

INVESTIGATION OF MECHANICAL PROPERTIES OF TITANIUM ALLOYS BASED ON GENETIC OPTIMIZATION AND PARETO FRONT

ИЗСЛЕДВАНЕ НА МЕХАНИЧНИТЕ ХААКТЕРИСТИКИ НА ТИТАНОВИ СПЛАВИ НА БАЗАТА НА
ГЕНЕТИЧНА ОПТИМИЗАЦИЯ И ФРОНТ НА ПАРЕТО

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Abstract: An approach to the study of the relationship between the extreme values of the mechanical properties of titanium alloys. The approach is based on the approximated dependence of the mechanical properties of the chemical composition of the alloy of the ANN model. Approximating dependencies are included in the genetic optimization model based on optimization algorithm NSGA II, which was built by Pareto - fronts, modeling the relationship between the studied mechanical parameters.

Keywords: METTALLURGICAL DESIGN, TENSILE PROPERTIES, COMPOSITION-PROCESSING-PROPERTY CORRELATION, APPROXIMATION WITH NEURAL NETWORKS, PARETO FRONT, NSGA II ALGORITHM

1. Introduction

The process of material selection gives meaning to a whole trend in the material science at the design stage. It is directly related to information integration of engineering activities and to their effectiveness, being related to methods for automated information processing.

The choice of material and the technology for its processing are necessarily concerned to formalize the product presentation and also in order to improve engineering automation. The purpose of this work is subjected to to this idea. It is based on a priori data used in the creation of approaches and software tools for the determination of control parameters of the examined system simultaneously assessing several of its contradictory parameters.

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 [1] [2], 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.

Introducing the dependencies between the extreme values of the physico-mechanical properties of titanium alloys can hardly be achieved based entirely on empirical research and also on the relevant statistical treatment of the results. In most cases, the experimental research can be difficult, too lengthy and much too expensive.

This work proposes a solution based on the use of a software model and techniques from the field of multicriteria analysis and optimization, and establishing regression relationships between the mechanical properties of the alloy and its chemical composition based on neural regression models.

At the base of the problematic links we find the set of non-dominated points with values of the investigated mechanical parameters - the so-called "Pareto front" and modeling relationships between the chemical composition and the mechanical properties with software tools. The task is presented as a typical multicriteria optimization problem. The main concepts in this task are described by the following relations:

General optimization problem - to be presented in the following form:

$$(1) \max(f_1(x), f_2(x), \dots, f_m(x)),$$

where:

$f_1(x), f_2(x), \dots, f_m(x)$ are the private optimization criteria (physical and mechanical characteristics);

$$(2) x \in D \subset R^n, m \leq 2, x = (x_1, x_2, \dots, x_n),$$

are the conditions defining the domain D vector solution $x = (x_1, x_2, \dots, x_n)$. In the specific task, the domain is given in the form:

$$(3) D : x_k \in [l_k, h_k] \subset R, k = 1, \dots, n, ,$$

where l_k and h_k are the lower and upper limits of the range of variation of each of the arguments (the percentage of the chemical element).

Relation of dominance between a pair of solutions $x^{(1)}$ and $x^{(2)}$ ($x^{(1)} \prec x^{(2)}$) - expressed in the following form:

$$(4) \forall i = 1, \dots, m \quad f_i(x^{(1)}) \geq f_i(x^{(2)}),$$

$$(5) \exists j = 1, \dots, m \quad f_j(x^{(1)}) > f_j(x^{(2)}),$$

i.e. dominance of $x^{(1)}$ to $x^{(2)}$ is when at least one of the criteria is a strict inequality (indicating orientation) for both alternatives, the remaining criteria in force non-canonical inequality (or at less equality).

Pareto-optimal set – the set of solutions $P^* \subset D$, non-dominated by any element of the set D . The Pareto-front is a graphic representation of the Pareto-optimal solution in the target space.

2. Methodology for solving the problem.

The definition of the purpose of the study leads to the formation of the general scheme of the model. The input parameters of the neural network are those of the alloy with composition and heat treatment according to Fig.1.

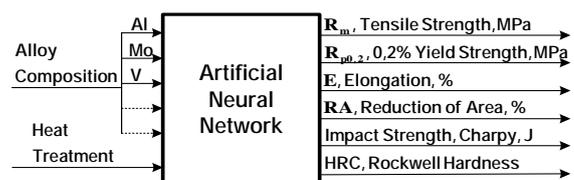


Fig.1. Input-output multicriteria research parameters.

Neural network (NN) input parameters are the chemical composition and the types of heat treatment.

The composition includes the most often used alloying elements, namely Al, Mo, V, Sn, Zr, Cr, Fe and O.

The methodology for solving the problem is based on some verified and validated research capacity [1]. It includes two main components:

- Modeling the links between mechanical parameters via neural models [1], [2];
- Applying a genetic model for multi-criteria optimization and constructing the Pareto front [4].

The approach of combining these two concepts has proven to be effective. It allows to overcome some limitations related to the inability easy to obtain good approximations of the relations between the problem variables, and also with respect to the search for appropriate (or optimal) solution in the definition domain of the problem. Both applied paradigms combine modern means of finding the solution.

Modeling relationships between the problem variables is performed by approximation with neural networks of the "multilayer perceptron" type with a single hidden layer. For this purpose we used an established software tool - package Statistica v.10 of corporation StatSoft. The inputs to the network are the values of percentage of the following elements: Al, Mo, Sn, Zr, Cr, Fe, V, Si and O. Another nine inputs to the neural model are determined for the nine nominal levels (with values 0 and 1) of parameter *HT*. The output of the model is a single value for the approximated mechanical parameter $f_i(x)$. The number of neuron models corresponds to the number of the modeled relationships between the chemical composition and the mechanical properties. The complete description of the methodology for modeling and analysis of the results is subject to another presentation in a separate publication.

The formation of the Pareto front, even in cases with just two competing criteria, is not at all a simple problem. The aspects of this problem are:

- "Non-convex" front - in this case the construction of the front via the direct use of a series of points calculated on the basis of the decisions taken in the domain space of the problem is impossible. Such is the case with Pareto-fronts approximating the links in the investigated problem.
- Concentration of ("clustering") the calculated points from the front in several clusters with significant empty spaces between them. This is a common problem of genetic algorithms used to determine the Pareto-fronts.

To overcome these problems there was used the popular algorithm to construct Pareto-front based on genetic optimization NSGA II (a non-dominated sorted genetic algorithm), described in [4] and [5]. Characteristic of this algorithm is the inclusion of a specific advanced procedure for building a set of non-dominated solutions and taking under consideration the distance (the compression ratio) between the calculated points [4] up this front. The algorithm is well-researched and successfully applied to the solution of problems of this type. In order to use it in our case, we made in it some improvements:

- Reduce the minimum distance between the points forming the front (in order to achieve their even distribution along the line forming the front);
- Filtration of the solutions frequently occurring with the same value - also in order to cover the whole range of possible values in the front and to improve the performance of the genetic algorithm.

The introduced algorithm is implemented as software code in programming language Java.

3. Survey results.

Data for constructing the studied relationships in the software model are taken from [3]. There have been approximated the values of parameters $Rp_{0,2}$, *E* and *IS*. Some of the research parameters manifest a significant scatter and low correlation between observed and modeled values, probably due to insufficient accuracy of the experimental results.

Despite the incompleteness of the data and their possible lack of precision there was achieved satisfactory approximation (the coefficient of correlation between observed and modeled values of *R* is in the range from 0.79 up to 0.87).

Approximating dependencies (neural regression models) are included as source code in the basic software model that implements the algorithm NSGA II [4]. The results of modeling the Pareto fronts of the parameters Rp_{02} , *E* and *IS* are shown in Fig. Fig. 1, 2, 3, 4 and 5. Fig. 6 shows a three-dimensional graph of the relationship between the parameters Rp_{02} , *E* and *IS*. Unfortunately, due to the peculiarities of the algorithm at this stage, it was impossible to obtain a three-dimensional graph of the general Pareto-front for these three parameters.

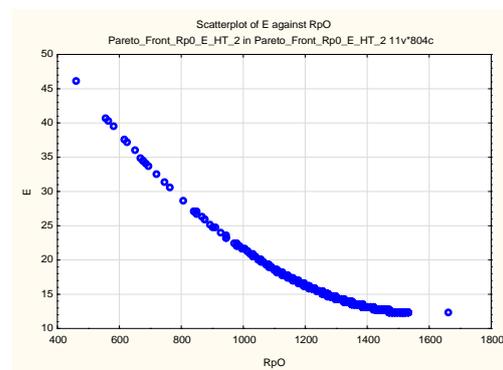


Fig.2. Pareto-front for parameters Rp_{02} and *E* for $HT=2$.

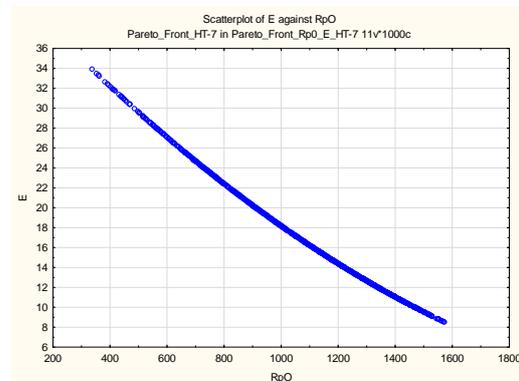


Fig.3. Pareto-front for parameters Rp_{02} and *E* for $HT=7$.

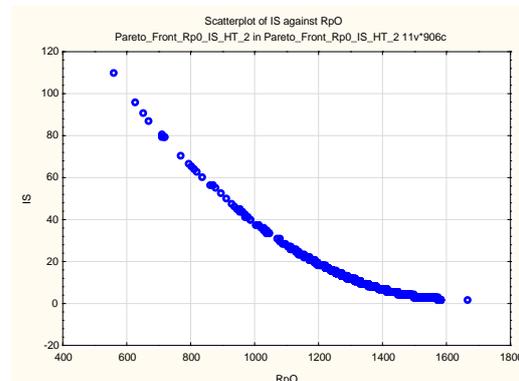


Fig.4. Pareto-front for parameters Rp_{02} and *IS* for $HT=2$.

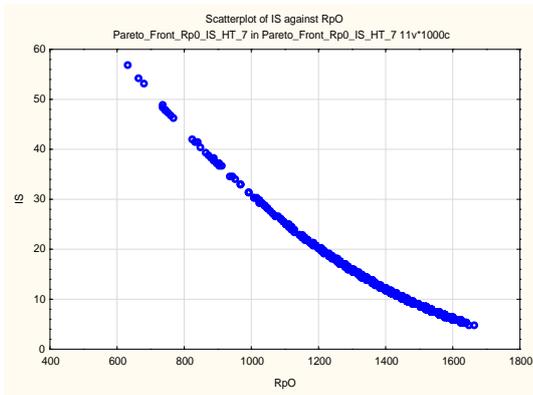


Fig.5. Pareto-front for parameters Rp_{02} and IS for $HT=7$.

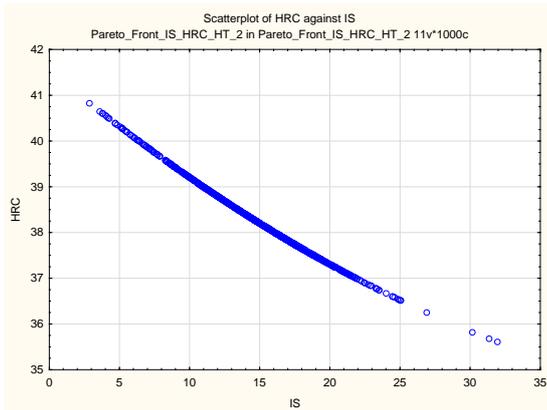


Fig.6. Pareto-front for parameters $Rp_{0.2}$, E and IS for $HT=2$.

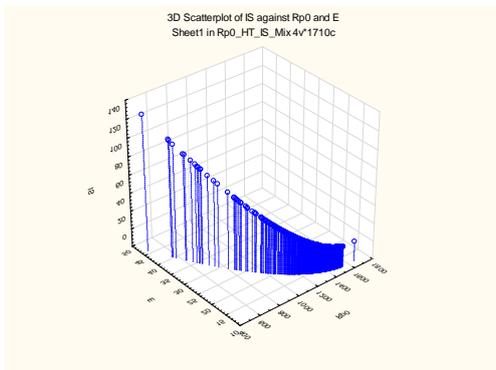


Fig.7. Pareto-front for parameters Rp_{02} , E and IS for $HT=2$.

The achieved results show that the proposed method can quite successfully be used to determine the substantial relations between the extreme values of the mechanical parameters.

Complementation of the database from the experimental measurements from [3] will allow improvement of the software model and the future refinement of the results. The proposed approach and the established relations may be used in the engineering practice.

4. Conclusion.

The new method offers a realistic possibility to significantly reduce the cost and time to predict chemical concentrations and multiple properties of a class of Ti alloys so that the new alloys will have improved properties.

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 cases of different titanium alloys. Pareto front is constructed and analyzed related to the system 'composition-processing- properties'.

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