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STRUCTURAL AND PHYSICAL CHARACTERIZATION OF NEW Ti-BASED ALLOYS

Production of Ti-based alloys with non-toxic elements give the possibility to control the market of medical applications, using alloys with appropriate properties for human body, contributing to improving the health of the population. Determination of parameters of atomic and magnetic structure of functional biomaterials demonstrating interesting physical phenomena and being promising for medical applications in a wide range of thermodynamic parameters; exploration of the role of cluster aggregation in the formation of physical properties. Paper is about the obtaining of the new titanium system alloys, the determining their characteristics and structure, and obtaining information concerning phase transitions and some mechanical properties. Ti15Mo7ZrxTa (5 wt.%, 10 wt.% and 15 wt.%) alloys developed shows a predominant β phase highlighted by optical microstructure and XRD patterns. A very low young modulus of alloys was obtained (43-51 GPa) which recommends them as very good alloys for orthopedic applications.

Keywords: new biomaterials; titanium alloys; biocompatible elements; β phase

1. Introduction

Metallic biomaterials is a class of materials used for different medical applications, because they have some good mechanical properties, are resistant to corrosion and have an acceptable biocompatibility [1]. The most known and used are metallic biomaterials are: stainless steels alloys, Co-Cr alloys and Ti-based alloys [2,3]. It is also possible to use Fe-based bulk amorphous alloys, which are characterized by good mechanical properties [4,5].

Stainless steels are a class of metallic materials that largely have the properties imposed on the materials used in the human body: biocompatibility, chemical, thermal and mechanical stability in the special conditions of the human environment [6]. Used for orthopedic implants have the disadvantage of a high modulus of elasticity [7].

Cobalt-based alloys are widespread in medical applications, such as orthopedics, but especially dentistry. However, Co-Cr alloys have problems with poor adhesion to bone tissue and allergic reactions caused by cobalt in the body, sometimes even 15 months after the removal of implants with high concentrations of cobalt in the blood and plasma [8]. Another disadvantage for Co-Cr alloys is Young's modulus of high values (210-232GPa), thus negatively influencing bioadhesion. Thus, the elastic deformations of the implants and the high pressing pressure are transferred to the bone, which is an important shortcoming [9].

Titanium and titanium-based alloys are the most widely used metal materials for implants. The most used titanium alloys are the Ti4Al6V alloy and C.P. Ti, which has good physico-mechanical, chemical and biocompatibility characteristics [10,11]. When many researches were discovered that vanadium is toxic, it started to be replaced with various biocompatible elements: Nb, Fe, Si, Ta, Mo, etc. [12].

Titanium alloys used as implant materials has the advantage that can form on their surface protective, stable passivity films, which "close" the metals to the corrosive environment [13,14]. The ability to form protective films is called passivation, and the state of high corrosion resistance is defined as passivity [15].

Aim for the present study is to design a new alloy for future medical applications. The paper presents the design and characterization of three original titanium-based alloys, improved

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with biocompatible elements like molybdenum, zirconium and tantalum. The addition of biocompatible elements such as Mo, Zr and Ta shows good mechanical properties (a lower modulus of elasticity), compared to other classical biomaterials.

We choose elements like Mo, Zr and Ta alloyed with Ti because are biocompatible elements, which do not cause side effects [8]. Also, molybdenum and tantalum are beta stabilizers for titanium alloys, elements that can bring improvements to the properties of the alloys [12]. Zirconium is a neutral element, but alloyed in the compositions of titanium alloys, refines the structure of the alloys [8,9].

2. Experimental Procedure

In order to obtain the experimental titanium alloys, it was chosen to use an arc remelting vacuum installation (RAV) MRF ABJ 900 type. to obtain alloys with uniform composition, by repeated remeltings. For the elaboration of Ti-Mo-Zr-Ta alloys, were used high purity elements as raw materials (Ti-99.8%, Mo-99.7%, Zr-99.2% and Ta-99.5%) and have been degreased and properly prepared for obtaining.

OPTIKA XDS-3 MET optical microscope was used for the structure analysis. The metallographic samples were properly prepared: cutted to appropriate dimensions, embedding in epoxy resin, grinding and polishing at specific speeds, chemical attack with reactive (10 ml HF, 5 ml HNO_3, 85 ml H_2O, for 30 s).

Phase determination was performed by qualitative analysis by X-ray diffraction, using a PanaticalX'Pert Pro MPD equipment. Thus, the phases and compounds that make up the investigated alloys were highlighted. Parameters used for the analysis of samples are: an angle range θ-2θ between 20-80°; continuous scan; step size of 0.0131303 (°), time per step: 60 (s); scan speed 0.054710 (°/s); number of steps: 6093. An X-ray tube with copper anode was used, which emits X-rays in linear mode, using a Pixcel type detector. The data obtained were processed with the Highscore Plus program, then they were imported and processed using an experimental data processing software in order to obtain the diffractograms of the experimental alloys.

Universal Micro-Tribometer CETR UMT-2 equipment was used for tribological and mechanical determinations.

3. Results and discussions

Elaboration of alloys in (RAV) MRF ABJ 900 type was efficiently, losses were minimal (max 1%). The metal load was 30 g per alloy and all alloys were followed to six remeltings to obtain homogeneous alloys. Table 1 presents the chemical composition of the alloys obtained. The percentages of the elements varying with small differences compared to the theoretical load calculation. The analysis bulletins regarding the chemical composition obtained, highlighted the fact that the main elements identified in the elaborated alloys are: Ti, Mo, Zr and Ta, without the existence of inclusions in alloys.

TABLE 1

Chemical compositions of elaborated alloys, expressed in mass percentages

Alloy	Ti [%]	Mo [%]	Zr [%]	Ta [%]
Ti20Mo7Zr5Ta	69.94	18.95	6.53	4.58
Ti20Mo7Zr10Ta	63.02	20.13	7.10	9.75
Ti20Mo7Zr15Ta	59.39	19.25	6.84	14.52

Figure 1 present optical microstructure of the elaborated alloys. As seen in all three images the structure is uniform. For

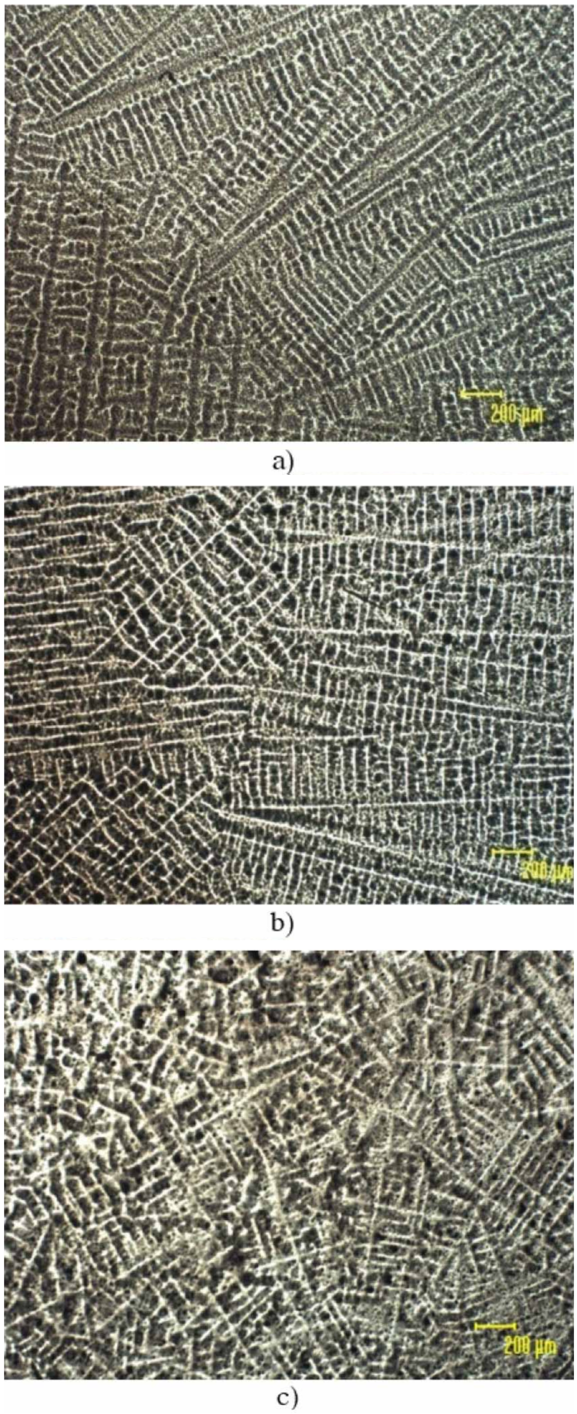

Fig. 1. Optical microstructure of the elaborated alloys at a magnification power of 50×: a) Ti20Mo7Zr5Ta; b) Ti20Mo7Zr10Ta; c) Ti20Mo7Zr15Ta

titanium alloys, percentage of beta or alpha stabilizing elements, contributes on the microstructures and mechanical properties. For Ti-Mo-Zr-Ta alloys, the formation of a β type structure is due the high percentage of β stabilizing elements (Mo, Ta) [16,17]. Zirconium is a neutral element in titanium alloys and contributes to the refining of the microstructure. Figure 2 shows a characteristic EDX spectrum for the alloys analyzed.

Thus, elements with tantalum percentages (5-15%), corroborated with the molybdenum concentration of 15-20%, contribute to the formation of the β phase. With the help of optical microscopy, a biphasic, uniform structure is highlighted, consisting of a high proportion of solid solution β, in which intergranular lamellar structures of dendritic type specific to orthorombicmartensite α" appear. Orthorombicmartensite α" frequently occurs in the case of titanium-based alloys in which there are β-stabilizers in the category of transition metals, which include the elements molybdenum and tantalum. In this case the presence of the α" phase is due to the decomposition of the β phase during cooling.

From Figure 3, the presented diffractograms confirm the β-type structures identified by optical microscopy, taking into account the fact that titanium is an allotropic element, presenting in different forms: up to temperature 882°C, having a compact hexagonal structure α-Ti and above 882°C, β-Ti, having a cube structure with centered volume [18-20]. In the composition of the investigated alloys there is a majority phase β with a cube structure with centered volume and a secondary phase α" with an orthorhombic structure [21,22].

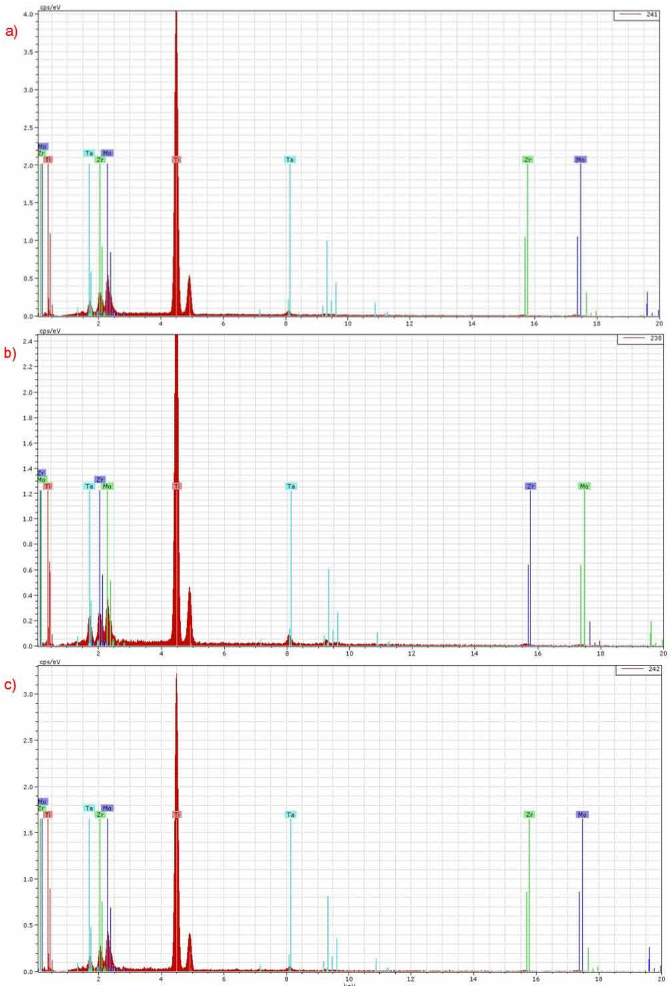

Fig. 2. EDX spectrum for investigated alloys: a) Ti20Mo7Zr5Ta; b) Ti20Mo7Zr10Ta; c) Ti20Mo7Zr15Ta

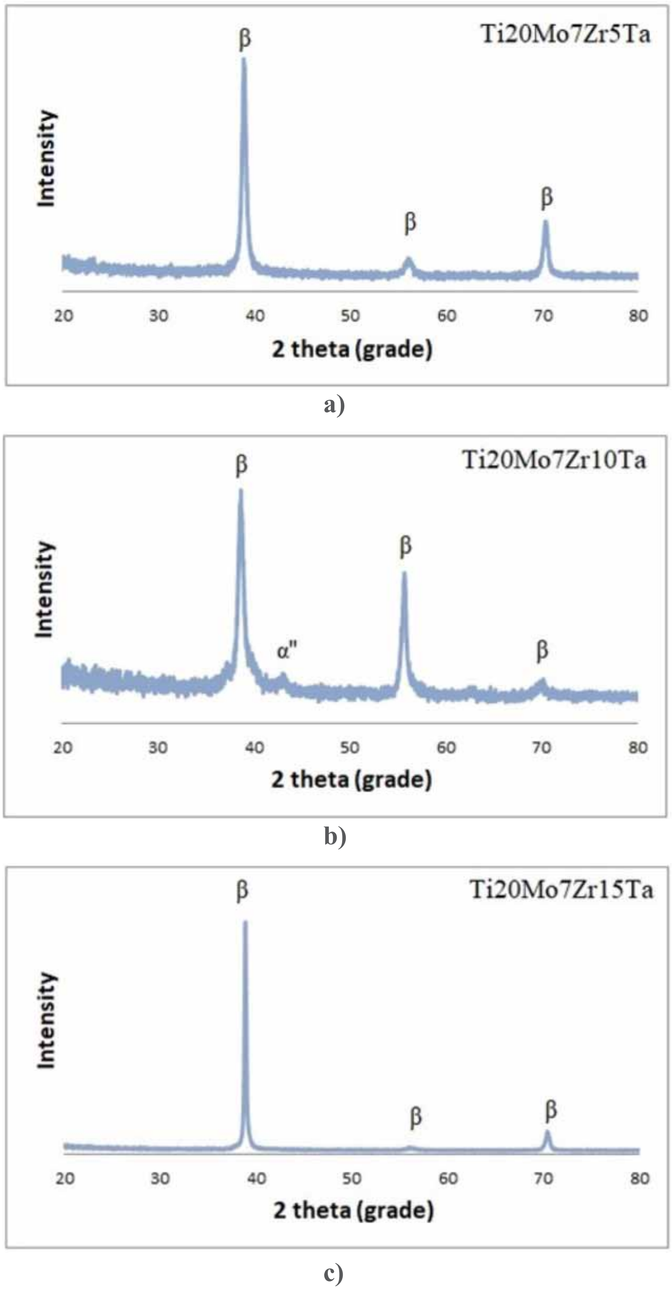

Fig. 3. Diffractograms of elaborated alloys: a) Ti20Mo7Zr5Ta, b) Ti20Mo7Zr10Ta, c) Ti20Mo7Zr15Ta

The predominant β phase (Fig. 2) for the investigated samples: Ti20Mo7Zr5Ta, Ti20Mo7Zr10Ta, Ti20Mo7Zr15Ta, was identified with the main maximum at angle 2θ = 58.7960°; 37.2459°; 38.9277°.

The parameters of the compounds, such as the crystallographic system, the network parameters or the cell volume are highlighted in Table 2. From Table 2 it can be seen that following the volume analysis of elaborated alloys, two solid solutions with the cubic crystallization system were identified.

TABLE 2

Crystallographic parameters for the phases identified following XRD analysis

Solid solution	Group space	System of crystallization	a (Å)	b (Å)	c (Å)	α (º)	ß (º)	γ (º)	Volume cell (10^6 pm^3)	RIR
TaTi	Fd-3m	Cubic	3.29	3.29	3.29	90	90	90	35.48	19.73
MoTi	Fd-3m	Cubic	3.17	3.17	3.17	90	90	90	31.86	14.59

TABLE 3

Elastic modulus values for Ti-Mo-Zr-Ta alloys measured by indentation test

Alloy	Ti20Mo7Zr5Ta	Ti20Mo7Zr10Ta	Ti20Mo7Zr15Ta
Young modulus (GPa)	51.68	45.41	43.57

Table 3 shows the values of the investigated Ti-Mo-Zr-Ta alloys measured by indentation tests, young modulus values between 51.68-43.57 GPa for the modulus of elasticity. It can be observed that with the increase of the Ta content from 5% to 15%, it leads to the decrease of the modulus of elasticity by about 8 GPa.

Figure 4 illustrates a graphical comparison of elaborate alloys versus classical alloys and the modulus of elasticity of human bone. The alloys elaborated from the Ti-Mo-Zr-Ta system have a 50% reduced modulus of elasticity compared to the classic alloy based on Ti6Al4V. The values of the modulus of elasticity are significantly reduced compared to other alloys due to the alloying elements, especially Mo and Ta which reduced the modulus of elasticity. Compared to human bone, the alloys obtained are ideal candidates for orthopedic applications, because the modulus of elasticity is close to that of human bone and thus avoids the phenomenon of stress shielding.

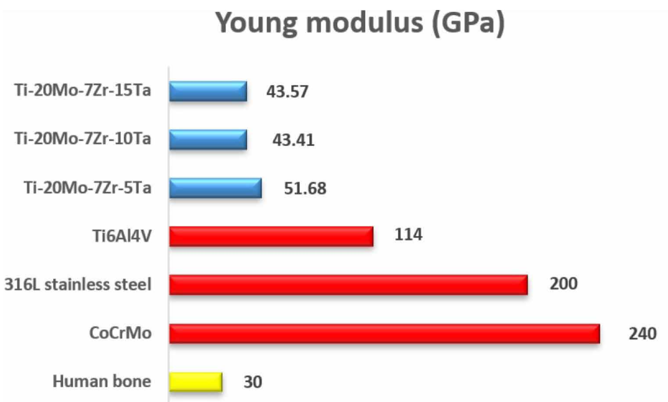

Fig. 4. Comparison of the modulus of elasticity between the classic alloys and the elaborated alloys

4. Conclusions

In the aim to design new alloys for future medical applications, three alloys from the Ti15Mo7ZrxTa (5wt.%, 10 wt.% and 15 wt.%) system were developed in an electric vacuum arc furnace (RAV) MRF ABJ 900 type. This type of equipment develops homogeneous alloys under to the special protection conditions required.

Due to the presence of beta stabilizing elements like Mo and Ta, observed both in diffractograms and in the microstructure of samples, alloys contain β phase (as matrix) and second phases α" (minor).

Indentation testing on the tested alloys showed low values of the elastic modulus between 51.68 - 43.57 GPa, close to the human bone (27GPa).

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