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MATHEMATICAL MODELING FOR CORRELATION OF THE RESISTANCE TO COMPRESSION WITH THE PARAMETERS Md, Bo AND e/a, FOR THE DESIGN OF TITANIUM β ALLOYS DEVELOPED FOR MEDICAL APPLICATIONS

Mihai BUZATU[1], Victor GEANTĂ[2], Radu ŞTEFĂNOIU[3], Mihai BUŢU[4], Mircea-Ionuţ PETRESCU[5], Mihai BUZATU[6], Ştefan-Ioan GHICA[7], Iulian ANTONIAC[8], Gheorghe IACOB[9], Florentina NICULESCU[10], Dragoş-Florin MARCU[11], Horaţiu MOLDOVAN [12 *]

In the scientific literature no attempts have been made to establish a correlation between the values of these important material parameters and the mechanical properties of the steady-state titanium β alloys. To determine a mathematical function that establishes a correlation between the parameters Md, Bo, e/a and the resistance to compression of titanium alloys, an active experimental program, a second-order orthogonal program (OP2) was used. Such a program is obtained by supplementing a program of the first type FFC type 2n (FFC = full factorial experiment) with certain points of the factorial space. On the basis of the experimental data and the initial conditions imposed, the mathematical model of the dependence Rc = f(Md, Bo, e/a) has been achieved.

Keywords: medical applications; titanium β alloys; mechanical properties; Md, Bo and e/a; mathematical modeling

1. Introduction

Metallic materials for medical applications represent an important part of materials engineering. All research channeled in this direction is aimed at increasing the life span of implants of this nature. Of the metallic materials for this purpose, titanium and its alloys account for over 40%. A documentation based on an extensive bibliographic study led to the choice of tungsten as an alloying element to obtain a more complex alloy starting from the well-known Ti15Mo binary alloy with outstanding properties [1-12].

In choosing a material for medical applications, a number of criteria (biocompatibility, osseointegration, mechanical properties, corrosion resistance, wear resistance, fatigue resistance) must be taken into account. Osseointegration

[1] Medical Center MedLife Victoriei, Bucharest, Romania, e-mail: buzatu.mihai@yahoo.com
[2, 3, 4, 5, 6, 7, 8, 9, 10, 11] Faculty of Materials Science and Engineering, University POLITEHNICA of Bucharest, Romania
[12 *] Corresponding author, Faculty of Medicine, *Titu Maiorescu* University, Bucharest, Romania, e-mail: h_moldovan@hotmail.com

has enhanced the science of medical bone and joint replacement techniques as well as dental implants and improving prosthetics for amputees. Titanium are often used for medical implants manufacturing, as this metal exhibit high tensile strength and corrosion resistance with excellent biocompatibility [13-24].

Of the wide range of titanium-based alloys the β-stable alloys have the most favorable properties, especially those that have alloying elements capable of providing a high electron density on the atom. Such alloys may be able to provide a low modulus of elasticity. A current trend in the acquisition of new materials with medical applications emphasizes the need for designing and selecting a metallic material for the purpose of serving safely for a long time, without rejection, as a metallic implant [4, 5, 8, 9, 26].

The new researches feature titanium alloys with outstanding properties such as super-elasticity, cold super-plasticity, etc.; Nb, Ta and other metals such as Zr, Mo, Cr, Mn, Sn, Fe, Sn and Al are present in the composition of these alloys. It has been shown, that the mechanical stability of β-phase was connected to several electronic parameters, including Bo and Md [25]. Bo, the bond order, measures the average covalent bond strength between Ti and an alloying element. Md is the average d-orbital energy level calculated on a body-centered cubic, and e/a the ratio between valence electron and atom [26]

In a paper of Saito et al. [27] is presented the obtaining of titanium biomaterials with low modulus of elasticity, and this property of "metallic gum" is related to the values of some material parameters, Md, Bo and e/a. This property of "metallic gum" is achieved at values around Bo = 2.87, Md = 2.45 and e/a = 4.24. The study was made on Ti12Ta9Nb6Zr1.5O and Ti23Nb0.7Ta2Zr1.2O, molar alloys. These alloys are superplastic and have a very low elastic modulus.

In the literature, no attempts have been made to establish a mathematical correlation between the values of these important material parameters and the mechanical properties of the stable structure alloy titanium alloys.

2. Materials and methods

To determine a function that establishes a correlation between the Md, Bo and e/a parameters and the resistance to compression of titanium alloys, an active experimental program was adopted [26, 28, 29] in order to calculate the optimum working conditions in the process of Ti-15Mo-W alloys development.

The second-order orthogonal program (PO2) 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):

- 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 established by means of the parameter α (the *star point*) whose value was determined 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

The results of the application of the model to the process are presented in Figs. 1-12 and Table 1. Based on the experimental data presented in Table 1 and the initial imposed conditions, the mathematical model *Rc = f (Md, Bo, e/a)* of the *Resistance to compression - Md, Bo, e/a,* was developed. According to the data obtained, 3D charts have been built showing the dependency of the resistance to compression response surfaces according to the three parameters considered, Md, Bo, e / a under various conditions.

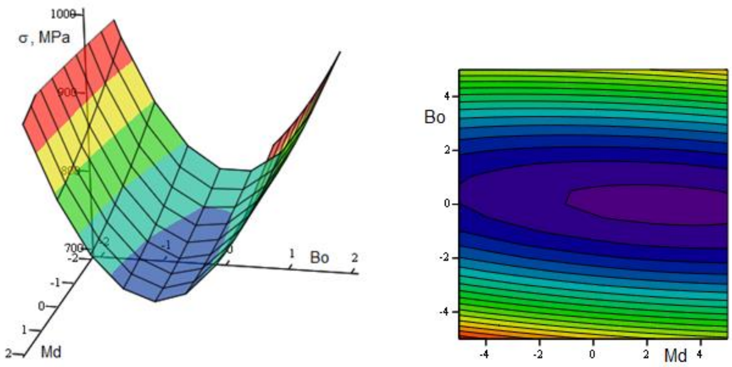

Fig. 1. Resistance to compression according to Md and Bo (coded units) at e / a of 4.1978 (-1, coded units)

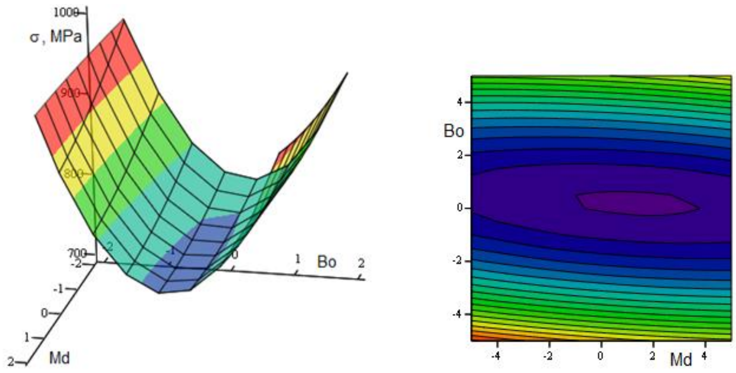

Fig. 2. Resistance to compression according to Md and Bo (coded units) at e / a of 4.2133 (0, coded units)

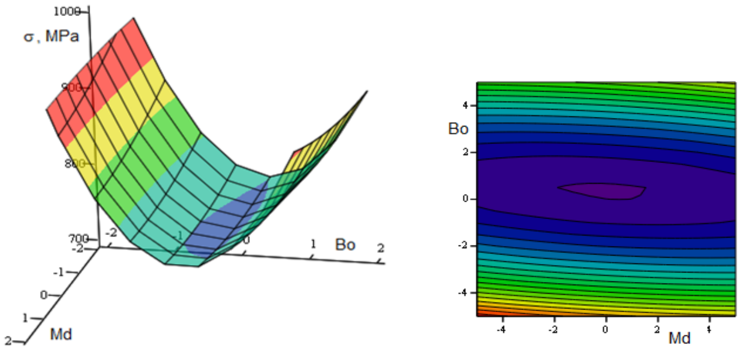

Fig. 3. Resistance to compression according to Md and Bo (coded units) at e / a of 4.2288 (+1, coded units)

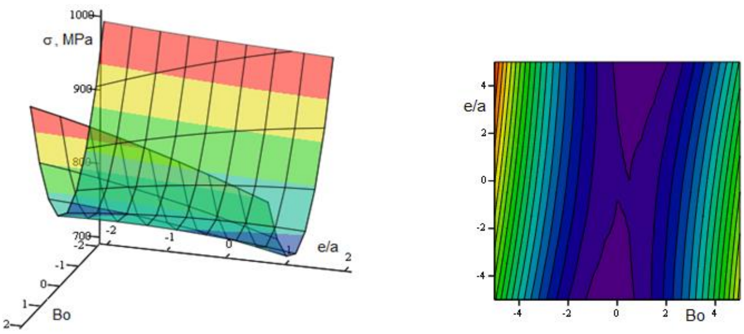

Fig. 4. Resistance to compression according to Bo and e/a (coded units) at Md of 2.3945 (-1, coded units)

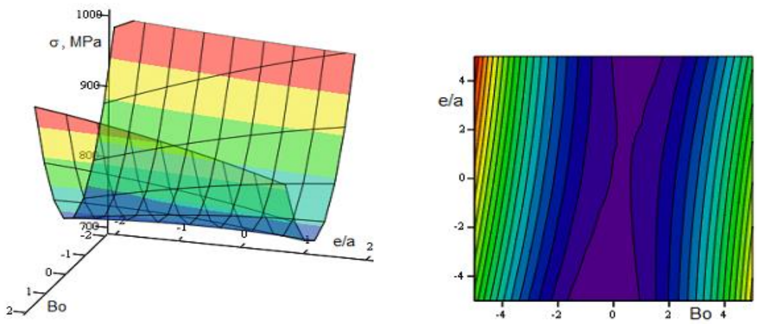

Fig. 5. Resistance to compression according to Bo and e/a (coded units) at Md of 2.3975 (0, coded units)

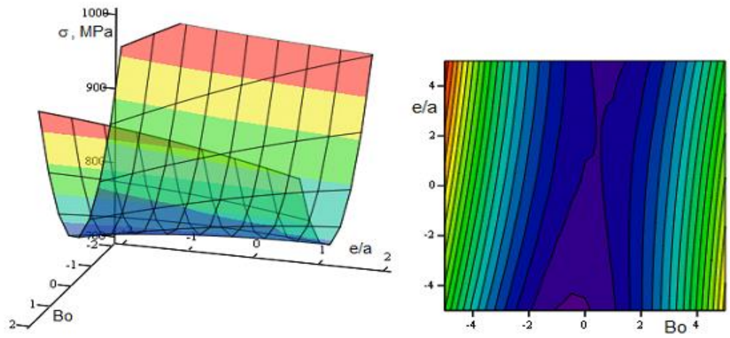

Fig. 6. Resistance to compression according to Bo and e/a (coded units) at Md of 2.4005 (+1, coded units)

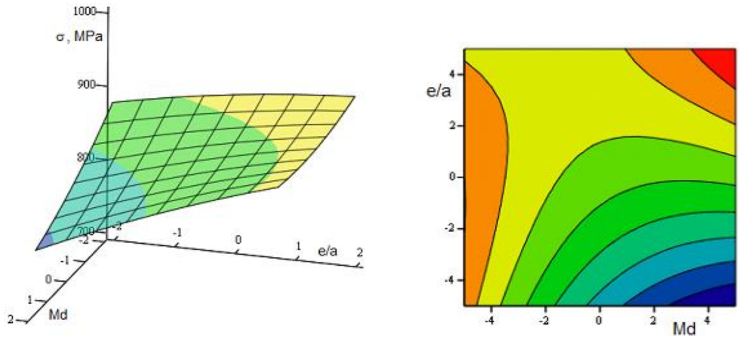

Fig. 7. Resistance to compression according to Md and e/a (coded units) at Bo of 2.8179 (-1, coded units)

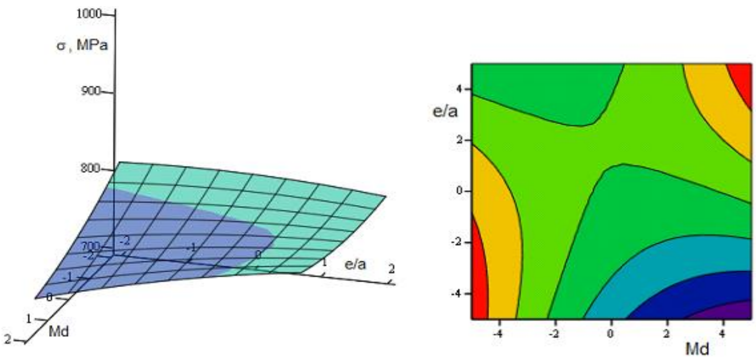

Fig. 8. Resistance to compression according to Md and e/a (coded units) at Bo of 2.8204 (0, coded units)

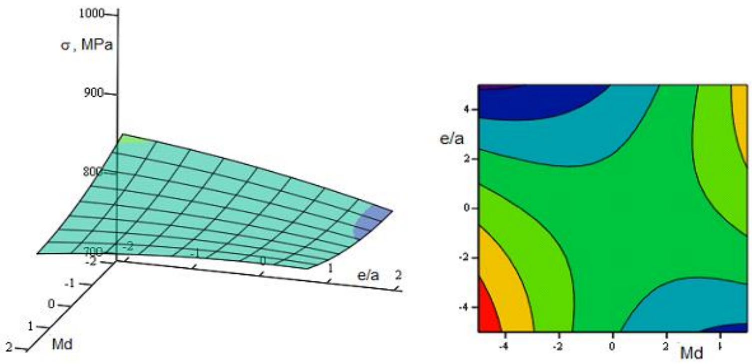

Fig. 9. Resistance to compression according to Md and e/a (coded units) at Bo of 2.8229 (+1, coded units)

Table 1

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

No.	Parameters (coded units)			Parameters (uncoded units)			Rc, MPa (experimental)	Rc, MPa (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	901	873.08
2	+1	-1	-1	2.4005	2.8179	4.1978	817	836.24
3	-1	+1	-1	2.3945	2.8229	4.1978	798	832.00
4	+1	+1	-1	2.4005	2.8229	4.1978	808	820.67
5	-1	-1	+1	2.3945	2.8179	4.2288	908	904.92
6	+1	-1	+1	2.4005	2.8179	4.2288	912	887.58
7	-1	+1	+1	2.3945	2.8229	4.2288	821	811.36
8	+1	+1	+1	2.4005	2.8229	4.2288	782	819.50
9	0	0	0	2.3975	2.8204	4.2133	781	794.16
10	0	0	0	2.3975	2.8204	4.2133	796	794.16
11	0	0	0	2.3975	2.8204	4.2133	780	794.16
12	0	0	0	2.3975	2.8204	4.2133	799	794.16
13	0	0	0	2.3975	2.8204	4.2133	800	794.16
14	-1.471	0	0	2.3931	2.8204	4.2133	801	809.67
15	+1.471	0	0	2.4019	2.8204	4.2133	815	788.58
16	0	-1.471	0	2.3975	2.8167	4.2133	921	949.73
17	0	+1.471	0	2.3975	2.8241	4.2133	916	869.46
18	0	0	-1.471	2.3975	2.8204	4.1905	801	779.35
19	0	0	+1.471	2.3975	2.8204	4.2361	798	801.91

In the situations (Figs. 1 to 6) where a variable parameter is Bo (the bond order), the resistance to compression presents quite large variations, this parameter considerably influences the resistance to compression, showing minimum values in the interval (-1.0) of encoded units. When Bo is constant (Figs. 7 to 9), the influence of the other two parameters is not so obvious, except when Bo = -1, coded units, Fig. 7, the resistance to compression is increasing for higher values of Md and e/a.

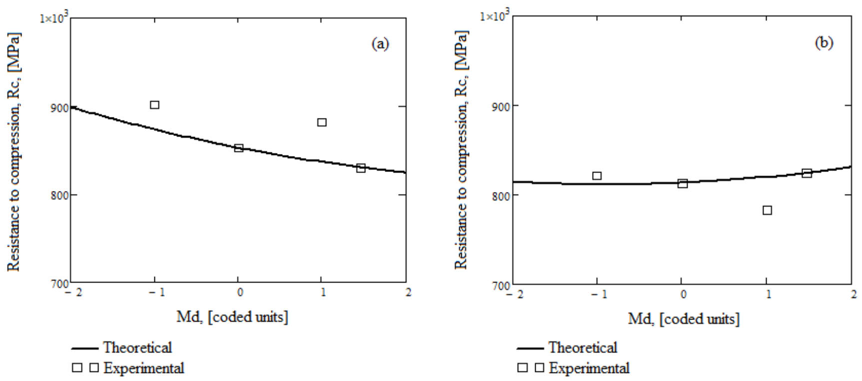

Fig. 10. Rc vs. Md for constant values of Bo and e/a: a) (1, 1) and b) (-1, -1)

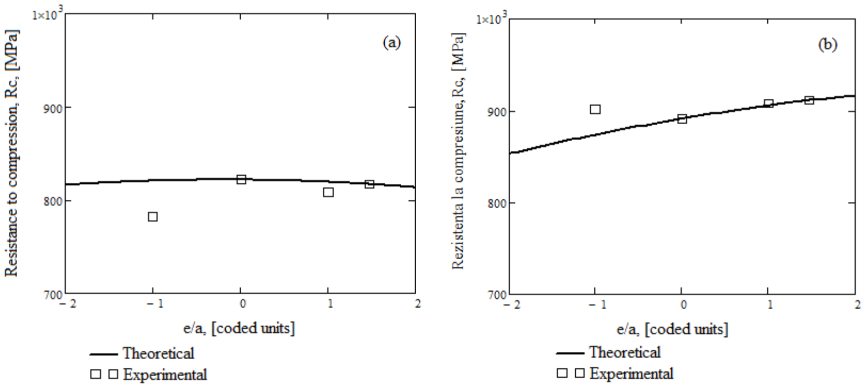

Fig. 11. Rc vs. e/a for constant values of Bo and Md: a) (-1, -1) and b) (1, 1)

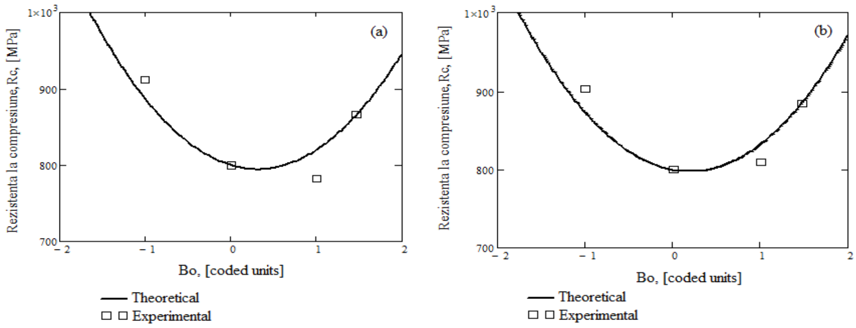

Fig. 12. Rc vs. Bo for constant values of Md and e/a: a) (-1, -1) and b) (1, 1)

These observations are also visible in Figs. 10 to 12, where the theoretical curves developed by the mathematical model are presented, compared to the experimental data.

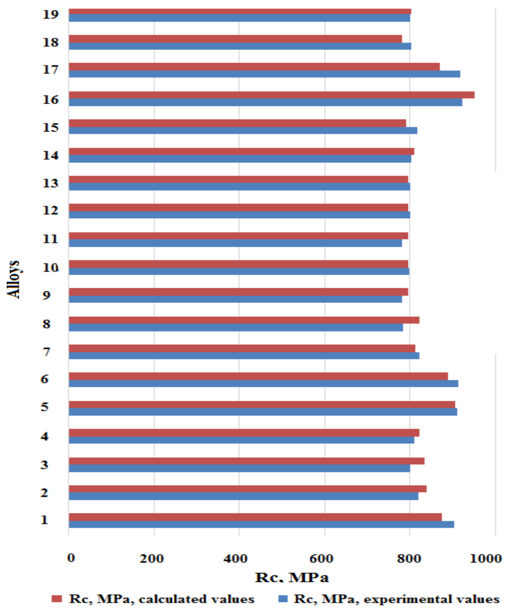

Fig.13. Comparison of the experimental values with the calculated values for the resistance to compression

Not all situations that can be generated from the mathematical model have been presented, but in all cases for all combinations of values for Md, Bo and e/a, the curves σ vs. Bo, σ vs. Md and σ vs. e a have the same aspect (alura), the experimental values being recorded on these curves, in the error margin of the theoretical model (δ = 13.657).

Calculated and experimental values are shown in Table 1 and compared in Fig. 13. It can be seen from Fig. 13 that there is a good concordance between the experimental values and the calculated values for the resistance to compression of all the studied alloys, the differences falling into the calculation error - δ = 13,657.

4. Conclusions

With this model, was obtained theoretical data on the resistance to compression of Ti-15Mo-W which are in very 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 - δ = 13,657. The nonlinearity all 3D charts demonstrates that there are interactions between each independent variable and the resistance to compression. Therefore, it can also be concluded that all contour surfaces of the three parameters considered, Md, Bo, e/a under various conditions were nonlinear.

R E F E R E N C E S

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