IMPACT OF CHEMICAL COMPOSITION ON ELASTIC MODULUS OF Ti-Zr-Nb ALLOYS

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Zr–Ti–Nb biomedical alloys with b.c.c. structure was produced by cold compaction and vacuum sintering of multicomponent powders. The influence of powder composition on microstructure and porosity was studied. Final porosity (6–9%) is linked to the Frenkel effect and depends on the blend composition.

Keywords: biomedical alloys, powder metalurgy, elastic modulus

Introduction. Currently, biocompatible alloys based on titanium and zirconium are widely used in medical applications. A key requirement for these materials is an elastic modulus comparable to that of human bone. Literature analysis [1–**Помилка! Джерело посилання не знайдено.**] identifies the Zr–Ti–Nb system as the most promising for developing biocompatible, low-modulus alloys. Achieving a reduced Young's modulus is associated with the formation of a single-phase β structure. Studies [2, 2] provide a list of ternary Zr–Ti–Nb compositions with low elastic modulus and stable β-phase, predicted through first-principles calculations. Based on these theoretical findings, several compositions were selected for experimental investigation of synthesis processes using heterogeneous powder blends. These compositions feature relatively high contents of zirconium, titanium, and niobium, which complicates the transformation of multicomponent powder systems into homogeneous alloys with the desired structural-phase characteristics. Therefore, understanding the general principles of their synthesis is of significant scientific and practical interest, particularly for biomedical applications and related industries [2, 2].

Materials and methods. Materials were produced by powder metallurgy methods. It was used zirconium and titanium hydride powders (less 100 μm) and metal niobium (less 63 μm). These blends were compacted at pressure of 640 MPa, room temperature. The powder compacts were heated in vacuum to 1250°C with isothermal holding for 4 hours.

Experimental. The alloy compositions selected for experimental study of the synthesis processes are given in Table 1. Achieving chemical and microstructural homogeneity of these highly alloyed alloys in the solid-phase sintering process is complicated by significant concentration gradients that arise between particles during the redistribution of elements, with a corresponding significant change in diffusion coefficients in the transitional diffusion zones.

Table 1. Compositions of alloys of the Zr-Ti-Nb system selected for the study of synthesis processes, their Young's moduli and characteristic porosity levels.

№	Alloy composition (mass. %)	Young's modulus according to theoretical calculations [2], GPa	Experimentally measured Young's Modulus, GPa	Porosity, %
1	20Zr-43Ti-37Nb	71	Not measured due to preservation of heterogeneous structure	8-14
2	35Zr-39,5Ti-25,5Nb	33	56	9-11
3	59Zr-19Ti-22Nb	49	55	6-10
4	39Zr-36,1Ti-24,9Nb	43	58	7-10
5	47,8Zr-32,7Ti-19,5Nb	65	64	6-8

Typical microstructures of these alloys are shown in Fig. 1. It was shown that the microstructures obtained for each studied composition have certain characteristic differences, which mainly concern the volume fraction and pore morphology. Also, depending on the general chemical composition of such systems, there is a noticeable difference in the rates of homogenization processes during the formation of homogeneous alloys.

Despite the use of two hydrides (zirconium and titanium), which should potentially significantly activate the pore healing processes in the synthesis of all the studied alloys, their microstructure still contains a significant volume fraction of pores, which varies within 6-14% by volume (depending on the chemical composition of the material, Table 1). The residual pores have an irregular elongated shape, and the sizes of some pores reach 100-120 µm in length. As shown by microstructural analysis (fig. 1), four out of five studied alloys achieved complete (fig. 1 b, c, d) or almost complete (fig. 1 e) microstructural homogeneity during high-temperature holding under the specified regime. An exception is the alloy 20Zr-43Ti-37Nb (fig. 1 a), in which, unlike other compositions, after isothermal holding, significant microstructural inhomogeneities still remain, which, as local microanalysis showed, are associated with undissolved niobium particles. For this composition of the powder system, achieving chemical homogenization obviously requires a higher sintering temperature or a significant increase in the isothermal holding time compared to other alloys.

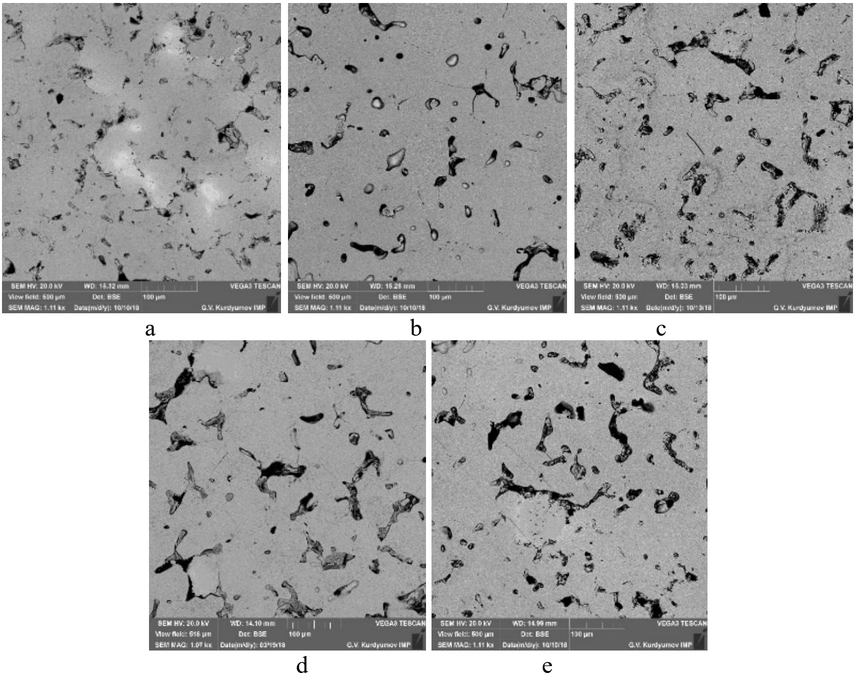

Fig. 1. Comparison of the microstructure of alloys synthesized at 1250 °C with exposure for 4 hours: a – 20Zr-43Ti-37Nb, b – 47.8Zr-32.7Ti-19.5Nb, c – 35Zr-39.5Ti-25.5Nb, d – 59Zr-19Ti-22Nb, e – 39Zr-36.1Ti-24.9Nb.

To compare with theoretical calculations and determine the prospects of synthesizing a particular composition, a preliminary assessment of Young's modulus was carried out. Experimentally measured values of Young's modulus depend on such basic factors as the chemical composition of the alloy and its residual porosity, therefore they differ significantly and are quite different from the values obtained by theoretical calculations for non-porous materials. An increase in porosity is a positive factor in terms of reducing Young's modulus, although at the same time it negatively affects strength and ductility.

Conclusions. The used multicomponent mixtures of titanium hydride, zirconium hydride and niobium powders in different proportions allow the formation of chemically and microstructurally homogeneous alloys for most of the studied compositions during the sintering process (Table 1). Since the 20Zr-43Ti-37Nb composition is characterized by a significantly lower rate of chemical homogenization, it was decided to abandon its further study. Among the alloys for which a homogeneous structure was achieved, the 47.8Zr-32.7Ti-19.5Nb composition with a slightly lower final porosity (6-8%) has a 6-9 GPa higher Young's modulus. This makes this composition less promising for research, since the ultimate main goal is to achieve minimized Young's moduli. The same is true for the 39Zr-36.1Ti-24.9Nb composition.

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