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 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 \(b_{ij}\) 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.

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Table 1. Coefficients of regression models of the examined target parameters.

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<th>A</th>
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\( R_p \quad R = 0.9880 \)  \( F_{cal.} = 18.8637 \quad (p=0.05,54,25) > 1.8367 = F_{tabl} \)

\( A \quad R = 0.9906 \)  \( F_{cal.} = 24.2416 \quad (p=0.05,54,25) > 1.8367 = F_{tabl} \)


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.
References

Yield strength, Rp 02 [MPa]

Relative elongation (A [%])