scale - the method of molecular dynamics was used to simulate processes of alloy crystallization under different temperature gradients conditions. Varying the temperature gradients was determined by the original temperature conditions of the system and by changing the heat sink intensity given by the thermo-physical properties of the substrate. Future the adhesion properties between particles of obtained Ti-Nb alloy, determines by the duration of the high-energy laser exposure were estimated.

2 Results of calculation

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 in the framework of the embedded atom method [7, 8], which had earlier been verified in test problems on the calculation of elastic and energy characteristics. The simulated system consisted of two spherical crystallites, one of which was corresponded to the lattice of titanium, and the second one - niobium. 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. The initial sample structure is shown in Fig. 1a.
In order to study the effect of varying duration of a laser beam exposure the high-

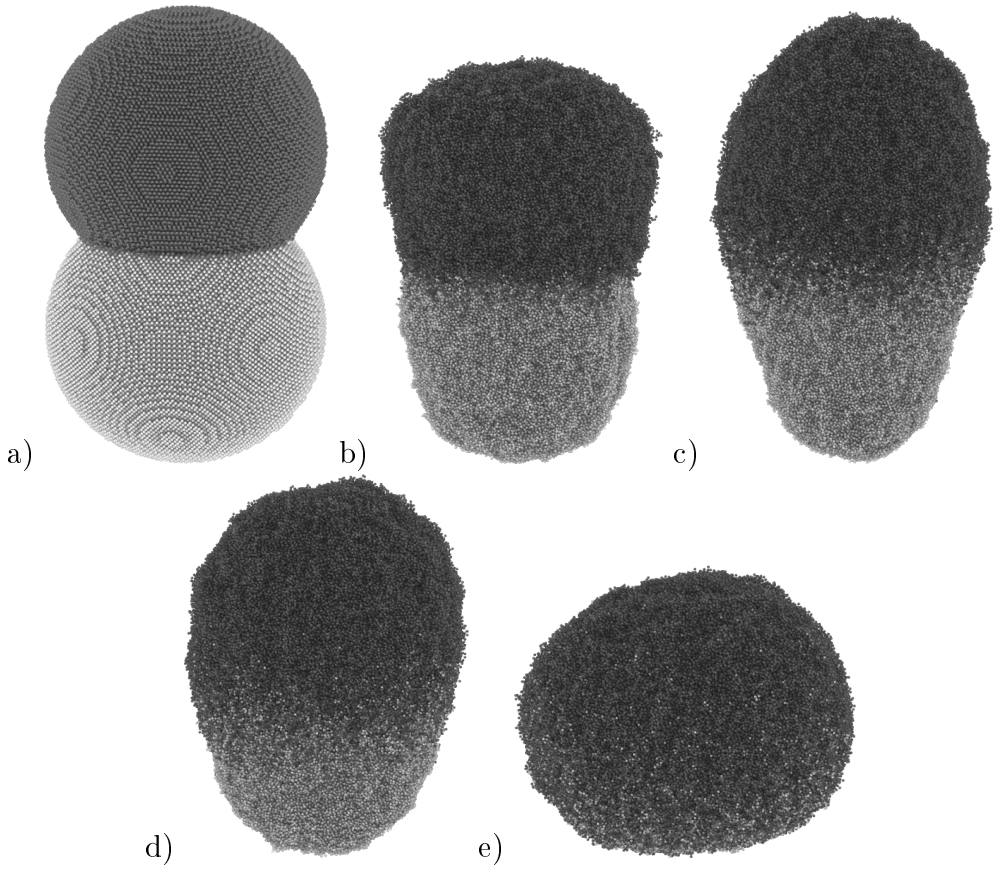

Figure 1: (a) The initial structure of the modeled particles of Ti (dark gray) and Nb (light gray) and structure corresponds to different moments of time of the high-speed heating process up to 6000 K: (b) 30 ps, (c) 70 ps, (d) 120 ps and (e) 220 ps.

speed warm-up of two particles up to temperature of 6000 K, 5000 K and 3000 K in various tasks was realized. Snapshots given on Figures 1b-d demonstrate the structure of the modeled system at different moments of time corresponding to the heating process. As a result of warm up stage the uniform melting for both metals within one particle was achieved as shown in Figure 1e.

The future solidification procedure during which a linearly decreasing of the system temperature from high value to ambient (300 K) one was carried out. The following cooling rates of the modeled ensemble of atoms were studied: 9.5, 5.7 and 3.1 K/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 K/ps the resulting temperature of the system after heating stage was decreased to 5000 K. The resulting structure of the sample after cooling was analyzed using the algorithm which allows one to determine the local topology of interatomic structure corresponding to bcc, fcc and hcp crystal lattices. The influence of cooling rate on the ratio of atoms with bcc local topology of Ti-Nb alloy was studied.

The resulting structures for considered variants of cooling rates are shown in Figures 3a-c. Percentage of bcc atoms for the resultant state depends on the cooling rate and amounts to 11.2%, 56.2% and 87.7%, respectively. A further reduction of

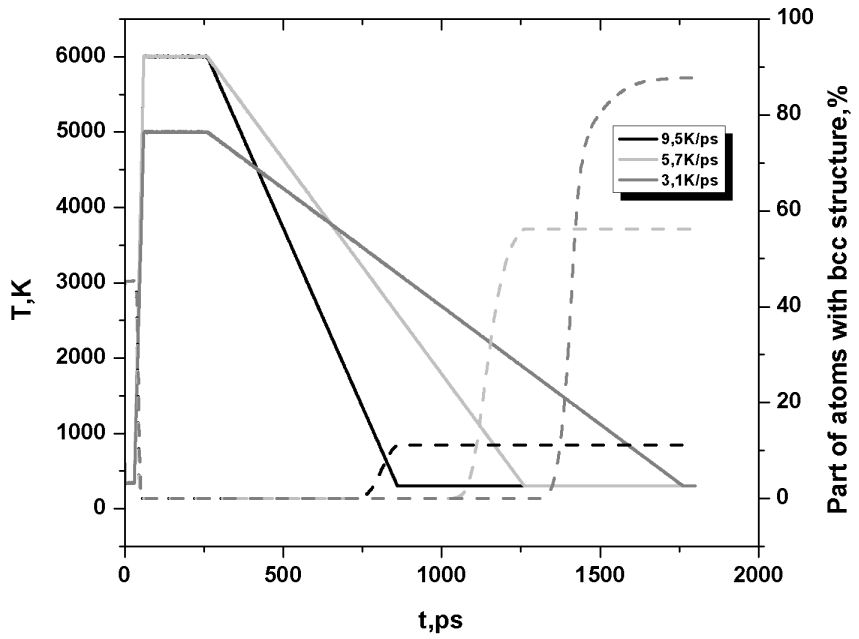

Figure 2: Time dependencies of the system temperature and parts of fcc atoms for three cooling rates.

the rate of the system cooling has not led to a noticeable change in the proportion of atoms with a bcc lattice in the resulting state. Thus, by trying of different cooling modes of the system we found that the cooling rate of 3.1 K/ps or less for two-component system is sufficient to ensure that to form the resulting polycrystalline structure of Ti-Nb beta-alloy. The remaining 12% corresponds to the surface atoms, and atoms located near the formed grain boundaries.

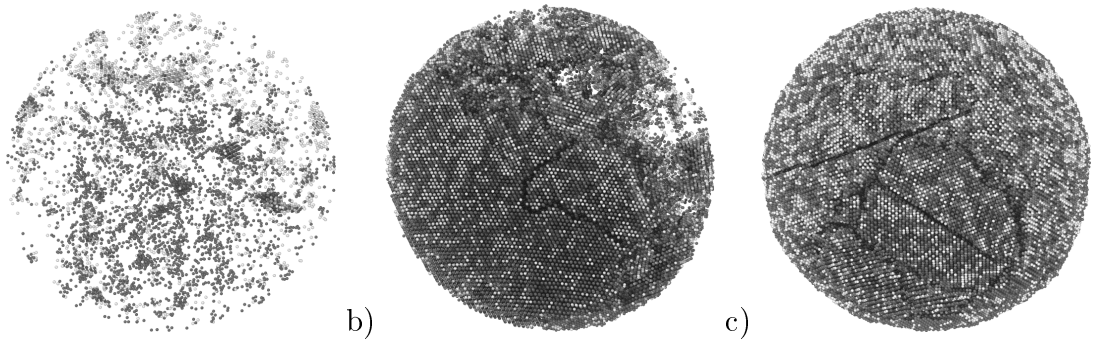

Figure 3: The final structure of the modeled sample after crystallization with different cooling rates: (a) 9.5 K/ps, (b) 5.7 K/ps and (c) 3.1 K/ps.

These results allow the use of mechanical and physical characteristics of the formed particles of the Ti-Nb alloy as the parameters needed to describe the interaction between particles for models of a mesoscopic scale. We can also note the qualitative agreement between results of simulation and existing experimental data on the effect of pre-heating the powder mixture and the use of the substrate during the preparation of beta-titanium-niobium alloy under selective laser sintering.

2.2 Adhesion properties of Ti-Nb particles

Next stage of research was devoted to study the influence of the alloy particle system heating duration 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 the β-alloy Ti-Nb system obtained by as a result of the crystallization process were simulated. Testing was carried out as follows. Initially hemisphere from their tops converged to a distance of about 1 nm. Obtained in this way configuration of the modeled system is shown in Figure 4a. The crystallographic orientation of the particles was chosen so that, in the area of convergence of the particles grain boundary was formed.
By the next stage of testing a local heating of both particles in the region of tops convergence by adding the kinetic energy to the surface atoms of the ratio of 1 eV/ps for the entire system was simulated. As a result melting of the hemispheres and their subsequent sintering were occurred. Depending on the duration of heating the sintering area has changed. The resulting structure, corresponding to the contact area of 8500 Å^2 is shown in Figure 4b.This configuration was obtained by heating the modeled system in the area of convergence of particles tops to $\approx$ 3000 K within 50 ps, followed by cooling.

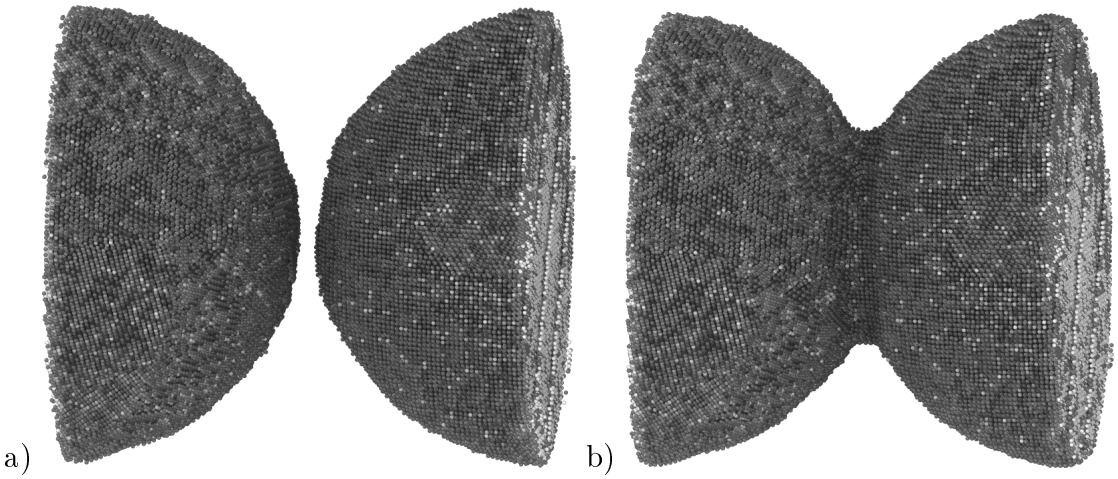

Figure 4: The structure of the modeled setup of Ti-Nb β-alloy at different stage: (a) before heating, (b) after heating.

To assess the adhesive force the configuration, not only with different values of the contact square, but 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 adhesive forces estimation consists into modeling of rupture of the formed coupling. To this end, the movement with constant velocities of atoms located at the base of the hemispheres was modeled. Velocities were oriented in opposite directions along axis X. Figure 5 shows the dependence of the resistance force on the initial value of the square of molten area. It can be seen very well pronounced linear dependence

between forces and squares 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.

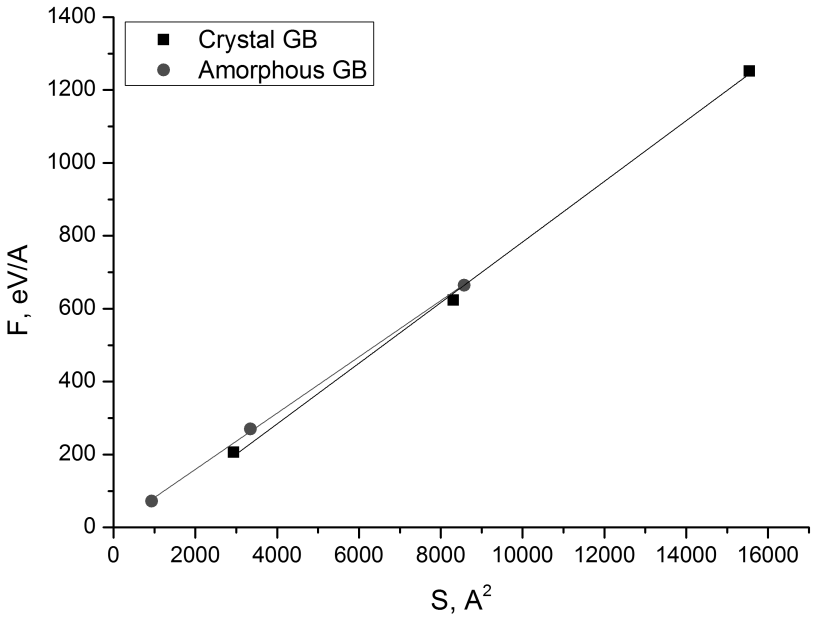

Figure 5: The dependence of adhesion strength on the square and the structure features of the molten area of two particles of Ti-Nb β-alloy.

Thus, the main factor determining the magnitude of the adhesive force is the square of the area 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 almost no effect on the resulting adhesion properties.

3 Conclusions

Computer simulation results of the melting process, followed by crystallization of a mixture of particles of titanium and niobium, for different values of the temperature gradient allowed to determine 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 K/ps or less for considered two-component system is sufficient to ensure that the resulting polycrystalline structure was beta alloy with a maximum content of the bcc lattice. At that variation of the temperature gradients determined by the initial system temperature and a different heat removal intensity defined by thermo-physical properties of the substrate. It should be noted that the obtained results qualitatively agree 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 the 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 almost no effect on the properties of the resulting adhesive. The obtained result will be used to specify the mechanical and physical characteristics of the formed powder particles of the alloy Ti-Nb in the description of the interaction between the particles in the model of a mesoscopic scale.

Acknowledgements

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Nikonov A.Yu., Akademichesky 2/4, 634055, Tomsk, Russia
Dmitriev A.I., Akademichesky 2/4, 634055, Tomsk, Russia
Sharkeev Yu.P., Akademichesky 2/4, 634055, Tomsk, Russia