MODELING AND OPTIMIZATION OF THE PROPERTIES AND COMPOSITION OF TITANIUM-BASED ALLOYS

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Abstract: *The possibilities of regression analysis to model the properties and the related to it multicriteria optimization of the composition of titanium alloys are introduced in the presented research. This is done after performing characteristics of established applications of various titanium alloys. To predict elongation in this paper there have been obtained nonlinear regression models that allow to estimate the strength properties and the plasticity depending on the equivalents for aluminum and molybdenum for titanium alloys.*

Key words: METALLURGICAL DESIGN, TENSILE PROPERTIES, COMPOSITION-PROCESSING-PROPERTY CORRELATION

1. Introduction

Analysis of international trends and forecasts in the use of metal alloys up to year 2020 shows that titanium alloys are promising materials of general-purpose worldwide engineering [1].

Despite the economic uncertainty in the world economy, over the past years there was a steady demand for titanium products, which was a result of high rates of development of the aerospace sector – the main consumer of titanium products. In the international scientific community there is a continuous research of new ideas about the applications of titanium alloys in various industries, and, above all, the emphasis is put on areas with importance of the quality of the final product, but not in commercial aerospace and aeromechanics [2, 3], military industry (Figure 1)

A lot of attention in the development and improvement of titanium alloys for various applications is dedicated to the problem of effective alloying materials the solution of which leads to improved basic operating parameters of the alloys. The structural strength of materials plays an important role in ensuring a reliable long-term operation of machine parts and assemblies. Creation of new equipment in aviation, engineering, oil-, gas- and other industries imposes more stringent requirements for higher performance of the designs. This necessitates the use of materials with a higher set of physical and mechanical properties. For metallic materials, this problem is solved either by creating new alloy compositions, or by the development of new high-performance thermomechanical methods targeting the structure of industrial production of alloys.

Over the years, the research of titanium and its led to much experimental, theoretical and practical experience in the metal science, thermal and mechanical treatment, such as: basic principles of alloying titanium alloys were well-grounded, the methods and modes of heat treatment were developed, the basic dependencies of various mechanical properties were established on the chemical composition, structure, modes of thermal, thermo-mechanical, etc. operation.

The results of these studies are summarized in a series of monographs and reference works [4]. As a result, to date there is collected extensive material for statistical research that can be used to elaborate methods for predicting mechanical and technological properties of titanium alloys according to different criteria, such as the chemical composition.

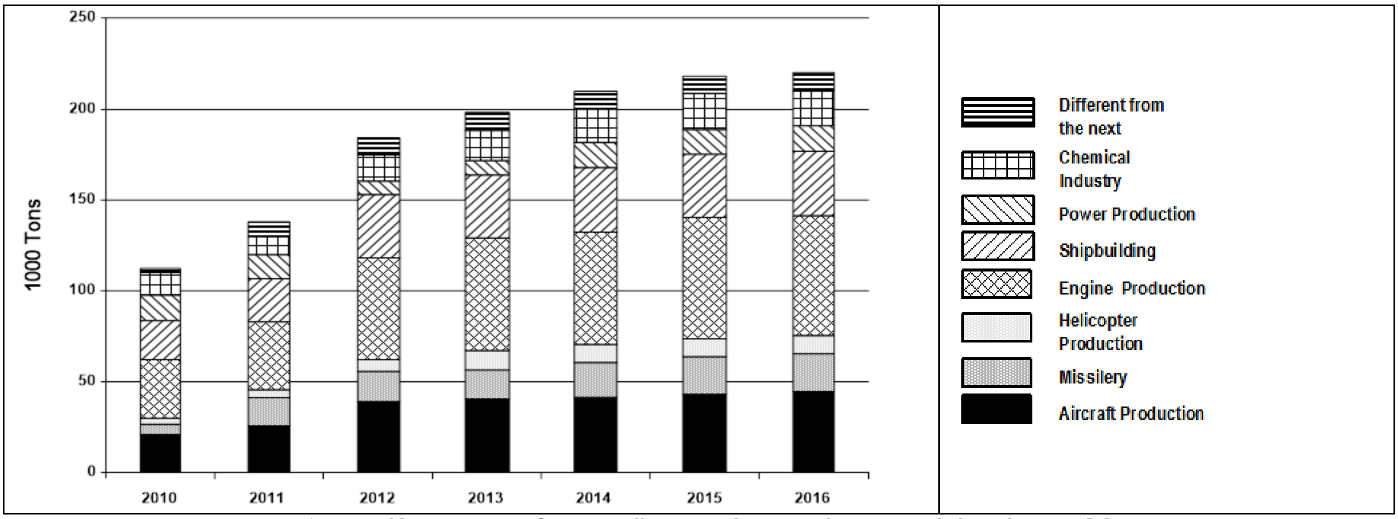


Fig 1. *World consumption of titanium alloys according to applications and along the years [1]*

2. Characteristics of titanium alloys and their superior criteria for classes

To obtain predetermined mechanical properties of titanium it is alloyed with aluminum, vanadium, manganese, molybdenum, chromium, iron and some other chemical elements. Introducing alloying elements in certain combinations and quantities, as well as targeted thermal effect, allow to change the properties of alloys in a wide range. The ultimate tensile strength of commercial titanium alloys can be varied from 400 MPa for low-alloyed soft alloys and up to 1600 MPa for the high-heat-strengthened alloys.

Relatively To obtain predetermined mechanical properties of titanium it is alloyed with aluminum, vanadium, manganese, molybdenum, chromium, iron and some other low density in combination with relatively high-strength characteristics of titanium alloys provides a higher specific strength (ratio of strength characteristics to density) in a wide range of temperatures, as compared to aluminum alloys, steels and heat-resistant nickel alloys.

This circumstance is the decisive factor in determining the preference of use of titanium in aircraft and aerospace engineering. Titanium alloys retain their inherent strength characteristics up to a relatively high temperature. Best heat-resistant titanium alloys can operate at temperatures 600-650 ° C.

Class of alloys		Rm, MPa	ρ g/cm^3	Rm/ρ, MPa cm^3/g
Titanium alloys	Low-strength Middle-strength High-strength	400-700 700-1000 >1000	4,5-4,55 4,4-4,5 4,65-4,75	88,4-154,6 157-225 >213
Alluminium alloys	Low-strength Middle-strength High-strength	130-300 350-500 >500	2,7 2,85 2,85	48,1-1 14 123-175 >175
Steels	Conventional Low-alloyed Middle-alloyed High-strength	300-700 400-850 850-1500 >1500	7,8 7,8 7,8 7,8	38,5-89,7 89,7-109 109-192 >192

***Table 1**. Comparison of the level of strength for steels, titanium and aluminum alloys [1]*

Table 1 presents a comparison between the strength and the density of steels, titanium and aluminium alloys.

Specific features and unusual functional characteristics of special titanium alloys significantly expand the scope of their use. Criteria for competitiveness for various titanium alloys are presented in Table 2.

Titanium alloys	Application criteria
Technical titanium	Mass, corrosion resistance, stiffness, deformability, appearance
α + β – alloys, titanium aluminides	Mass, high-temperature strength/resistance, oxidation resistance, durability, strength
β –alloys	Mass, high strength, spring characteristics, cold formability
Titanium aluminides	Heat resistance
Titanium-nickel alloys	Mass, corrosion resistance
Titanium-nickel alloys	The shape memory effect

***Table 2.** Criteria for various titanium alloys, related to their competitiveness*

The numeric design of the composition and the operative technological parameters in metallurgy is a problem of particular complexity due to its multivariate nature. There is a need for continuous improvement of the whole industry in order to improve the properties of alloys with broad application.

This research is part of series of approaches and methodologies that at the stage of generating the decision do not use the knowledge gained in the field of metallurgy. The proposal has the potential to predict the mechanical properties of alloys, like in [t13], using prior information of data linking composition, processing and properties. The cited monograph explores the iron-based alloys, thus confirming the thesis for evaluation of these alloys numerically and experimentally. This methodology is the way to design alloys at a predetermined database.

3. Formulation of the problem

The results from the analysis of the models and the optimization can provide a guideline for further experimental and computational investigation [6, 7].

Instead of performing real experiments, the computational design approach combines physical models of known interactions, compositions, processing, properties to predict the alloy composition and the related to it set of characteristics [8].

The increase in the number of variables is considered usually to lead to a drastic increase in the complexity of physical models, which causes the calculation to be much more time-consuming and demanding for computation capacity [9].

That is why the developed by us procedures and algorithms [5] are realized for a fixed processing mode. Therefore it is of practical importance and also it is necessary to expand the task to understand the relation between the composition, the processing and the properties which would allow a quick evaluation for the alternation of composition and of the processing route.

The purpose of this research was the statistical comparison of strength and plastic properties for titanium alloys of different classes depending on their chemical composition, expressed as equivalents for aluminum and molybdenum.

This paper includes an example illustrating the relationship between the composition and the properties and modeling capabilities in this direction. Thereby it is possible to evaluate the basic properties depending on a popular summary of the alloy composition based on two widely used equivalents [1].

To calculate equivalents for aluminum and molybdenum there was used the average chemical composition of 18 industrial alloys. In references [4] on the basis of summarizing a large amount of literature and experimental data there are cited the most typical values of the mechanical properties, i.e. values close to the average estimates. The used data base is presented in Table3. Related to the specific composition of each alloy there are defined two quantities of aluminum and molybdenum equivalents described as follows [1]. The mechanical properties of titanium alloys strongly depend on the thermal treatment. The data shown in Table 3 are derived from the same heat treatment - Annealing (α + β)

$$Al = \%Al + \%\frac{Sn}{3} + \%\frac{Zr}{6} + 10\left(\%O + \%C + 2(\%N)\right);$$

$$Mo = \%Mo + \%\frac{Ta}{4} + \%\frac{Nb}{3{,}3} + \%\frac{W}{2} + \%\frac{V}{1{,}4} + \%\frac{Cr}{0{,}6} + \%\frac{Ni}{0{,}8} + \%\frac{Mn}{0{,}6} + \%\frac{Fe}{0{,}4}.$$

These two equivalents carry information for alloying, because they are calculated for the various combinations of the alloying elements.

For comparison and optimization of titanium alloys it is possible to use structural and strength equivalents to aluminum and molybdenum, proposed in [1]: molybdenum and aluminium equivalents are integral characteristics describing the effect of alloying elements on the structure, the phase composition and the strength of titanium alloys. The structural equivalent to the total effect of aluminum characterizes the impact of α- stabilizers and neutral reinforcers on the phase composition of alloys (intermetallic formation conditions α). The formation of phase α leads to a sharp decrease in ductility, and in the thermal stability of alloys. The phase is not formed if the equivalent structure on aluminum does not exceed 9%. α- stabilizers are alloying elements that increase the temperature of the polymorphic transformation of titanium. These include aluminum, carbon, nitrogen, oxygen. The structural equivalent of molybdenum characterizes the total effect of β-stabilizing elements on the phase composition of alloys (number of β-phase, its stability, the ability to phase transformations). β- stabilizers are elements that reduce the temperature of the polymorphic transformation of titanium. They can be divided into zoomorphic (vanadium, tungsten, molybdenum, etc.) and eutectoid (chromium, manganese, cobalt, etc.).

This example shows the effect from alloying complexity related to the quantities and also to the alloy elements, over the basic mechanical parameters - Rm - ultimate tensile strength, Rp0.2 - tensile yield strength, E - elongation.

№	alloy	Mo –ekv X_1	Al-ekv X_2	Rm [MPa]	Rp0.2 [MPa]	E [%]
1	Ti-6Al-2Sn-1.5Zr-1Mo-0.35Bi-0.1Si	**1,375**	**8,12**	**937**	**848**	**16,0**
2	Ti-3Al-2.5V	**2,161**	**4,2**	**690**	**627**	**20,0**
3	Ti-6AI-2Sn-4Zr-2Mo	**2,375**	**8,53**	**1000**	**930**	**15,0**
4	Ti-8Al-1Mo-1V	**2,089**	**9,2**	**1000**	**930**	**12,0**
5	Ti-10V-2Fe-3Al	**12,14**	**4,2**	**970**	**900**	**9,0**
6	Ti-13V – 11Cr-3Al	**27.99**	**4.2**	**950**	**860**	**18**
7	Ti-6AI-2Sn-4Zr-6Mo	**6,375**	**8,53**	**1030**	**970**	**11,0**
8	Ti-6Al-4V (Grade 5)	**3,232**	**7,2**	**950**	**880**	**14,0**
9	Ti-6Al-6V-2Sn	**4,661**	**7,87**	**931**	**807**	**18,0**
10	Ti-7Al-4Mo	**4,375**	**8,2**	**1030**	**970**	**12**
11	Ti-5Al-5Sn-2Zr-2Mo-0.25Si	**2,375**	**8,2**	**730**	**552**	**20,0**
12	Ti-5Al-6Sn-2Zr-1Mo-0.25Si	**1,375**	**8,53**	**720**	**550**	**17,0**
13	Ti-4Al-3Mo-1V	**4,089**	**5,2**	**860**	**860**	**10,0**
14	Ti-5Al-1.5Fe-1.4Cr-1.2Mo-	**7,283**	**6,2**	**1061**	**1020**	**14,0**
15	Ti-5Al-2.5Fe	**6,25**	**6,2**	**860**	**780**	**9,0**
16	VT14	**4,475**	**6,1**	**883**	**873**	**10,0**
17	VT16	**8,589**	**3,5**	**814**	**716**	**8,0**
18	Ti (99.5)	**0,375**	**1,2**	**331**	**241**	**30**

Table 3. *Relationship between variables and equivalents percentage*

4. Results

Based on this information from Table 3, nonlinear regression models are derived establishing the relation between the complex composition and the properties.

The software package DSTAT [10] was used for statistical analysis.

Table 4 presents the coefficients of the regression models derived for coded values of the variables. Passive-experiment data affect the accuracy of the models, but nevertheless the models are adequate and they can be used for prediction. Fig. 2 introduces graphical interpretations of the displayed models

Characteristics / Coefficient	Rm [MPa]	Rp_{02} [MPa]	E [%]
Free coefficient	990.168	1008.96	10.7753
$b_1 * X_1$ (Mo ekv)	179.100	185.366	-2.29775
$b_2 * X_2$ (Al ekv)	342.250	380.970	-5.27148
$b_{11} * X_1^2$	-102.675	-185.659	8.37208
$b_{12} * X_1 X_2$	85.8673	202.658	-
$B_{22} * X_2^2$	-106.736	-123.784	-
R	0.8834	0.8016	0.6753
F computing	8.5277	4.3135	3.9131
F tabl. meaning	3.1059 (α = 0.05, 5, 12)	3.1059 (α = 0.05, 5, 12)	3.3439 (α = 0.05, 3, 14)

Table 4. *Coefficients and parameters of regression models describing properties depending on molybdenum and aluminum equivalents*

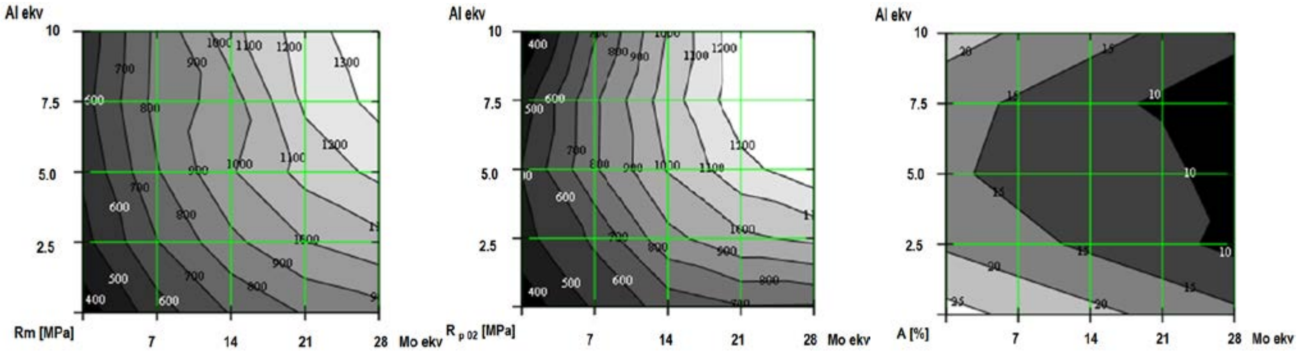
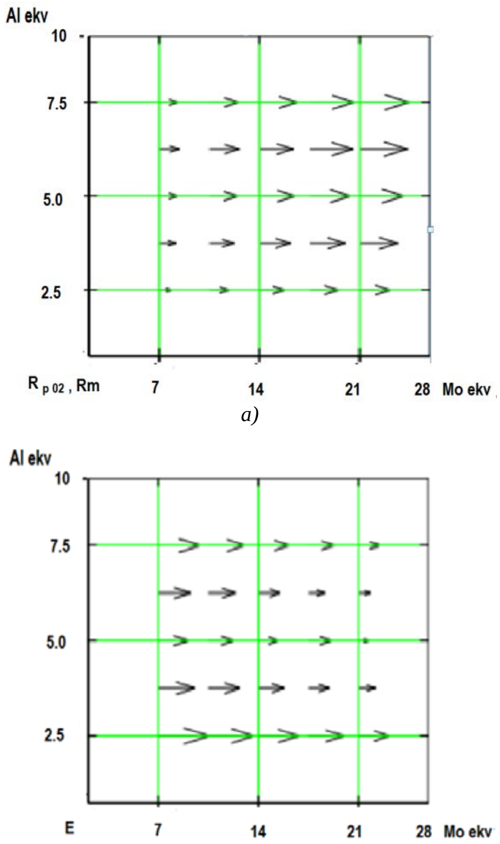


Fig. 2.*Changes of mechanical properties - Rm - ultimate tensile strength, Rp0.2 - tensile yield strength, E-elongation depending on the aluminum and molybdenum equivalents.*

The contradiction between plastic and strength characteristics stands out from all attached graphics, including vector graphics depicted in Fig. 3. High strength is observed for high values of aluminium and molybdenum equivalents. Plasticity is relatively low for these values of the equivalents.



a)

b)

Fig. 3*. Vector representations of: Rp0.2 – tensile yield strength, Rm – ultimate tensile strength – a) and for E – elongation b), depending on molybdenum and titanium equivalents.*

The resulting regression models listed in Table 3 make it possible to define the multicriteria problem, by means of which to determine optimal values of aluminum and molybdenum equivalents for which strength and plastic properties are relatively maximal. This procedure is described in detail [11]. As a result of applying the procedure in Table 5 are shown the following optimal values.

Input parameters of optimal characteristics		Optimal values of the investigated characteristics	
		for elongation E	For yield strength $R_{p\,02}$
Mo ekv /X_1/	Al ekv /X_2/	16.8 [%]	1008 [MPa]
28 % /1/	5.2 % /0/	Percentage of the determined decision related to the maximum value	
		53.6 [%]	60.60 [%]

Table 5*. Optimal values of the investigated characteristics*

Conclusion.

In the presented research are introduced the possibilities of regression analysis to model the properties and the related to it multicriteria optimization of the composition of titanium alloys. This is done after performing characteristics of established applications of various titanium alloys. For clarity of results the option is a bidimensional case, expressed by aluminum and molybdenum equivalents. The applied methodology is solved for ten variables

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