# MODELING AND OPTIMIZATION OF THE COMPOSITION OF TITANIUM -BASED ALLOYS BY APPROXIMATION WITH REGRESSION MODELS

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***Abstract:*** *The article is dedicated to an approach optimizing a task of statistical modeling of the mechanical properties of products in real production metallurgy design. The approach is designed for the benefit of producers-metallurgists aimed at providing panels of Ti - alloys of a specific set of eventual industrial properties. This is accomplished by a procedure of composition optimizing based on existing certificates of brands Ti - alloys. The article presents an approach using mathematical models of optimization problem following the implementation of approach the classical methodology capable of decision-making in the production practice.*

**Keywords:** METALLURGICAL DESIGN, TENSILE PROPERTIES, COMPOSITION-PROCESSING-PROPERTY CORRELATION, OPTIMIZATION OF THE COMPOSITION

## *1. Introduction*

An effective approach at metallurgical design is to use data from previous experience, processed up to a statistical model, based on a large amount of data related by composition, processing and properties. The design of the alloy composition and the optimization of the technological-process parameters are directly related to the resolution of the compromise between the measured values related to certain selected indicators of the quality of a set of materials for a test group or a class [1]. The most characteristic for these approaches is that they do not use the principles of metallurgy and metal physics. It is relied mainly only on an a priori information about the relation "composition and processing and their influence on the properties." Compared with physical models, the advantage of statistical models is their ability to explore a complex of properties and to obtain information in a timely and effective manner, even when there are no well-established physical theories and models.

The aim of this study is to present a robust approach for determining the influence of alloying elements on the properties of Ti - alloys that ensures better results than the input ones used to obtain a mathematical model.The formulated optimization models are used at the stage of modeling the mechanical properties of the composition of Ti - alloys during the production metallurgy process.

The multidimensional regression analysis is one of the most popular data-mining methods. It has been applied successfully to the study of multiple relationships in metallurgical industry, [2] – [4]. Due to the nature of each statistical analysis, the coefficients of limitations imposed by the regression analysis are known only approximately. That should be reflected in the mathematical model of the optimization problem.

## *2. General description of the approach*

The analysis presented in this paper is related to the analysis of mechanical properties of Ti - specimens described by the following parameters: yield strength, Rp 02 [MPa], tensile strength and relative elongation (A [%]). The limitations connected with these

parameters are due to Ti grade characteristics and customer's specifications. However, the main problem is that these parameters cannot be under direct observation during the manufacturing process, so any limitations associated with them cannot be clearly defined in the optimization model. That means that we must develop models linking the final mechanical properties of the specimen/sample of the steel chemical composition as well as the parameters of the production process.

The regression analysis allows describing the relation between the variables of input and output, without going into the phenomenon nature during the process.

The regression models presented below have been created based on the data collected during the industrial production process.

The statistical analysis described in this section is based on a data set of 300 records extracted from the whole database.

The Pareto front was built based on this initial information related to the couple of parameters yield strength, $Rp_{02}$ [MPa] and relative elongation (A [%]). The chemical composition of the various compositions is given in an implicit form in the case. From the list of compositions in the full range of variations there have been selected Pareto compositions for which the sum of the basic elements had a relatively small value. The selection is focused on compositions for which the relatively small price of their expensive elements does not affect the values of the explored parameters for optimization. The obtained regression models are related to this information. In respect to the problem under examination, nonlinear regression dependencies have been identified for each of the mechanical properties of alloys. The regression dependencies are of the following kind:

Here bij are the regression model parameters. The coefficients in equations are defined in Table 1. The models can be used for prediction if the check-up $F > F(0.5, \nu 1, \nu 2)$ described in details has been made.

The relationship between the derived coefficients in Table 1 and the specific chemical elements is described in the regression elements.

$Rp_{02}$ = 1211.88 + 51.5221 Al - 24.9734 Mo - 80.7796 Sn + 96.9246 Zr + 209.828 Cr + 80.3385 Fe + 72.0976 V - 21.4625 Si + 40.3190 O - 6.81555 $Al^2$ - 106.347 Al Mo - 69.9600 Al Sn - 43.6439 Al Zr + 15.4261 Al Cr -61.9896 Al Fe -81.5665 Al V + 10.3925 Al Si + 47.3631 Al O + 31.7825 $Mo^2$ - 24.5042 Mo Sn - 19.5766 Mo Zr - 43.8777 Mo Cr - 34.0499 Mo Fe - 70.3951 Mo V - 51.3807 Mo Si + 60.8373 Mo O + 6.35824 $Sn^2$ - 62.3299 Sn Zr - 49.0562 Sn Cr + 47.2030 Sn Fe - 84.9186 Sn V + 7.34492 Sn Si + 47.5112 Sn O + 44.0214 $Zr^2$ -39.5834 Zr Cr - 34.9639 Zr Fe + 19.4983 Zr V + 34.0014 Zr Si + 1.40613 Zr O + 109.626 $Cr^2$ - 26.3554 C Fe + 12.6771 Cr V + 0.829980 Cr SI - 24.8476 Cr O - 75.0358 $Fe^2$ + 3.91375 Fe V + 25.5956 Fe Si - 67.2523 Fe O - 6.09390 $V^2$ + 19.2299 V Si + 17.1889 V O -51.7804 $Si^2$ +19.0743 Si O -38.5409 $O^2$

***Table 1.*** *Coefficients of regression modelds of the examined target parameters.*

| № | designation | $Rp_{02}$ | A | № | designation | $Rp_{02}$ | A |
|---|---|---|---|---|---|---|---|
| 1 | b( 0 0) | 1211.88 | 43.4377 | 29 | b( 3 4) | -62.3299 | 7.48801 |
| 2 | b( 1 0) | 51.5221 | -12.4873 | 30 | b( 3 5) | -49.0562 | 3.57374 |
| 3 | b( 2 0) | -24.9734 | 5.83605 | 31 | b( 3 6) | 47.2030 | -13.2362 |
| 4 | b( 3 0) | -80.7796 | 16.1346 | 32 | b( 3 7) | -84.9186 | 18.1995 |
| 5 | b( 4 0) | 96.9246 | -26.5634 | 33 | b( 3 8 | 7.34492 | 2.45297 |
| 6 | b( 5 0) | 209.828 | -41.6628 | 34 | b( 3 9) | 47.5112 | -7.84135 |
| 7 | b( 6 0) | 80.3385 | -11.3614 | 35 | b( 4 4) | 44.0214 | -12.5869 |
| 8 | b( 7 0) | 72.0976 | -12.2634 | 36 | b( 4 5) | -39.5834 | 11.2109 |
| 9 | b( 8 0) | -21.4625 | 9.45284 | 37 | b( 4 6) | -34.9639 | 11.6078 |
| 10 | b( 9 0) | 40.3190 | -7.32094 | 38 | b( 4 7) | 19.4983 | -1.06720 |
| 11 | b( 1 1) | -6.81555 | 4.99262 | 39 | b( 4 8) | 34.0014 | -5.39692 |
| 12 | b( 1 2) | -106.347 | 32.8537 | 40 | b( 4 9) | 1.40613 | 3.89560 |
| 13 | b( 1 3) | -69.9600 | 13.9749 | 41 | b( 5 5) | 109.626 | -11.8927 |
| 14 | b( 1 4) | -43.6439 | 6.60931 | 42 | b( 5 6) | -26.3554 | 18.2370 |
| 15 | b( 1 5) | 15.4261 | 2.81458 | 43 | b( 5 7) | 12.6771 | 12.9706 |
| 16 | b( 1 6) | -61.9896 | 24.7026 | 44 | b( 5 8) | 0.829980 | 0.427527 |
| 17 | b( 1 7) | -81.5665 | 26.9275 | 45 | b( 5 9) | -24.8476 | 8.14636 |
| 18 | b( 1 8) | 10.3925 | -4.94533 | 46 | b( 6 6) | -75.0358 | 22.7628 |
| 19 | b( 1 9) | 47.3631 | -7.11438 | 47 | b( 6 7) | 3.91375 | 14.6460 |
| 20 | b( 2 2) | 31.7825 | -8.72509 | 48 | b( 6 8) | 25.5956 | -10.9786 |
| 21 | b( 2 3) | -24.5042 | 3.37836 | 49 | b( 6 9) | -67.2523 | 18.1532 |
| 22 | b( 2 4) | -19.5766 | 1.36551 | 50 | b( 7 7) | -6.09390 | 1.46032 |
| 23 | b( 2 5) | -43.8777 | 13.8703 | 51 | b( 7 8) | 19.2299 | -4.26022 |
| 24 | b( 2 6) | -34.0499 | 13.3358 | 52 | b( 7 9) | 17.1889 | -6.80520 |
| 25 | b( 2 7) | -70.3951 | 18.9816 | 53 | b( 8 8) | -51.7804 | 14.9821 |
| 26 | b( 2 8) | -51.3807 | 9.02304 | 54 | b( 8 9) | 19.0743 | -5.02353 |
| 27 | b( 2 9) | 60.8373 | -3.70434 | 55 | b( 9 9) | -38.5409 | 1.21278 |
| 28 | b( 3 3) | 6.35824 | 2.60378 | | | | |
| **$Rp_{02}$** | | R = 0.9880 | | F cal. = 18.8637 $_{(a=0.05,54,25)}$ > 1.8367 = F tabl | | | |
| **A** | | R = 0.9906 | | F cal. = 24.2416 $_{(a=0.05,54,25)}$ > 1.8367= F tabl | | | |

A = 43.4377- 12.4873 Al + 5.83605 Mo + 16.1346 Sn - 26.5634 Zr - 41.6628 Cr -11.3614 Fe - 12.2634 V + 9.45284 Si - 7.32094 O + 4.99262 Al $^2$ + 32.8537 Al Mo + 13.9749 Al Sn + 6.60931 Al Zr + 2.81458 Al Cr + 24.7026 Al Fe + 26.9275 Al V- 4.94533 Al Si - 7.11438 Al O - 8.72509 Mo $^2$ +3.37836 Mo Si + 1.36551 Mo Zr + 13.8703 Mo Cr + 13.3358 Mo Fe + 18.9816 Mo V + 9.02304 Mo Si -3.70434 Mo O + 2.60378 Sn$^2$ +7.48801 Sn Zr + 3.57374 Sn Cr- 13.2362 Sn Fe + 18.1995 Sn V +2.45297 Sn Si-7.84135 Sn O - 12.5869 Zr $^2$ + 11.2109 Zr Cr + 11.6078 Zr Fe - 1.06720 Zr V - 5.39692 Zr Si + 3.89560 Zr O - 11.8927 Cr $^2$ + 18.2370 Cr Fe + 12.9706 Cr V + 0.427527 Cr Si + 8.14636 Cr O + 22.7628 Fe $^2$ + 14.6460 Fe V - 10.9786 Fe Si + 18.1532 Fe O + 1.46032 V $^2$ - 4.26022 V Si - 6.8052 V O + 14.9821 Si$^2$ - 5.02353 Si O + 1.21278 O $^2$

The numerical experiment [6] has proved the ability to improve the quality of Ti alloy of a certain class. Mathematical models suitable for forecasting and optimization have been derived. The approach of Taguchi applied has lead to a desired result, to separate variables Xi for the examined parameters that do not influence significantly on the final result. With this limit, the numerical optimization for maximum search has been conducted with each chemical composition. That allows improving it. Relative elongation A turned to be less variable index and yield strength Re requires caution with extreme selecting. The decision of bi-criteria problem set has been defined thus proving that the Taguchi approach is applicable to a similar class of problems.Following the applied optimization procedure and based on the derived models, a solution was formulated. According to it, the content of aluminum and molybdenum is about 8-9 percent, and the values of vanadium, chromium and silicon are negligible. Fig. from 1-8 visualizes an interpretation of the main alloying elements and their effect on the investigated variables at fixed values of the rest of the elements that are equal to the determined optimal

## *Conclusion*

It has been proven that during the design of the properties of the materials it is possible to determine effective solutions via defining a multicriteria problem. It has been proven that during modeling process costs for the different Ti - alloys grades in aggregate, it is possible to evaluate equally possible for realization technological routes.Optimal compositions of a Ti-alloys have been determined grade by Pareto-front in terms of strength and ductility that are experimentally verified for a particular application. The number and the amount of alloying elements in low-alloy steels are determined. For Ti - alloys with economic alloying there are constructed models defining the relationship.

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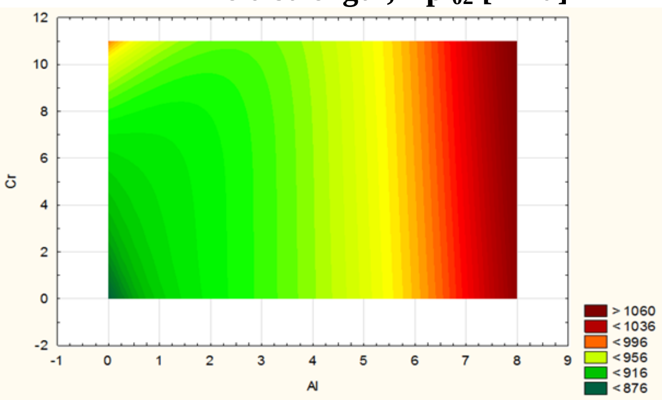
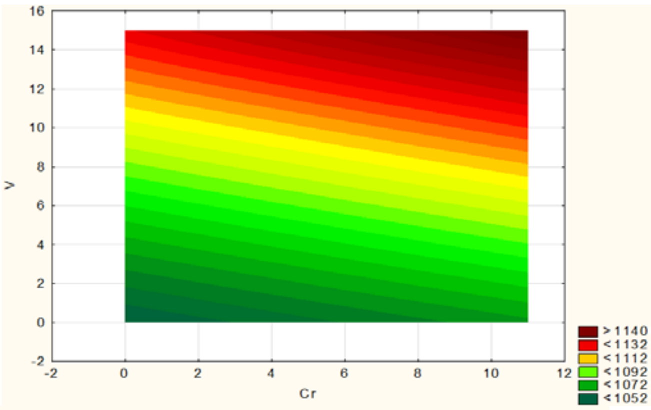
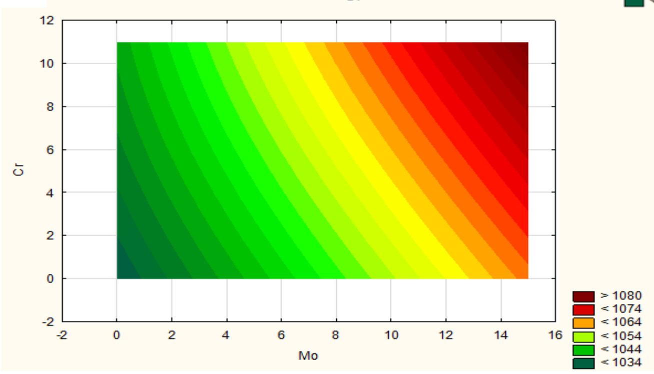
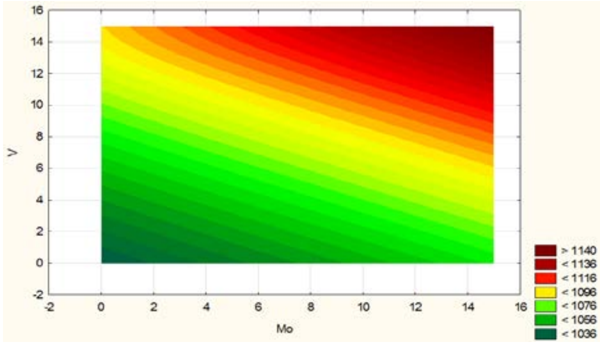
## Yield strength, Rp $_{02}$ [MPa]




## Relative elongation (A [%])