ROBUST BI-CRITERIA APPROACH TO OPTIMIZE THE COMPOSITION AND PROPERTIES OF TITANIUM ALLOY

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Abstract: *The numerical experiment has proved the ability to improve the quality of titanium alloys. 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.*

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

1. Introduction

Titan and its alloys was originally intended for use in military and defense industry, but over time they are becoming more common in peaceful areas – the economy, civil aviation, medicine and marine studies, sports and automotive industry. [1]

Thanks to the development of large lean production titan became more accessible and cost-effective material. Its high performance coupled with modern technological and industrial advances have opened vast opportunities for use in transport machinebuilding.

Very small quantities of the concentration of alloying elements and their combinations may result in significant changes in the physical and mechanical properties of the alloys. This fact determines the need to seek the most appropriate for the specific concentrations of alloying elements. Probably the most famous center for research in the field of modeling and regression analysis of super-alloys is the one in the University of Cambridge UK [2-4]

The traditional alloy-development strategy consists of producing numerous samples with varying composition and set of the elements, the processing mode included, to define an alloy with optimal properties [5].

The approach resulted in high costs of experimentation [6].

This is the reason that the methods of directed search and the ‘trial and error’ method reside the lowest level in the hierarchy of methods.

An alternative effective approach is to use data from past experience worked to a statistical model – based on a large amount of data associated by composition, processing and properties.

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 [7], 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.

Not only does each element strengthen alloys through more than one mechanism, but sometimes two or three elements can combine together to influence the strength.

In addition, the realization of strengthening effects of these elements strongly relies on the processing conditions.

2. Formulation of the problem

The ambition consists in building an approach and validation techniques to determine the trade-offs in meeting specific requirements are the properties of titanium alloys. For these specific properties there are indicated the possible combinations of alloying elements for different types of heat treatment. Regression and neural models are designed for the properties and optimization is performed for the composition and the processing parameters for a large database with more than 300 monitorings of different titanium alloys.

The creation of mathematical models to analyze the objects of metallurgical process under examination is an important stage. These models contribute to improve the set of properties and the final product quality. It is confirmed that it is possible to meet the requirements of the current market by implementation of such models. The wide range of problems, which Taguchi method has been applied to, is shown in [7].

The core of Taguchi approach consists of the method for reducing the influence of factors called noise (disturbing) that impair the quality parameters of the product/process. It is where the radical difference from the traditional technique of quality, which provides identification of existing sources and conduction of measurements that are often costly due to their control. The parametric design of Taguchi ensures non-sensitivity to noise along the way to the proper selection of certain parameters called controllable factors.

The aim of this paper is to present a robust approach for determining the influence of alloying elements on the properties of iron-based alloys that ensures better results than the input ones used to obtain a mathematical model.

The statistical analysis presented in this article is based on of data collected during the real production process described in [8]

The ranges of change of the used alloying elements of ferrous alloys are listed in Table 1.

Input parameters – Alloyng components		**Al [%]**	**Mo [%]**	**Sn [%]**	**Zr [%]**	**Cr [%]**	**Fe [%]**	**V [%]**	**Si [%]**	**O [%]**
min		0,00	0,00	0,00	0,00	0,00	0,15	0,00	0,00	0,05
max		8,00	15,00	11,00	11,00	11,00	5,00	15,00	0,50	0,25
mean		4,13	3,11	1,46	1,92	1,24	0,49	3,29	0,03	0,12
St. Dev.		2,14	4,25	2,08	2,54	2,77	0,75	4,62	0,08	0,02
Number of data pairs containing this element at output parameters	**Rp_{02}**	277								
	E	252								

Table 1 *Minimum and maximum values of alloying components*

Heat treatment

№	Heat treatment
1.	Without heat treatment
2.	Annealing (β)
3.	Annealing (α + β)
4.	Annealing (α)
5.	Solution treatment (β)
6.	Solution treatment (α + β)
7.	Solution treatment
8.	(β) + ageing
9.	Solution treatment
10.	(α + β) + ageing
11.	Duplex annealing

***Table 2.** Heat treatments used in the database*

3. General description of the approach

The analysis presented in this paper is related to the analysis of mechanical properties of titanium specimens described by the following parameters: yield strength, *Rp02* [MPa] and relative elongation E [%]. The limitations connected with these parameters are due to Ti alloys 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 alloys 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 Least Squares method, LS is used to estimate the regression parameters. The estimated models of parameters Rp_{02} , E obtained in the examinations are given below.

In respect to the problem under examination, nonlinear regression dependencies have been identified for each of the mechanical properties of titanium alloys. The regression dependencies are of the following kind:

$$f_i(x) = b_{00}^i + \sum_{j=1}^{10} b_{j0}^i x_j + \sum_{j=1}^{10} b_{jj}^i x_j^2 + \sum_{j=1}^{10} \sum_{l=j+1}^{10} b_{jl} x_j x_l$$

Here b_{ij} are the regression model parameters. The coefficients in equations are defined in Table 2. The models can be used for prediction if the check-up F > F (0.5, ν_1,ν_2) described in details has been made. .

No	Coef	Rp02 [MPa]		No	Coef	Rp02 [MPa]	
1	C_0	396.2381	20.93544	**36**	$X_4 X_5$	9.379346	-0.01963
2	X_1	-32.0791	1.38401	**37**	$X_4 X_6$	15.51388	-0.37177
3	X_2	112.122	-7.84864	**38**	$X_4 X_7$	-10.5601	0.331122
4	X_3	78.1541	-0.16339	**39**	$X_4 X_8$	-16.6893	1.854779
5	X_4	130.7104	10.20102	**40**	$X_4 X_9$	-2.24882	-0.20250
6	X_5	-68.973	-6.45484	**41**	$X_4 X_{10}$	-48.3878	-2.56518
7	X_6	-730.192	21.26902	**42**	$X_5 X_6$	-2587.76	2.647485
8	X_7	-298.681	21.50194	**43**	$X_5 X_7$	44.56953	-0.80710
9	X_8	-3.12209	5.387568	**44**	$X_5 X_8$	-82.9475	-0.31884
10	X_9	-198.672	-31.7729	**45**	$X_5 X_9$	-6.13139	0.313483
11	X_{10}	-54.3129	2.672808	**46**	$X_5 X_{10}$	745.7955	-4.73098
13	$X_1 X_2$	-4.43718	-0.01702	**47**	$X_6 X_7$	-8.27673	-0.77459
14	$X_1 X_3$	-1.97432	-0.09657	**48**	$X_6 X_8$	263.0571	-9.12352
15	$X_1 X_5$	3.394209	-0.09768	**49**	$X_6 X_9$	-1.48548	-0.09670
16	$X_1 X_6$	7.171607	-0.03038	**50**	$X_6 X_{10}$	833.1564	-14.9056
17	$X_1 X_7$	2.889379	-0.17456	**51**	$X_7 X_8$	-87.6232	2.552293
18	$X_1 X_8$	9.00349	-0.19287	**52**	$X_7 X_9$	-16.70463	-0.32755
19	$X_1 X_9$	-1.1397	-0.05656	**53**	$X_7 X_{10}$	990.25321	-34.7130
20	$X_1 X_{10}$	-160.918	1.594115	**54**	$X_8 X_9$	-223.4617	2.604354
21	$X_2 X_3$	20.43437	0.487606	**55**	$X_8 X_{10}$	0	0
22	$X_2 X_4$	20.43437	0.487606	**56**	$X_9 X_{10}$	-585.6379	-0.988713
23	$X_2 X_5$	28.43656	-1.36517	**57**	X_1^2	84.742546	-3.812744
24	$X_2 X_6$	-18.7498	1.221792	**58**	X_2^2	6.993687	-0.133356
25	$X_2 X_7$	57.55664	-2.47272	**59**	X_3^2	-13.60908	0.8324983
26	$X_2 X_8$	21.12227	-0.48067	**60**	X_4^2	-6.65281	0.0710407
27	$X_2 X_9$	4.359865	-0.31536	**61**	X_5^2	-.168734	-0.20634
28	$X_2 X_{10}$	-164.874	14.12199	**62**	X_6^2	6.283372	0.0988364
29	$X_3 X_4$	443.6655	-0.54792	**63**	X_7^2	38.88832	-0.777694
30	$X_3 X_5$	-3.52382	-0.35718	**64**	X_8^2	71.03410	-6.386223
31	$X_3 X_6$	14.67915	0.115228	**65**	X_9^2	13.38640	-0.417462
32	$X_3 X_7$	48.49843	-0.50207	**66**	X_{10}^2	-549.354	-48.96597
33	$X_3 X_8$	78.61216	0.752812	**R**		0.7071	0.7312
34	$X_3 X_9$	-16.0990	-0.30255	**F cal**		3.246	3.467
35	$X_3 X_{10}$	366.2553	2.326692	**F tabl**		1.37	1.37

***Table 2** Coefficients of regression models of the examined target parameters*

By Taguchi methodology (Khosrow Dehnad, 1989) an experiment modeled on orthogonal matrices developed by him is carried out. The experiment can be accomplished in two ways by:

- a real experiment leading to obtaining results for processing;
- a numerical experiment with the presence of adequate regression models.

The availability of the described model coefficients, which can be used to predict, give a possibility to make a numerical experiment involving Taguchi method. The noise matrix is selected from orthogonal matrix I (27,13) with 27 rows and 13 columns developed by Taguchi [7]. The matrix is worked out with factors at three levels.

Specifically for the data of the experiment, eight of columns are used since the regression models are obtained on the basis of eight variables. In the matrix X_1 corresponds to parameter heat treatment, X_2 corresponds to aluminum , X_3 corresponds to molybdenum, X_4 corresponds to tin, X_5 - corresponds to zirconium, X_6 corresponds to chromium, X_7 corresponds to iron, X_8 corresponds to vanadium, X_9 corresponds to silicon and X_{10} corresponds to oxygen.

The methodology proposed is implemented for yield strength Rp_{02} and relative elongation E. To take out the models of these two target functions, 277 measurements that form the data matrix Rp_{02} (277, 10 +1), and - E (252, 10+1) have been used. Here the added column "1" is for the output target function Rp_{02} or E stored compactly in the matrix.

To optimize the computing process, the scheme, which having been processed for the particular case takes the following kind, is selected.

In numerical experiments that use models based on the chemical composition the noise can be expressed only in the change of the respective components. It is assumed to express noise Δ in the following way $\Delta_i = \frac{\overline{x}_i}{k}$ where further calculations are made for k equal to 100.

Here $\overline{x}_i$ is the mean value of relevant variable "i".

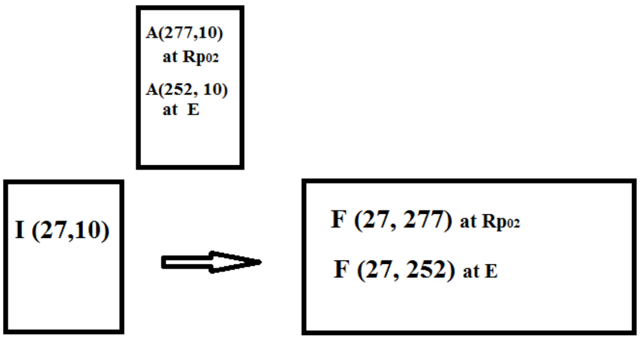

Fig. 1. *Organizing experiments with parametric planning with matrices I, A and F*

For level "1" of I (27,10) noise is subtracted from relevant x_i taking the value of $x_i - \Delta_i$. With level "2" no correction is applied, the value of x_i is preserved. With level "3" noise is added to relevant x_i taking the value of $x_i + \Delta_i$. In numerical experiments where models based on chemical composition are used, noise can be expressed only in the change of the respective components.

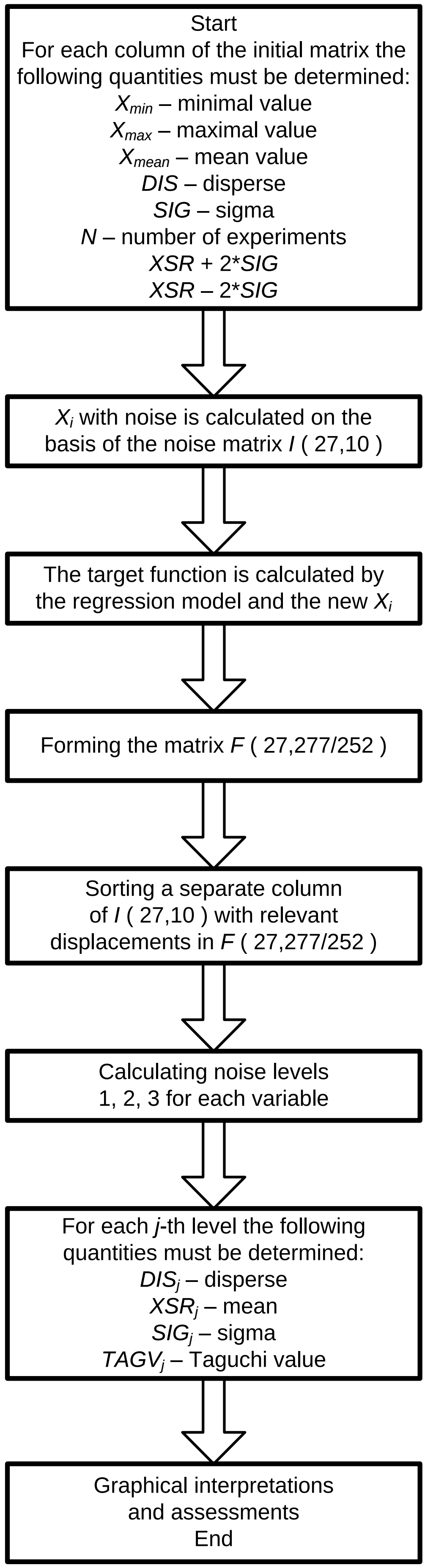

Fig. 2 *Computational algorithm*

Noise Δ is assumed to be expressed as follows $\Delta_i = \frac{\overline{x}_i}{k}$, where the further calculations are made for k equal to 100. Here $\overline{x}_i$ is the average value of the respective variable "i". In level "1" I (27,10) noise is subtracted from respective x_i taking the value of $x_i - \Delta_i$. In level "2" no correction is applied, the value of x_i is preserved. In level "3" noise is added to respective x_i taking the value of $x_i + \Delta_i$.

Thus, noise is expressed in the change of chemical composition. The calculation process is organized as follows:

A row of matrix I (27,10) is taken (for example, row 1 - I (1,10)). In this row level "1" is assigned for each x_i, i.e. noise will be taken out from each value x_i.

Thus F (1,1) of the matrix F (27,277) at Rp_{02} (F(27, 252) at E) is obtained from the first row of A (277,10). The same rule is applied to the rest of the series F (277,10) /F (252,10)/ and it forms F (27,277) /F (27,252)/.

It is continued with the next row of matrix I (27,10) performing the following sequence. Each row of matrix I (27,10) forms a relevant row of matrix F (27,277) /F (27,252)/.

Calculations are performed according to the following algorithm.

If we take the first column of matrix I (27,10) relevant to X_1, it is seen that the first nine rows correspond to level "1" of noise, the second nine lines correspond to level "2" and the third nine rows correspond to level "3" of noise. This makes possible to use the values of the first nine rows of matrix F (27,277) / F (27,252) / to calculate level "1", to use the second nine rows to calculate level of "2" and the third nine rows for calculation at level "3" for X_1. For other columns from 2 to 10 it is necessary to sort in ascending order Xi from I (27,10). After sorting the column obtains the kind of the first column. If changes are made with sorting, they are reflected also in matrix F (27,277) / F (27,252) /– fig.1.

After sorting of the respective variable, calculations for different levels can be made. It is continued with the next matrix row I (27,10) performing the following sequence. Each row of matrix I (27,8) forms a corresponding row of matrix F (27,277) / F (27,252) /. If we take the first column of matrix I (27,10) corresponding to the X_1 , it is seen that the first nine rows correspond to noise level "1" of noise, the second nine rows correspond to level "2" and the third nine rows correspond to noise level "3". That allows using the values of the first nine rows of matrix F (27,277) /F (27,252) / to calculate level "1", the second nine rows to calculate level "2" and the third nine rows to calculate level "3" for X_1. For the rest columns from 2 to 10 it is necessary to sort by ascending order of Xi of I(27,10). After sorting the column takes the kind of the first column. With sorting, if shifts are made, they are reflected in matrix F (27,277) /F (27,252)/. After sorting the corresponding variable it is possible to make calculations for different levels.

Variable	Input parameters	Noise level	
		R_{p02}	E
X_1	№ HT	1	2
X_2	Al	1	1
X_3	Mo	1	1
X_4	Sn	2	3
X_5	Zr	3	1
X_6	Cr	1	1
X_7	Fe	3	2
X_8	V	1	3
X_9	Si	3	3
X_{10}	O	3	1

Table 3 *Levels of noise factors for the research parameters*

After the analysis of assessments of the respective graphics for yield strength (R_{p02}) and relative elongation (E), the generalization of the solution is shown in Table3.

The conclusion that can be made on the boundary of yield strength R_{p02} based on the results in the table is that tin do not significantly affect the ultimate outcome within the range of variation examined. Zirconium, iron, silicon and oxygen influence significantly on R_{p02} as it is expected that these elements will change in direction to increase of their values. Aluminum, chromium, molybdenum, vanadium in direction to decrease of their values.

4. Search of optimal composition

As the experiment is numerical, it is possible to perform numerical optimization with the mathematical models obtained as the values of X_i are remained to change within the limits defined by the output data (Table 3).

From the performed Taguchi analysis (presented as a summary in Table 3) for the research quantity Rp 02 it is evident that the maximum of X4 (Zr) occurs at level 2; this means that X4 (Zr) must be maintained at a constant level. It is clear from the output data described in Table 1 that this parameter takes values in the range $0 \leq X4 \leq 11.0$.

Different methods for numerical optimization are described in [9]. The simplex method of Nelder and Mead with a deformable polyhedron has been selected for the purpose. It is a method of direct searching extremes, so it is suitable for the case of ravine surface of the target function.

After fixing X4 in the cited range optimization is applied to the rest of the parameters with in the range from Table 1. The values of the optimized parameters are shown in Table. 4. An increase in X4 leads to increasing the extremum value for Rp 02.

For elongation E the performed Taguchi analysis suggested fixing two variables X1 and X7.

Three cases were formed:

-Parameter X1 takes values in the range $1 \leq X_1 \leq 8$ as X_7 remains constant with a value of 0.15;

-Parameter X1 takes values in the range $1 \leq X_1 \leq 8$ as X_7 remains constant with a value of 2;

-Parameter X1 takes values in the range $1 \leq X_1 \leq 8$ as X_7 remains constant with a value of 1.

After optimization with the method of Nelder and Mead for various combinations of X_1 and X_7 it was clear that the increase of X1 leads to an increase of the extremum of E for each of the three cases. The obtained values are bigger than the biggest quantity in the output data in three cases.

This circumstance guarantees an improvement of these indicators.

An interesting result is obtained if model Rp 02 is calculated for the extrema values of E in the cases with fixed X_1 and X_7 – Table 4.

Parameters		Rp_{02}	
X_1	X_7	calculated F	F max data
1	0.15	868.8	945
0	1.0	2451.3	945
0	2.0	2627.5	945

Table 4. Optimal *parameters*

This indicates that there is a case where an increase in E leads to an increase of Rp 02 and this leads to the requirement for implementing an improvement of both of these criteria simultaneously, which proved that the task is feasible and executed..

Conclusion

The numerical experiment has proved the ability to improve the quality of Ti alloys 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 Rp_{02} 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.

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