

Impact of Machining and Phase Composition Change of Titanium Alloyed with Molybdenum

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Abstract. The titanium samples alloyed with molybdenum and aluminum are used to conduct full high-precision X-ray experiments enabling to determine the characteristic of the atomic interrelations - the unit cell dimension, and to establish the phase components of the doped single crystal. An orthorhombic phase is found, the volume of which increases after the deformation impact.

Introduction

The refractory elements added to the alloys of titanium with aluminum change their strength and other functional characteristics. The alloying significantly extends the application of these materials in biomedicine and other applications. Currently, in order to create new compositions based on titanium, a comprehensive study of these alloys by various methods and modeling of their characteristics based on quantum-mechanical calculations is used [1-2].

The concentration dependence of microhardness, corrosion as well as other characteristics of the atomic and electronic structure are studied in [2] for alloys of the Ti-Mo binary system. Both the calculations and the experimental data allowed to establish the factors of the relationship between the energy chains of composition-structure properties, ranging from the atomic and electronic level to the meso-, micro- and macrolevels of the real macroscopic properties of products made of these alloys. The influence of molybdenum additions on the phase composition, microstructures, and mechanical properties of initial composition of the Ti6Al4V with a gradual increase in-the Mo content up to 6 wt.% is studied in [3]. It is shown that the element hardening the solid solution such as Mo improves mechanical properties like yield strength, ultimate tensile strength, ductility, and hardness, compared with the pre-alloyed Ti6Al4V alloy.

The impact of mechanical treatment on the strength properties of samples of titanium with a higher molybdenum content is studied in this work. For the beta-phase of the samples, high-precision experiments were carried out for the first time, using single crystal X-ray diffractometry, and the comparison was made with the undoped composition. These experiments enabled to determine the basic thermodynamic characteristic of atomic interrelation after crystallization of alloys – the unit cell dimension (the parameter of the formed crystal lattice) [4].

Samples and procedure

To investigate microhardness by the Vickers (HV50) method the plates cut from ingots were used. The electric spark cutting was followed by electropolishing with the surface layer of 20 μm and

60 μm being removed. Then the surface was treated with an emery cloth coated with corundum of an average size of 40 μm , after which the surface was polished using diamond paste (with the particle size of 9 μm) and colloidal silicon. 49 times the measurements (matrix 7*7 on each plate) were carried out using a PMT3 microhardness-meter with the applied load of 50 grams. The deformed layer having been measured, the electropolishing was again carried out bringing the surface to the initial state, and the measurements of the microhardness of the same samples were repeated.

For the measurements performed on a four-circle single-crystal diffractometer ("Xcalibur" Rigaku-Oxford Diffraction) cubes with the face size of 1 mm were cut from large grains of a composition containing 15% Mo and 6% Al. To improve the measurement accuracy, spherical samples with a diameter of no more than 0.3-0.4 mm were prepared from them. After rolling, the surface layer was removed by etching. The preliminary diffraction patterns exhibited high quality of the analyzed samples and suggested a reliable and detailed analysis of the intensity distribution in each recorded Bragg reflection.

In the measurements a short-wavelength MoK α 1 radiation with a wavelength of 0.070932 nm was used, which enabled the recording of the diffraction pattern of total volume analyzed samples. The samples were sequentially rotated making possible to record the intensity of the reflected beams on the CCD-detector with a full display of the Ewald sphere, during 80-180 hours (two control reflections were recorded every 50 frames to take into account possible drifts; however, voltage fluctuations did not exceed 0.1 V at a voltage of 50 kV).

From 8 to 24 sets of the independent system of Bragg reflections were obtained (depending on the Miller indices of these reflections), which ensured additionally an increase in the accuracy and reliability of the measurement results. The lattice parameters of the beta-phase were calculated in accordance with the Bragg-Wolf law and cubic symmetry of the unit cell. Unlike powder diffractometry, when from 6 to 40-60 averaged reflections are recorded, the use of the geometry of 4-circle diffractometer and a single-crystal form of the samples made possible to record more than 2600 Bragg reflections in the diffraction pattern of each sample at room temperature (297-300) K.

Results and discussion

The study of alloys based on titanium, including bimetallic products, showed the presence of synergy of effects at the micro- and macro-level of the material structure during various kinds of machining [5-8]. For the investigated composition, also considered sequentially were the data at the microstructural and then at the atomic level of the structure.

The microhardness of the samples remained invariable after a layer of thickness of 20 μm and 60 μm was removed. The use of diamond pastes for surface treatment increased microhardness and the use of larger corundum particles of an average size of 40 μm , which are commonly used in surface treatment technology, led to an additional increase in microhardness more 11%.

It was shown in [3] that phase shifts of diffraction reflexes occurred when the stabilizer Mo from 2 to 6 wt.% was added, exhibiting the occurrence of the lattice distortion. It was found that the lattice parameter changed from 0.3228 nm for Ti6Al4 to 0.3232 nm, 0.3243 nm, and 0.3251 nm for Ti6Al4V-2Mo, -4Mo, and -6Mo, which the authors considered was due to the increase of stabilizer Mo content from 2 to 6 wt.%, which acting as hardening agent in the solid-solution in the pre-alloyed Ti6Al4V alloy, and which is seen in the improved mechanical properties of the alloys - microhardness. Ti6Al4V-6Mo had the highest value among these compositions.

The lattice parameters for our alloy containing 15% molybdenum and 6% aluminum, demonstrated a further increase in the crystal lattice parameters of the beta-phase - 0.330595 (2) nm and 0.330628 (2) nm for two studied samples.

An analysis of references was also carried out, for related to the crystal lattice parameters of the alpha-phase of pure hexagonal titanium [9] and the beta-phase [10] of titanium. Two methods were used to estimate the values of the lattice parameter of the beta-phase at room temperature. For the undoped beta phase, in one method the lattice parameter at room temperature was determined by extrapolating the values measured for the beta-phase at high temperature, which gave a value of $a_{\text{extr}} = 0.3276$ nm; in the other method it was near this values of $a_{\text{extr}} = 0.3279-0.3282$ nm. They were obtained by extrapolating data from the dependences of the lattice parameters on the concentration of substituent varied elements (Mo, Nb, V, Zr, Cr, Ta, Fe, Al).

The experimental data in [11] indicate that as the Mo content increases, on parts of the volume of sample a martensitic transformation can occur, including under the action of the applied stress. The martensite has a hexagonal structure denoted as α' -martensite, in dilute compositions with a higher solute content as orthorhombic α'' -martensite in alloys.

It should be noted that in this study the full diffraction pattern from the analyzed sample is recorded. The use of single-crystal samples increases the intensity of the observed reflections by 3-4 orders of magnitude. The software (CrysAlis) allows for such samples to detect the presence of a second phase, though it may be in small quantities. In fact, along with the predominant beta-phase, a family of reflections was found in the samples, with a unit cell belonging to the orthorhombic phase. The amount of this phase may differ in different parts of the sample and probably be the cause of small scattering of values of the parameters of the two studied samples. Preliminary estimates show that the number of reflections of this second phase can be more than 25% of the number of reflections of the beta phase.

It is well known that the presence of a metastable anisotropic phase in samples leads to the appearance of noticeable distortions in the matrix and to an increase in the density of dislocations in the matrix. This, in turn, can be one of the reasons for the observed increase in strength characteristics during deformation action on the surface of the samples.

Summary

The use of single crystal samples enables to increase the accuracy and reproducibility of the results of diffraction experiments. The addition of molybdenum results in an increase in the crystal lattice parameter of the beta-phase of titanium and in the appearance of a second metastable orthorhombic phase in this alloy. The mechanical surface treatment, inducing more micro-distortions and providing the formation of a second phase, leads to an increase in the strength characteristics of the surface of products made from this alloy.

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