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Elastic and mechanical properties of Ti–Nb–Zr based alloys

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ABSTRACT The elastic properties and mechanical characteristics of Ti–Nb_{22}–Zr_6 based alloys were calculated using the exact muffin-tin orbital method with the coherent potential approximation. Alloying by metals such as Hf, Mg and their combination were considered, and their concentration did not exceed 5 at.%. It was shown that addition of Hf and Mg leads to a decrease in Young's modulus due to both size effect and electronic factor. The calculated Young's modulus for the ternary Ti–Nb_{22}–Zr_6 alloy (70.1 GPa) is found in good agreement with experimental one (70 GPa). The smallest value of Young's modulus was calculated for the Ti–Nb_{22}–Zr_6–Hf_5–$Mg_{2.5}$ alloy, achieving 57 GPa. Further increase in Mg concentration leads to a negative C' and alloy destabilization. Additionally, alloying of the Ti–Nb_{22}–Zr_6 alloy results in a decrease in hardness, fracture toughness, but brittleness index is increased.

KEYWORDS titanium alloys, elastic moduli, mechanical properties, ab-initio calculations

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1. Introduction

Ti–Nb based alloys are very promising materials for biomedical applications [1–7] because of their low Young's modulus (E) and biochemical compatibility with bone tissues. Our calculations of binary Ti–Me alloys (Me = V, Nb, Mo, Ta) demonstrated that near critical concentration of second component ($\beta \rightarrow \alpha$ transformation) all alloys have sharp decrease of E. However, prolonged contact of vanadium ions with biological tissues can provoke allergic reactions and have a negative effect on the nervous system [6]. Molybdenum, although is not considered cytotoxic, has an extremely detrimental effect on the rate of cell proliferation, mitochondrial activity and the volume of cells cultured on it [6]. So, the Ti–(Ta,Nb) based system can particularly suitable for orthopedic implants due to a reduced Young's modulus. Indeed, modern low-modulus alloys are mainly developed based on the Ti–Nb system with alloying elements such as Zr/Hf, Ta and Sn [5–7]. These elements, like Ti, are characterized by high biocompatibility and are β-stabilizing or neutral elements [6, 8]. Besides, the atomic radii of these elements exceed the size of the Ti atom that can also decrease the Young's modulus. At present, quantum mechanical methods allow one to calculate elastic moduli with sufficient accuracy and in a reasonable time in comparison with experiments and do not require significant expenditures. In order to estimate the elastic constants and moduli of disordered alloys several approaches are used. One of them is using the supercell approach, in which the larger the supercell, the lower the possible concentration of the alloying element [9, 10]. A significant drawback of this approach is the dependence of the total energy on the configuration of impurity atoms, although it is often neglected. Another approach is to use the so-called special quasirandom structures (SQS) [11]. In this case, supercells are generated to simulate a random distribution of atoms in terms of the correlation function, minimizing calculation errors relative to real random structures. Further, the exact muffin-tin orbital method with the coherent potential approximation (EMTO–CPA) [12] can be used also. This method is more suitable to structures with chemical disorder, since it eliminates the issue of configuration altogether, and calculations are performed for a unit cell containing a minimum number of atoms (one atom in the case of the β-phase). Nevertheless, studies using the EMTO–CPA method remain relatively rare. In any case, the problem to verification of obtained results is common one for all theoretical approaches. The latter is connected with a large scatter of experimental results, difference in the component concentration, the absence of information about phase compositions, etc. Recently the β-alloy with composition Ti–Nb_{22}–Zr_6 (at.%) was detailed studied in the paper [13]. Both experimental and theoretical values of Young's modulus are presented in this study.

The aim of this work is to study the electronic structure and mechanical characteristics of ternary β-Ti–Nb_{22}–Zr_6 alloy and to compare with available data as well as to investigate the influence of Hf and Mg on the lowering Young's modulus.

2. Method

Calculations of the electronic structure of disordered ternary and many component Ti–Nb_{22}–Zr_6 based alloys were performed using the exact MT-orbital method with the coherent potential approximation (EMTO–CPA) [12], which utilizes a random distribution of alloy atoms. The Green's function formalism and a $15\times15\times15$ k-point grid were used to calculate the total energies of alloys. The convergence criterion for the total energy was 10^{-7} Ry.

The finite displacement method was used to estimate the elastic constants. It is known that in the harmonic approximation, the change in total energy during deformation can be written as follows:

$$\Delta E\left(V,\{\varepsilon_i\}\right) = E\left(V,\{\varepsilon_i\}\right) - E\left(V_0,\ 0\right) = \frac{V_0}{2}\sum_{i,j=1}^{6} C_{ij}\varepsilon_i\varepsilon_j, \tag{1}$$

where $E(V,\ \varepsilon_i)$ and $E(V_0,\ 0)$ are the total energies of the deformed and equilibrium alloy cells with volumes V and V_0, respectively; ε_i is the strain; C_{ij} are the elastic constants. The total energies of the alloys, calculated for three different strains (isotropic, orthorhombic, and monoclinic), were used to estimate the bulk modulus (B) and the elastic constants C' and C_{44}, respectively. The other two elastic constants were calculated using the following formulas:

$$\begin{aligned} C_{11} &= B + 4C'/3, \\ C_{12} &= B - 2C'/3. \end{aligned} \tag{2}$$

Based on the elastic constants, the values of the shear and Young's moduli were calculated within the Voigt–Reuss–Hill approximation using standard formulas [14]:

$$\begin{aligned} G &= \frac{1}{2}\left[\frac{2C' + 3C_{44}}{5} + \frac{5C_{44}C'}{2C_{44} + 3C'}\right], \\ E &= \frac{9BG}{3B + G}. \end{aligned} \tag{3}$$

For the Vickers hardness (H_V) the following formula was used [15]:

$$H_V = \frac{E}{15.76}. \tag{4}$$

The choice of this expression is due to good agreement between the calculated value of 2.8 GPa for the Ti–Nb_{20} alloy and the experimental values of 2.7 [16] and 2.8 GPa [17] for the Ti–$Nb_{21.7}$ alloy.

The fracture toughness was calculated using the formula [18]:

$$K_{IC} = (1+\alpha)\sqrt{BGV_0^{1/3}}, \tag{5}$$

where V_0 is the volume per atom, and α is the enhancement factor due to peculiarities of metallic bond compared to covalent and ionic bonds.

Finally, the brittleness index M_{dt}, which reflects the machinability of the materials, can be defined as the ratio of the Vickers hardness to the fracture toughness [19]:

$$M_{dt} = \frac{H_V}{K_{IC}}. \tag{6}$$

3. Results and discussion

The calculated values of elastic constants and moduli for the binary alloys Ti–Nb_{20} and Ti–Nb_{25} are given in the Table 1. It is seen that the C' constant of the Ti–Nb_{20} alloy has small negative value that indicates mechanical instability of the β-phase. Indeed, the critical concentration for the $\beta \to \alpha$ transformation is equal to 22.5 at.% of Nb in accordance with experimental data [20]. Further, the calculation of C' for Ti–Nb_{25} demonstrates the positive value of 2.48 GPa that is in good agreement with estimation using C_{11} and C_{12} constants obtained in the paper [9]. In this paper [9] the elastic constants of β-Ti–Nb_{25} alloy were calculated using the PAW method with 16-atom supercell constructed by SQS technique. It is seen from Table 1 that EMTO–CPA method overestimates C_{44} constant in comparison with results in [9, 10]. In the paper [10], the elastic properties of Ti–Nb alloys were also obtained within the supercell approach, and the electronic structure of the alloys was calculated using the augmented plane wave plus local orbital (APW+lo) method implemented in the Wien2k software code [21]. In general, calculated C_{11} and C_{12} constants and elastic moduli are also in good agreement with results obtained in earlier papers [9, 10]. Our value of the Young's modulus is between the values calculated in [9, 10]. However, it is lower than experimental value of 73.9 GPa obtained for Ti–Nb_{25} alloy in [22] but closer to experimental value of 64 GPa [23] for the Ti–Nb_{26} alloy.

TABLE 1. Lattice parameter (in Å), elastic constants and moduli (in GPa) and Poisson's ratio of Ti–Nb_{22} based alloys

Alloy	a	C_{11}	C_{12}	C_{44}	C'	B	E	G	ν
Ti–Nb_{20}	3.338	125.0	128.1	59.3	−1.58	127.1	44.4	15.4	0.442
Ti–Nb_{25}	3.342	133.2	128.3	58.2	2.48	129.9	59.4	20.9	0.424
Ti–Nb_{25} [9]	—	140±11	116±13	34±10	—	124±13	63±13	22±13	—
Ti–Nb_{25} [10]	—	137.6	121.9	32.2	7.84	127.2	52.7	18.4	—
Ti–Nb_{22}–Zr_6	3.363	124.4	125.2	58.4	−0.40	125.0	48.7	17.0	0.435
Ti–Nb_{22}–Zr_6	3.304	157.7	150.4	65.7	3.6	152.9	70.1 70 [13]	24.6	0.424
Ti–Nb_{22}–Zr_6–Hf_5	3.329	147.9	146.6	65.4	0.6	147.1	58.7	20.5	0.433
Ti–Nb_{22}–Zr_6–$Mg_{2.5}$	3.307	152.8	147.4	66.6	2.7	149.2	67.5	23.7	0.425
Ti–Nb_{22}–Zr_6–Mg_5	3.311	150.1	146.0	67.2	2.0	147.4	65.4	22.9	0.426
Ti–Nb_{22}–Zr_6–$Hf_{2.5}$–$Mg_{2.5}$	3.320	138.9	136.2	66.3	1.3	137.1	62.0	21.7	0.425
Ti–Nb_{22}–Zr_6–Hf_5–$Mg_{2.5}$	3.333	144.5	144.3	65.9	0.1	144.4	57.0	19.9	0.434
Ti–Nb_{22}–Zr_3–Hf_5–Mg_5	3.325	142.8	143.0	66.7	-0.1	143.0	57.0	19.9	0.434

The theoretical lattice parameter obtained within PBE approximation for exchange-correlation functional is slightly higher than experimental value. In particular, the value of 3.304 Å given in the experimental paper [13] for the alloy Ti–Nb_{22}–Zr_6 is by 0.059 Å lower than that obtained by EMTO–CPA method (Table 1). The calculation of the ternary alloy with experimental lattice parameter leads to increase of both elastic constants and moduli. In particular, the theoretical value of 70.1 GPa the alloy Ti–Nb_{22}–Zr_6 is in good agreement with experimental one of 70 GPa [13].

Let us turn attention to experiments [13]. Two states of material were considered in this paper: 30 min heating at 600 °C to form the polygonized dislocation substructure (P state) with a subgrain size of ∼100 – 300 nm and 30 min heating at 750 °C to form the recrystallized structure (R state) with a grain size of ∼10 μm. To measure the Young's and shear moduli torsional pendulum experiment and mechanical test were performed. More details can be found in [13]. The value of $E = 110 \pm 10$ GPa obtained in the latter case is significant higher than that found by the torsional pendulum experiment. It should be noted that the obtained value mentioned above is a static "engineering" apparent elastic modulus which depends on the crystallographic texture and loading scheme and thus cannot be directly compared to its dynamical "physical" equivalent determined using a torsional pendulum or numerical simulations. The Poisson's ratio was also measured in [13] and the values of $\nu = 0.41 \pm 0.03$ (P state) and $\nu = 0.32 \pm 0.04$ (R state) were obtained. Our value (Table 1) is closer to one obtained in P state rather than in the R state.

The results of the atomistic simulations using molecular dynamic were also presented in the mentioned above paper [13]. Since the presence of lattice defects do not consider in the theoretical calculations, the comparison was made in the R state of the Ti–Nb_{22}–Zr_6 alloy. The atomistic simulation of Young's modulus allows one to obtain the value of 75±3 GPa within Voigt approach that is in good comparison with torsional pendulum experiment. However, it is higher by ∼55 GPa than that obtained within Reuss approach that leads to average value of ∼48 GPa at the low temperatures ∼50 °C. Besides, the values of elastic constants are significantly lower than those obtained in the present study. Thus, we can conclude that the present EMTO–CPA study with use of the Hill approach [14] allows obtaining Young's modulus for ternary Ti–Nb_{22}–Zr_6 alloy in good comparison with experiment. Therefore, we can consider the influence of some alloying elements on further lowering of E that is necessary for medical application of the Ti–Nb_{22}–Zr_6 based alloys.

In our previous paper [24], the influence of alloying elements on the Young's modulus was studied in the Ti–Mo_5–Me_x ternary alloys. We considered Zr, Hf, In, Sn, Mg, Mn, Ta as alloying elements with concentration changed from 1 to 5 at.%. Only Zr, Hf and Mg were shown as elements which can lower the elastic moduli. This lowering was interpreted as a combined effect of size and electron factors. Therefore, in present paper we consider only Hf, Mg and their combinations. It is seen from Table 1 that all alloying elements lead to increase in the lattice parameter. As a result, alloying by 5 at.% of Mg or Hf causes a decrease in E with the most pronounced effect of Hf. In the case of alloying by Hf, we observe the lowering of C' up to 0.6 GPa. It is interesting that for the Ti–Nb_{22}–Zr_6–Hf_5 alloy size effect is most pronounced and both C' and C_{44} constants are lower in comparison with the ternary alloy. In the case of Mg, elastic constant C' decreases but, on the contrary, C_{44} is increased. This trend is valid for the alloy with both Hf and Mg alloying

elements if their concentrations are 2.5 at.%. The growth of Hf concentration up to 5 at.% alongside with Mg alloying affects considerably C' constant, which lowers to 0.1 GPa. It should be noted that decrease in the concentration of Zr (Table 1) leads to instability of β-phase.

In the paper [25], it was demonstrated that some features of densities of states (DOS) can be connected with changes in C' and C_{44}. In particular, the first DOS peak near the Fermi level (E_F) reflects the changes in C', whereas the second peak shifted towards negative energy is connected with changes in C_{44}. Authors of [25] insist that hybridization of Nb with alloying elements and, as a consequence, increase of states in the second peak leads to stability of β-phase of the alloy. In turn, a decrease in the constant C' was associated by the authors [25] with a decrease in the states of *s*,*p*-metals at energies from -1.5 to 0.5 eV. Thus, the inverse relationship between the constants C_{44} and C' was explained by the opposite change in the peak heights upon alloying with *s*,*p*-elements. However, in the work [25], the change in the states under the DOS curves was estimated from the shape of the curves, and the division of the curves into two peaks was rather arbitrary. From Table 1 one can see that in the alloy with Mg the constant C' decreases, whereas C_{44} increases, but both constants are decreased in case of Hf as was mentioned above. Furthermore, a decrease in the number of states at the Fermi level indicates stabilization of the alloy and, consequently, an increase in C'.

Figure 1 shows the local DOS's of the Ti–Nb_{22}–Zr_6 alloys with alloying metals Hf and Mg. It is seen that the changes of the local DOS's at the Fermi level, $N(E_F)$, are insignificant in case of these elements. However, the addition of Hf in the alloy increases $N(E_F)$ more pronounced that *s*,*p*-element (lowest panel in Fig. 1). At the same time, the addition of fourth component means the decrease of Ti concentration. Since Ti contributes to a number of states at the Fermi level more than Hf or Mg, the alloying results in decrease of $N(E_F)$ shown in Fig. 2. This figure demonstrates difference of total DOS of doped and undoped ternary alloys. It is seen that decrease in $N(E_F)$ is significantly lower in the case of Hf. In general, states are decreased in the regions from -1.0 up to 0.5 eV and from -3.2 up to -1.7 eV, and they are increased in the region from -1.7 up to -1.0 and below -3.0 eV.

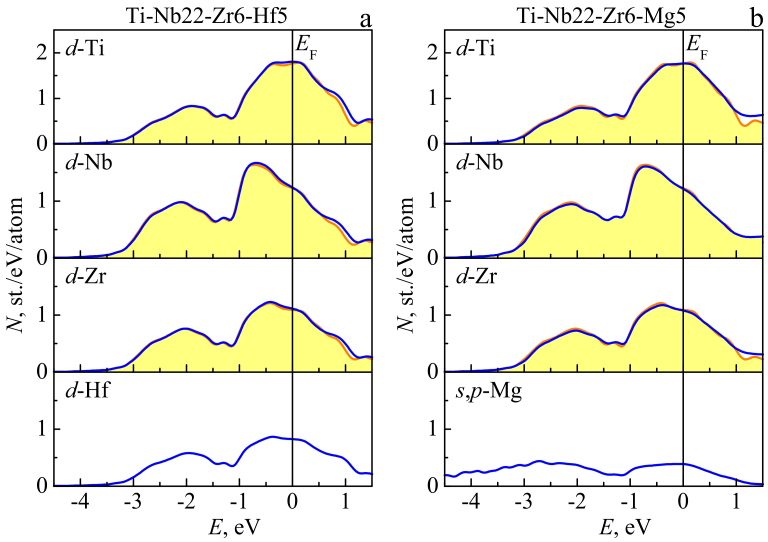

FIG. 1. Density of states of the Ti–Nb_{22}–Zr_6–Me_5 alloy components (blue line) in comparison with that of the Ti–Nb_{22}–Zr_6 alloy (orange line and yellow color fill): Me is Hf (a) and Mg (b)

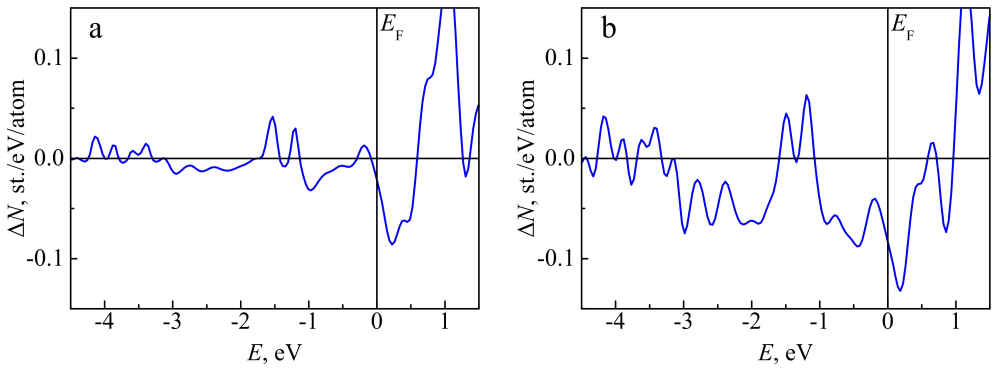

FIG. 2. Difference in the total DOS of the Ti–Nb_{22}–Zr_6–Me_5 alloy and Ti–Nb_{22}–Zr_6 one: Me is Hf (a) and Mg (b)

It should further be pointed out that in the case of Hf, the e/a concentration remains unchanged, whereas it decreases for the Mg doped alloy. It is seen from Table 1 that Hf, which is isoelectronic to Ti, causes a large decrease in E due to primarily its size effect. In the case of Mg doped alloys, the size effect is less pronounced in comparison with Hf but alongside with a decrease in the valence electron concentration, it contributes to a decrease in E as well.

The obtained results can be interpreted on the base of cluster-plus-glue-atom model, which was suggested in [26] for alloys with XY_3Ti_{11} composition, i.e. as approximately in our case. The basis of the structure is the cell (2×2×2) with the bcc Ti lattice. In the center of this cell, the Ti atom is replaced by an X element, and Y atoms are located in the middles of the cube edges with vacancies at the vertices. In our case, Y atoms are Nb ones, whereas X atom is Mg or Hf. A stronger bonding between X–Y atoms leads to a higher value of C_{44} in accordance with [25] and, as consequence, to stabilization of β-phase and to increase in E. However, the distance between X–Y atoms is great (Y is atom in the third coordination sphere in respect to X atom). So, their interaction can be indirect due to hybridization with Ti and Zr atoms. We have shown in [27, 28] that a weaker Y–Ti chemical bond leads to a lower value of E in the case of *s*,*p*-elements on X site, whereas in the case of *d*-elements on X site, a weak bonding X–Ti correlates also with a low value of E. Since Hf has larger atomic radius than Ti, its interatomic Hf–Ti bonds are weakening. In general, our simulations show that the smallest Young's modulus equaled to 57 GPa can be achieved for the Ti–Nb_{22}–Zr_6–Hf_5–$Mg_{2.5}$ alloy.

It should be noted that alloying of Ti–Nb_{22} alloy by 6 at.% Zr results in a decrease in hardness, fracture toughness but an increase in brittleness index (Table 2). Further addition of Hf and Mg in any combination enhances the changes in these mechanical characteristics. At the same time, the effect of Hf is more pronounced. The decrease in H_V is explained by the decrease in Young's modulus due to an increase in the metallic contribution in chemical bonding, while K_{IC} decreases due to a decrease in both factors in eq. (5). Since decrease in K_{IC} is larger than that in H_V, M_{dt} is increased. The highest value of M_{dt} obtained for the Ti–Nb_{22}–Zr_6–Hf_5–$Mg_{2.5}$ alloy, remains very low (0.279 $\mu m^{-1/2}$) that indicates high ductility of the alloys.

TABLE 2. Vickers hardness (H_V), fracture toughness (K_{IC}) and brittleness index (M_{dt}) for the Ti–Nb_{22} based alloys

Alloy	H_V, GPa	K_{IC}, MPa·$m^{1/2}$	M_{dt}, $\mu m^{-1/2}$
Ti–Nb_{22}	4.50	21.56	0.209
Ti–Nb_{22}–Zr_6	4.45	18.05	0.246
Ti–Nb_{22}–Zr_6–Hf_5	3.73	14.71	0.253
Ti–Nb_{22}–Zr_6–$Mg_{2.5}$	4.28	16.92	0.253
Ti–Nb_{22}–Zr_6–Mg_5	4.15	16.19	0.256
Ti–Nb_{22}–Zr_6–$Hf_{2.5}$–$Mg_{2.5}$	3.93	14.71	0.267
Ti–Nb_{22}–Zr_6–Hf_5–$Mg_{2.5}$	3.62	12.96	0.279
Ti–Nb_{22}–Zr_3–Hf_5–Mg_5	3.62	14.96	0.242

4. Conclusion

The elastic and mechanical properties of disordered titanium alloys Ti–Nb_{22}–Zr_6–Me alloyed with Hf, Mg and their combination were studied using the EMTO–CPA method. We demonstrate that the addition of Hf, which is isoelectronic to Ti, reduces Young's modulus by increasing the lattice parameter and weakening the chemical bonds. In the case of Mg, both structural and electronic factors also contribute to a reduction in Young's modulus. The smallest value of Young's modulus equaled to 57 GPa was calculated for the Ti–Nb_{22}–Zr_6–Hf_5–$Mg_{2.5}$ alloy. The decrease of Zr concentration and increase of Mg one leads to instability of β-phase of the alloy. The mechanical properties of the alloys, such as Vickers hardness, fracture toughness and brittleness index, were also calculated using the elastic moduli. It was shown that the hardness of the alloys decreases with the alloying by Hf and Mg, and effect of the former is more pronounced. Although the brittleness index increases for all alloying elements, its highest value, obtained for Ti–Nb_{22}–Zr_6–Hf_5–$Mg_{2.5}$, is only 0.28 $\mu m^{-1/2}$ indicating high ductility of the alloys.

References

[1] Niinomi M. Mechanical properties of biomedical titanium alloys. *Mater. Sci. Eng. A*, 1998, **243**, P. 231-236.
[2] Long M., Rack H.J. Titanium alloys in total joint replacement – a materials science perspective. *Biomater.*, 1998, **19**, P. 1621–1639.
[3] Geetha M., Singh A.K., Asokamani R., Gogia A.K. Ti based biomaterials, the ultimate choice for orthopaedic implants – A review. *Prog. Mater. Sci.*, 2009, **54**, P. 397–425.
[4] Niinomi M. Mechanical biocompatibilities of titanium alloys for biomedical applications. *J. Mech. Behav. Biomed. Mater.*, 2008, **1**, P. 30–42.

[5] Yu Z. *Titanium alloys for biomedical development and applications. Design, microstructure, properties, and application*. Elsevier, Amsterdam, 2022, 245 p.
[6] Biesiekierski A., Wang J., Gepreel M.A.H., Wen C. A new look at biomedical Ti-based shape memory alloys, *Acta Biomater*., 2012, **8**, P. 1661–1669.
[7] Illarionov A.G., Nezhdanov A.G., Stepanov S.I., Muller-Kamskii G., Popov A.A. Structure, phase composition, and mechanical properties of biocompatible titanium alloys of different types. *Phys. Met. Metall.*, 2020, **121**, P. 367–373.
[8] Li Y., Yang C., Zhao H., Qu S., Li X., Li Y. New developments of Ti-based alloys for biomedical applications. *Materials*, 2014, **7**, P. 1709–1800.
[9] Marker C., Shang S.L., Zhao J.C., Liu Z.K. Effects of alloying elements on the elastic properties of bcc Ti-X alloys from first-principles calculations. *Comput. Mater. Sci.*, 2018, **142**, P. 215–226.
[10] Yao Q., Sun J., Xing H., Guo W. Influence of Nb and Mo contents on phase stability and elastic property of β-type Ti-X alloys. *Trans. Nonferrous Met. Soc. China.*, 2007, **17**, P. 1417–1421.
[11] Zunger A., Wei S.H., Ferreira L.G., Bernard J.E. Special quasirandom structures. *Phys. Rev. Lett.*, 1990, **65**, P. 353–356.
[12] Vitos L. *Computational quantum mechanics for materials engineers. The EMTO method and applications*. Springer, London, 2007, 238 p.
[13] Dubinskiy S., Baranova A., Markova G., Prokoshkin S., Zelenina A., Kolotova L., Starikov S., Korotitskiy A., Bazlov A., Brailovski V. Atypical intrinsic elinvar behavior of beta Ti-22Nb-6Zr alloy in high and wide temperature range: atomic mechanism and control of the effect. *Trans. Nonferrous Met. Soc. China*, 2026, in press.
[14] Hill R. The elastic behaviour of a crystalline aggregate. *Proc. Phys. Soc., Sect. A*, 1952, **65**, P. 349–354.
[15] Jiang X., Zhao J., Wu A., Bai Y., Jiang X. Mechanical and electronic properties of B_{12}-based ternary crystals of orthorhombic phase. *J. Phys.: Condens. Matter.*, 2010, **22**, 315503.
[16] Lee C.M., Ju C.P., Chern Linn J.H. Structure-property relationship of cast Ti–Nb alloys. *J. Oral Rehabil.*, 2002, **29**, P. 314–322.
[17] Fikeni L. *Microstructural evolution and its influence on mechanical properties of Ti–Nb binary alloys*. University of Pretoria, Pretoria, 2021, 95 p.
[18] Niu H., Niu S., Oganov A.R. Simple and accurate model of fracture toughness of solids. *J. Appl. Phys.*, 2019, **125**, 065105.
[19] Boccaccini A.R. Machinability and brittleness of glass-ceramics. *J. Mater. Process. Technol.*, 1997, **65**, P. 302–304.
[20] Lütjering G., Williams J.C. *Titanium*, second ed. Springer, Berlin, 2007, 442 p.
[21] Schwarz K., Blaha P., Madsen G.K.H. Electronic structure calculations of solids using the WIEN2k package for material sciences, *Comput. Phys. Commun.*, 2002, **147** (1–2), P. 71–76.
[22] Raabe D., Sander B., Friák M., Ma D., Neugebauer J. Theory-guided bottom-up design of β-titanium alloys as biomaterials based on first principles calculations: Theory and experiments. *Acta Materialia*, 2007, **55**, P. 4475–4487.
[23] Boyer R.R., Welsch G., Collings E.W. *Materials properties handbook: titanium alloys*. ASM Int., Mater. Park, 1994, 1176 p.
[24] Kasparyan S.O., Bakulin A.V., Kulkova S.E. The influence of alloying elements on the elastic properties of β-Ti. *J. Exp. Theor. Phys.*, 2026, **169**, P. 71–81. (in Russian)
[25] Kwasniak P., Wróbel J.S., Garbacz H. Origin of low Young modulus of multicomponent, biomedical Ti alloys – Seeking optimal elastic properties through a first principles investigation. *J. Mech. Behav. Biomed. Mater.*, 2018, **88**, P. 352–361.
[26] Hao C.P., Wang Q., Ma R.T., Wang Y.M., Qiang J.B., Dong C. Cluster-plus-glue-atom model in bcc solid solution alloys. *Acta Phys. Sin.*, 2011, **60** (11), 116101.
[27] Kasparyan S.O., Ordabaev A.E., Bakulin A.V., Kulkova S.E. Elastic and thermal properties of some ternary β-Ti based alloys. *Nanosystems Phys. Chem. Math.*, 2025, **16** (2), P. 225–234.
[28] Kasparyan S.O. *Electronic structure and elastic moduli of binary and ternary β-titanium alloys. Cand. Sci. (Phys.-Math.) Dissertation*. Nat. Res. Tomsk State Univ., Tomsk, 2025, 154 p. (in Russian).

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