FULL FACTORIAL DESIGN FOR Ti-Mo-W BETA ALLOYS TO CORRELATE THE MODULUS OF ELASTICITY WITH THE MATERIAL PARAMETERS Md, Bo AND e/a

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Obtaining a metallic material based on titanium with the modulus of elasticity close to that of bone, was the main goal of the work. The design of the material was led in this direction, the choice of tungsten as an alloying element was conducted meeting the conditions for obtaining the values of the Md, Bo and e/a parameters that would ensure obtaining a reduced modulus of elasticity. The mathematical model was created to reflect the connection between the modulus of elasticity and these material constants, necessary for the design of a metallic material with imposed properties. To find a function to set up a correlation between the parameters Md, Bo, e/a with the modulus of elasticity of titanium-based alloys, an active experimental program, a second-order orthogonal program (PO2), was used. The obtained theoretical data about the modulus of elasticity are in particularly good agreement with the experimental data.

Keywords: titanium β alloys; modulus of elasticity; Md, Bo and e/a; full factorial design

1. Introduction

Titanium alloys are widely used in many applications such as aircraft, spacecraft, automotive and in manufacturing of orthopedic and dental implants, bicycles, consumer electronics and premium sports equipment due to their special properties such as: high tensile strength and toughness even at extreme temperatures, low density, extraordinary corrosion resistance and a low thermal expansion coefficient [1, 2].

The classification of titanium alloys is conducted in four main categories: alpha alloys (not treatable); near-alpha alloys (hold small amount of ductile beta-phase); alpha and beta alloys (metastable and can be heat treated); beta and near beta alloys (metastable and hold sufficient beta stabilizers) [2, 3].

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According to the equilibrium diagram, the formation of beta alloys requires the introduction of sufficient amounts of beta-stabilizers such as molybdenum, vanadium, niobium, tantalum, zirconium, manganese, iron, chromium, cobalt, nickel, and copper [4]. The beta alloys are readily heat treatable, with increased hardenability compared with alpha or alpha-beta alloys. The strength at room temperature of this alloys is high (but low at increased temperatures) and is expected to own an excellent formability in the solution-treated condition [5].

Their increased hardenability is also highly desirable for hardening of thick sections. Problems may arise due to beta stabilizers in the alloying process, such as the occurrence of segregation that requires successive melts as well as increasing the density of the developed alloy [6].

Recently, these alloys have attracted the attention of the medical industry to produce diverse types of orthopedic implants because they can achieve a low elastic modulus in conjunction with superior resistance to corrosion and excellent biocompatibility [7, 8, 9, 10].

The design of a metallic material with imposed properties (low modulus of elasticity), from the Ti-Mo-W system, was carried out based on the values of the material parameters, *Md – the energy level of the d orbital, eV, Bo – the bond order* and *e/a – electron density - the number of valence electrons per atom*. Some conclusions from the specialized literature were considered, which state that titanium alloys with a low modulus of elasticity can be obtained if some conditions regarding the values of the parameters mentioned above are met: 4.20-4.24 for *e/a*, 2.80-2.83 for *Bo* and 2.39-2.45 for *Md* [10, 11, 12, 13, 14, 15].

2. Materials and methods

After the elemental and chemical composition was decided by design, a series of alloys were developed starting from the Ti15Mo binary alloy, namely Ti15Mi5W, Ti15Mo7W, Ti15Mo9W and Ti15Mo11W. The process of melting in a vacuum arc furnace was chosen for the elaboration, mainly because the shape of the crucible plate allowed obtaining all 15 compositions of the Ti-Mo-W alloy system through a single melting followed by a remelting [16]. The furnace model ABD MRF 900 (RAV) was used, which reaches a maximum temperature of 3700^{o}C [16]. To find the modulus of elasticity, the universal mechanical testing machine EDZ 40 was used with the following characteristics:

- Capacity: 400kN/40985 KgF.
- Return speed: 0.001 to 600mm/min adjustable in steps of 0.001mm/min.
- The length of the clamping head: 1300mm, neck 600mm.

To find a function that proves a correlation between the *Md*, *Bo* and *e/a* parameters and the modulus of elasticity of titanium alloys, a second-order orthogonal program (PO2) was adopted [16, 17, 18] to calculate the best working conditions in development of Ti-Mo-W alloys. Based on the obtained experimental data and the imposed first conditions, the mathematical model of the dependence of the modulus of elasticity *E* with the material parameters *Md, Bo, e/a*, *E = f (Md, Bo, e/a)* was developed.

Such a program is obtained by supplementing a first-order program type *EFC 2n* (EFC = complete factorial experiment) with certain points of the factorial space [19]. The second-order orthogonal program (OP2) applied in this paper was obtained by adding some specific points of the factorial space to a simpler program order one type *CFE* 2^n (complete factorial experiment) [19]:

- Using the results obtained experimentally we have selected a point in the factorial space having the coordinates:

$$z_1^0 = 2.3975;\ z_2^0 = 2.8204;\ z_3^0 = 4.2133$$

As well as the following variation ranges:

$$\Delta z_1 = 0.003;\ \Delta z_2 = 0.0025;\ \Delta z_3 = 0.0155$$

- Then we have determined the value of the factors in the 8 points of the CFE 2^3 program which is a component of the OP2 program. Therefore, we have used the following relationships:

$$z_i^{(-1)} = z_i^0 - \Delta z_i\ ;\ z_i^{(+1)} = z_i^0 + \Delta z_i$$

- The coordinates of the 6 „star-points" ($z_i^{-\alpha}$, $z_i^{+\alpha}$) have been set up with the parameter α (the *star point*) whose value was found from the biquadrate equations:

$$\alpha^4 + 2^n \cdot \alpha^2 - 2^{n-1} \cdot (n + 0.5 \cdot N_0) = 0 \text{ and } \alpha^4 + 8 \cdot \alpha^2 - 22 = 0$$

- The mathematical model works with a different type of variables than the experimental ones, so the next step in developing the program was to change the variables. The *natural* variables z_1, z_2, z_3 were replaced by the *encoded* variables x_1, x_2, x_3, using to this purpose the following relationships:

$$x_i^{(-1)} = \frac{z_i^{(-1)} - z_i^0}{\Delta z_i} = -1, \qquad x_i^{(+1)} = \frac{z_i^{(+1)} - z_i^0}{\Delta z_i} = +1,$$

$$x_i^{(-\alpha)} = \frac{z_i^{(-\alpha)} - z_i^0}{\Delta z_i} = -\alpha, \qquad x_i^{(+\alpha)} = \frac{z_i^{(+\alpha)} - z_i^0}{\Delta z_i} = +\alpha .$$

3. Experimental results and discussion

Based on the experimental data presented in Table 1 and the imposed first conditions, the mathematical model of the dependence *E = f (Md, Bo, e/a)* of the *Modulus of elasticity - Md, Bo, e/a*, was developed.

Table 1

Experimental results and program matrix for *E = f (Md, Bo, e/a)*

No.	Parameters (coded units)			Parameters (uncoded units)			E, GPa (experimental)	E, GPa (calculated)
	Md x_1	***Bo*** x_2	***e/a*** x_3	***Md***	***Bo***	***e/a***		
1	-1	-1	-1	2.3945	2.8179	4.1978	43.14	42.205
2	+1	-1	-1	2.4005	2.8179	4.1978	42.78	40.442
3	-1	+1	-1	2.3945	2.8229	4.1978	43.05	40.373
4	+1	+1	-1	2.4005	2.8229	4.1978	45.35	44.261
5	-1	-1	+1	2.3945	2.8179	4.2288	23.27	28.898
6	+1	-1	+1	2.4005	2.8179	4.2288	19.55	26.466
7	-1	+1	+1	2.3945	2.8229	4.2288	17.86	24.438
8	+1	+1	+1	2.4005	2.8229	4.2288	22.48	27.655
9	0	0	0	2.3975	2.8204	4.2133	25.78	31.511
10	0	0	0	2.3975	2.8204	4.2133	31.11	31.511
11	0	0	0	2.3975	2.8204	4.2133	30.51	31.511
12	0	0	0	2.3975	2.8204	4.2133	30.29	31.511
13	0	0	0	2.3975	2.8204	4.2133	33.32	31.511
14	-1.471	0	0	2.3931	2.8204	4.2133	32.19	28.398
15	+1.471	0	0	2.4019	2.8204	4.2133	33.51	29.468
16	0	-1.471	0	2.3975	2.8167	4.2133	36.36	32.108
17	0	+1.471	0	2.3975	2.8241	4.2133	35.22	31.636
18	0	0	-1.471	2.3975	2.8204	4.1905	44.23	48.856
19	0	0	+1.471	2.3975	2.8204	4.2361	43.32	42.854

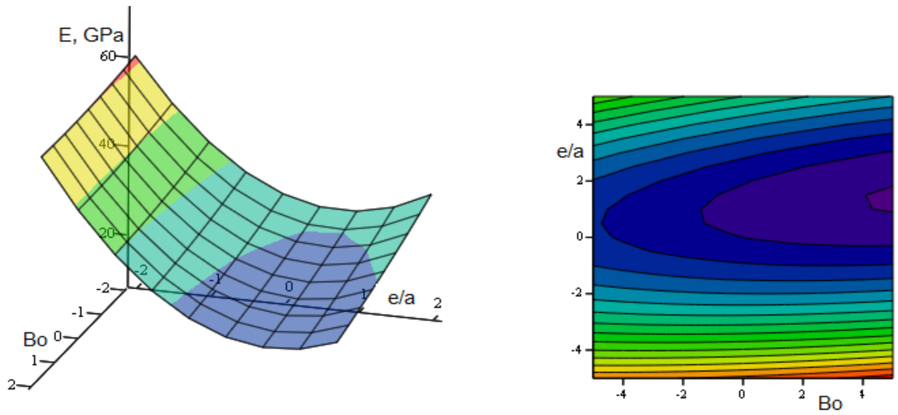

Fig. 1. Modulus of elasticity, *E* as a function to *e/a* and *Bo* (coded units) at *Md* of 2.3945 (-1, coded units)

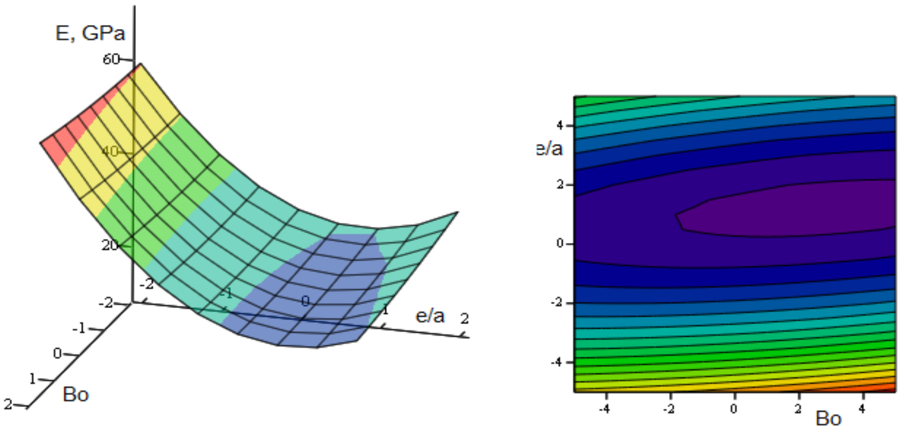

Fig. 2. Modulus of elasticity, *E* as a function to *e/a* and *Bo* (coded units) at *Md* of 2.3975 (0, coded units)

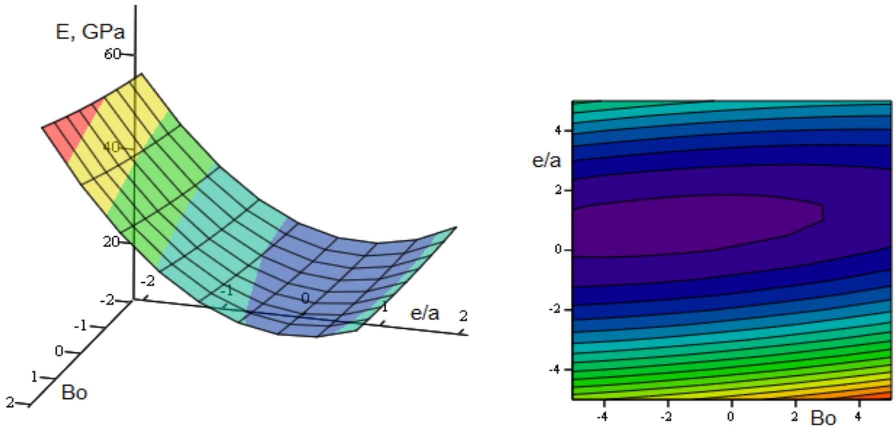

Fig. 3. Modulus of elasticity, *E* as a function to *e/a* and *Bo* (coded units) at *Md* of 2400 (1, coded units)

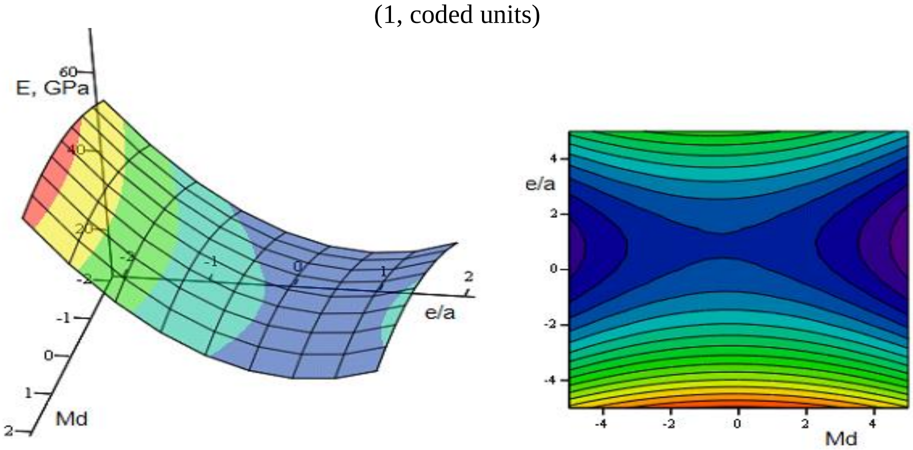

Fig. 4. Modulus of elasticity, *E* as a function to *e/a* and *Md* (coded units) at *Bo* of 2.8179 (-1, coded units)

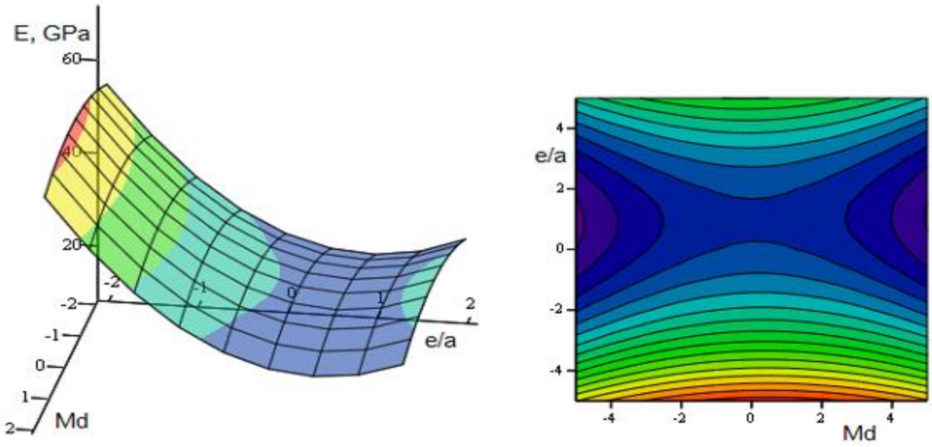

Fig. 5. Modulus of elasticity, *E* as a function to *e/a* and *Md* (coded units) at *Bo* of 2.8204 (0, coded units)

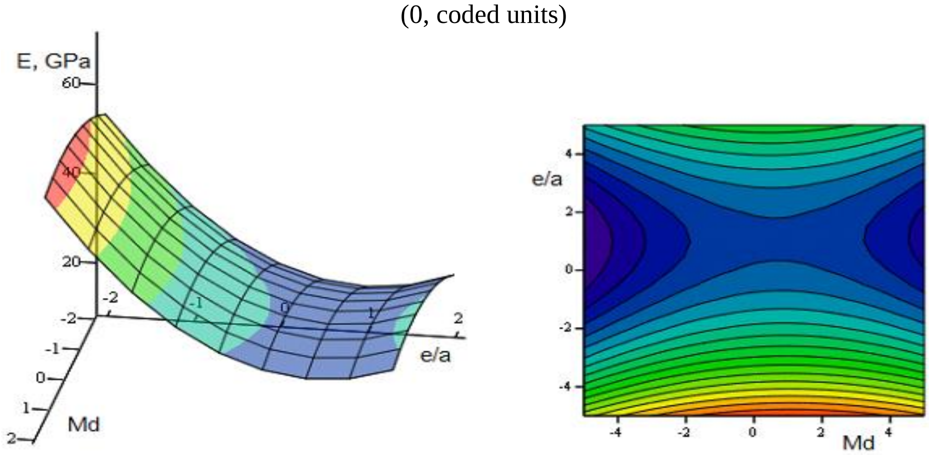

Fig. 6. Modulus of elasticity, *E* as a function to *e/a* and *Md* (coded units) at *Bo* of 2.8229 (1, coded units)

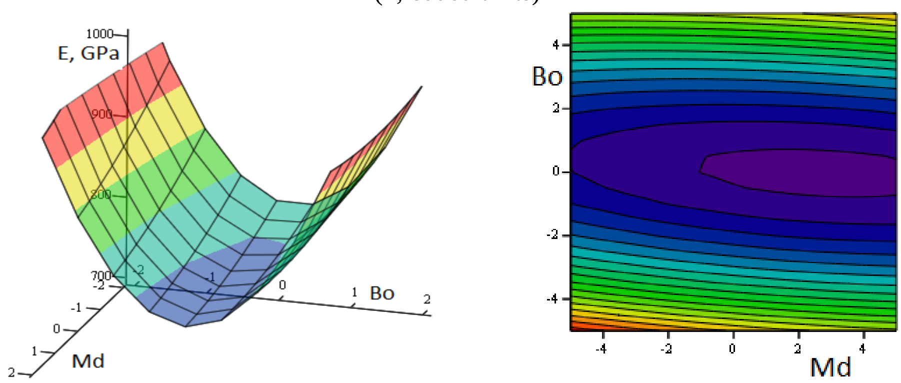

Fig. 7. Modulus of elasticity, *E* as a function to *Bo* and *Md* (coded units) at *e/a* of 4.1978 (-1, coded units)

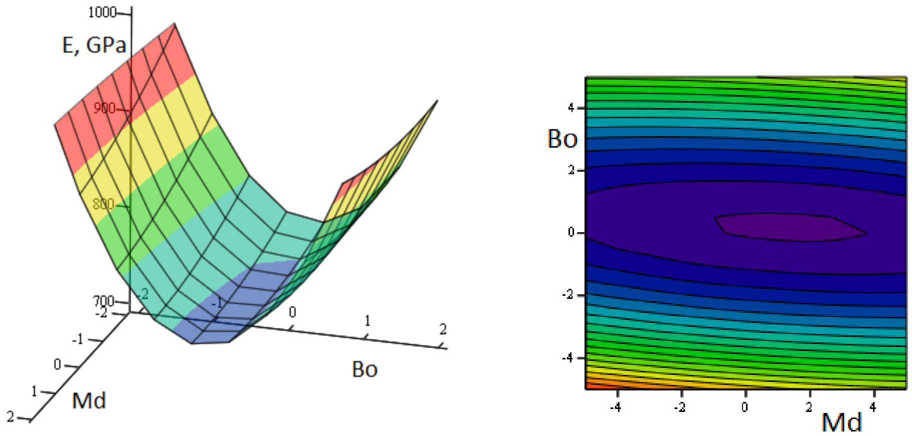

Fig. 8. Modulus of elasticity, *E* as a function to *Bo* and *Md* (coded units) at *e/a* of 4.2133 (0, coded units)

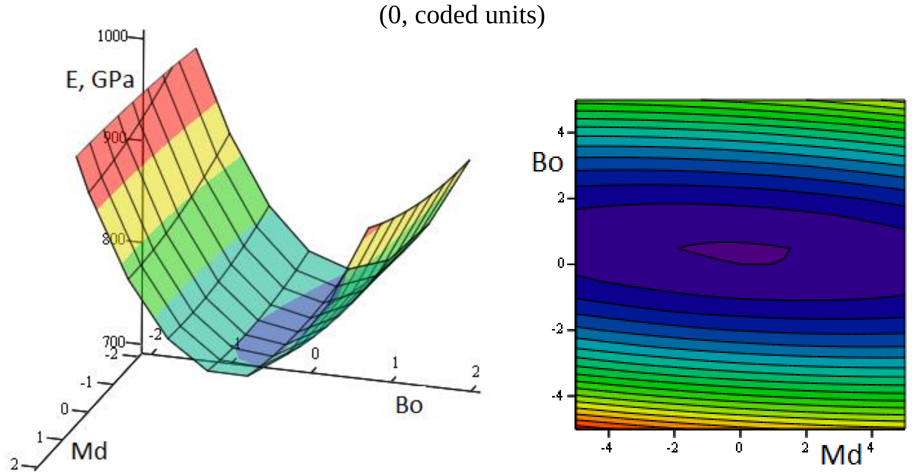

Fig. 9. Modulus of elasticity, *E* as a function to *Bo* and *Md* (coded units) at *e/a* of 4.2288 (1, coded units)

In the case of variation of *Bo* (bond order) and *e/a* (electron density per atom) parameters, at constant *Md* (energy level of the d orbital), Figures 1 to 3, the surface shows a minimum that moves from higher values as 1 to 0 (encoded units), when *Md* moves -1 to 1, the influence of *Bo* being very small.

In the case of the variation of parameters *Md* and *e/a* at constant *Bo* (Figures 4 to 6), the surface shows approximately the same shape, i.e. there is a minimum for the modulus of elasticity around the 0 value of *e/a* and a small maximum at values around of 1 and over 1 of *Md*. Shifting *Bo* between -1 and 1 does not significantly influence the shift of these extremes.

The same does not happen when the variable parameters are *Md* and *Bo* (Figures 7 to 9). The surface shows a minimum for *Bo* around its 0 value, with a fairly strong influence, and at a value of *Md* moving from 0 to 2 as e/a decreases from 1 to -1, but with an influence smaller than it.

These observations are also visible in Figures 10 to 12 where the variations of the modulus of elasticity according to a single parameter when the other two are kept constant are presented. It should be noted in these figures the agreement of the experimental data with the theoretical data, the deviations, as mentioned before, falling within the margin of error of the mathematical model.

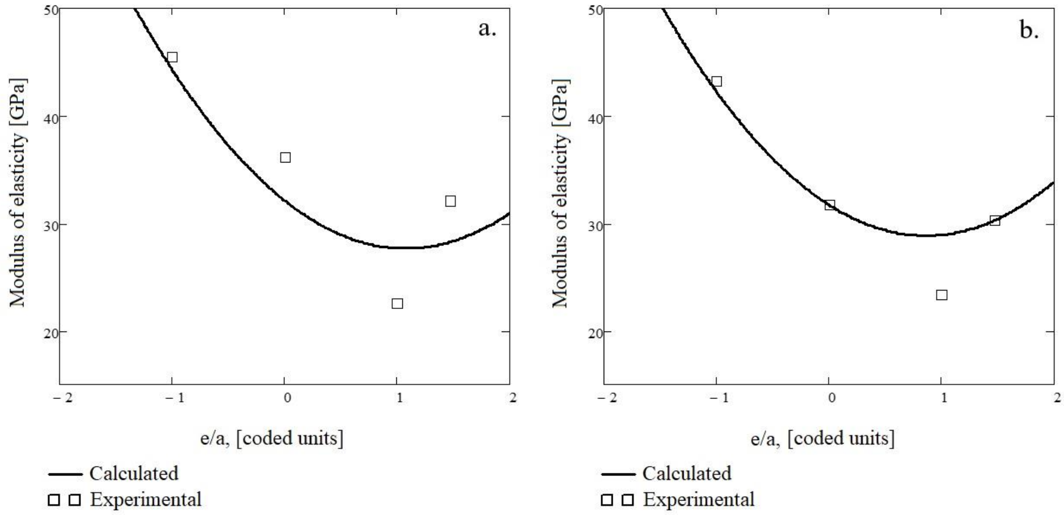

Fig. 10. *E* Vs *e/a* for constant values of *Bo* and *Md*: a) -1,-1 and b) 1, 1)

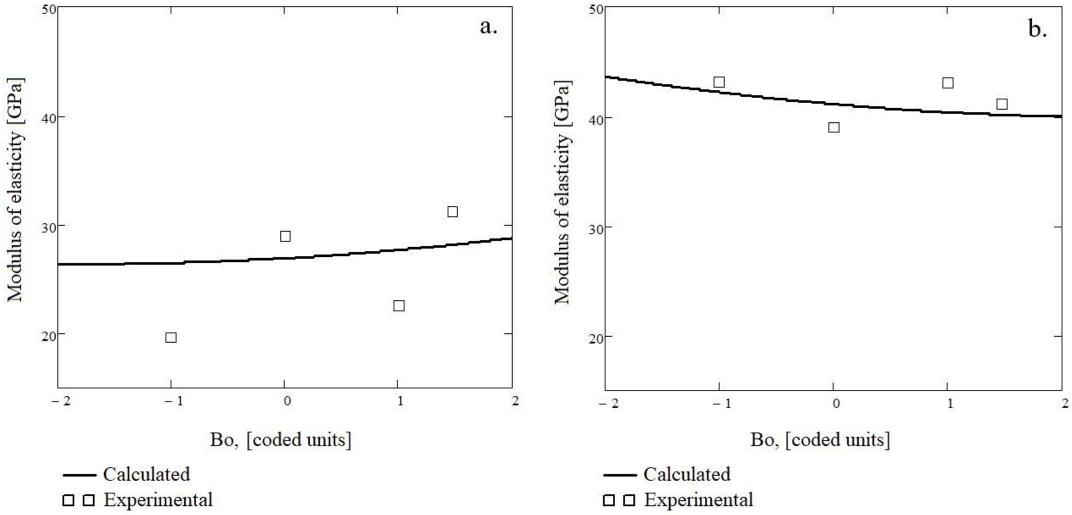

Fig 11. *E* Vs *Bo* for constant values of *Md* and *e/a*: a) -1,-1 and b) 1, 1)

Based on the data provided, we can conclude that to obtain an alloy from the Ti-Mo-W system, with the smallest modulus of elasticity, a composition of the elements can be chosen, considering the values of the three material parameters, *Md = 2.39-2.40, Bo = 2.82-2.83, and e/a = 4.22-4.23*, values that also correspond to the theoretical ones, determined by mathematical modeling.

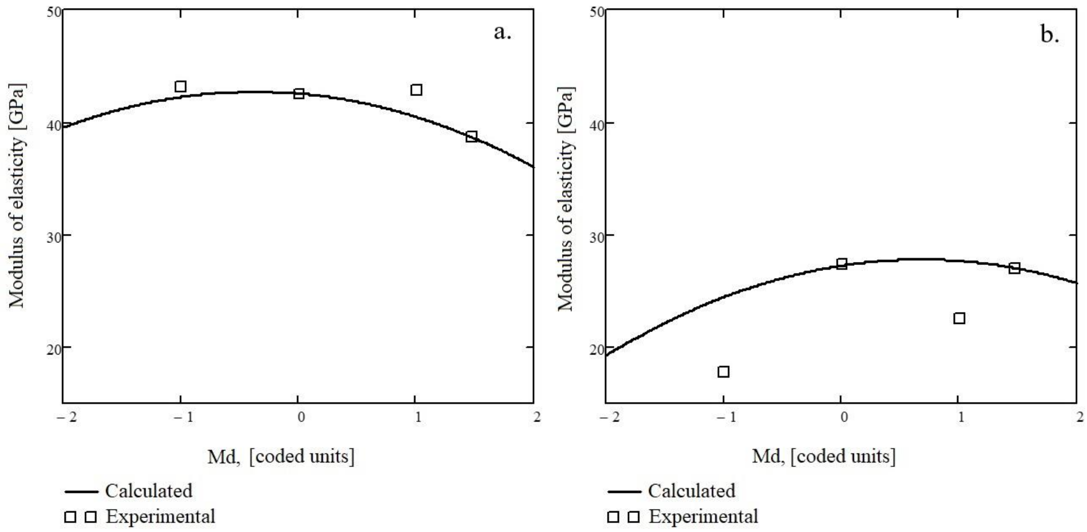

Fig. 12. *E* Vs *Md* for constant values of *Bo* and *e/a*: a) -1, -1 and b) 1, 1)

4. Conclusions

Of all the wide range of titanium-based alloys, the β-stable alloys have the most favorable properties, especially those that have in their composition alloying elements capable of ensuring a high density of electrons per atom. Such alloys may be capable of supplying a low modulus of elasticity.

With this model, was obtained theoretical data on the modulus of elasticity of Ti-Mo-W alloys which are in particularly good concordance with the experimental data. In addition, a comparison was made between the theoretical data obtained with these equations and the experimental data. There is a good concordance of the experimental data with the calculated data, the deviations falling within the calculated error - $\delta = 3,963$. The nonlinearity all 3D charts proves that there are interactions between each independent variable and the modulus of elasticity. Therefore, it can also be concluded that all contour surfaces of the three parameters considered, *Md, Bo, e/a* under various conditions were nonlinear.

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