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# MODELING AND PREDICTION OF COMPOSITION PROPERTIES OF TITANIUM-BASED ALLOUYS MEANS OF ARTIFICIAL NEURAL NETWORKS

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***Key words:*** *metallurgical design, modelling ANN, optimization, titanium alloys.*
***Abstract****: This message is a recommendation for an approach for adequate prediction of the properties of titanium-based alloys with defined composition and mode for heat treatment.*

*Based on a priori determined optimal experimental compositions and beyond the used proxy database, an approximation is defined most accurately fulfilling the determined conditions.*

*The approximation is carried out by means of neural models. The approach allows for a more precise automated prediction of the alloy features according to the composition and the heat treatment of the alloy.*

## 1. Introduction

Innovation and development of new technologies and the widespread use of modern materials is important for economic development. Increasing requirements for quality products in the production of materials necessitates the use of advanced tools for analysis and modeling.

Scientific references present a variety of models with varying degrees of complexity, mathematical description and with varying degrees of correlation between the predicted and the actual value in the field of metallurgy.

The models are a reflection of the system with logical connections between the variables describing them. The determination of the interaction of these variables allows to carry out an analysis of the behavior of the model in certain conditions.

Computational models are sets of information about the materials related to their properties, formulated as mathematical rules. Consequently modeling formalizes the description of these properties limited to a set of properties expressed by the mathematical model as formulas and relations [1-3].

The application of artificial neural networks is an approach with an increasingly important role in modeling the process. The main advantage of this method is that in most cases the development of the model with artificial neural networks leads to the analysis of long measurement data in databases as well as to processing parameters measurable in the laboratory.

The present study aims to recommend an approach for adequate prediction of the properties of titanium-based alloys at the given composition and heat treatment regime. An approximation is defined most accurately fulfilling the determined conditions with predetermined optimal and experimentation compositions outside the used database.

## 2. Formulation of the problem.

Stages of creation (design), research, production and implementation of titanium alloys involves the specification of: the chemical composition, the parameters of the heat treatment mode and the final mechanical properties.

Alloys with their components and features for heat treatment are a technological object and therefore it is possible for them to apply the approach with modeling their properties and optimizing the composition depending on the particular application. The procedure for argumented refinement of the chemical composition by the number and the quantity of alloying elements is relatively new related to search of dependencies with the final mechanical properties.

Artificial Neural Networks (ANN) [5 - 7] are very effective as a computational tool for solving problems without alternative. This is due to the advantage of neural networks over other computing systems that calculations with ANN are in parallel, thus exceeding successive calculations with their computational speed. Neural networks always act as a system of connected elementary units where all elements are important for the network function. One of the consequences of such activities is known as “graceful degradation”, the possibility of correct operation at the destruction of much of the ANN elements. The current trend of increasing use of ANN leads to more complex and intelligent design tools.

The research is funded on a database with 300 number of alloys, appearing in [2]. The cited database contains the relations between the chemical composition and the mechanical properties of the alloys included in it.

The design of the alloy is based on modeling neural networks that approximate satisfactorily the relations between the chemical composition of the alloy and the mechanical parameters yield strength $Rp_{0,2}$ and elongation E.

**Table 1.** Range of variation for the elements of the scope steels.

| Element | 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 |

For this purpose the following conditions were applied for modeling:

a. Type of neural models - the study is mainly focused on classic FF (Feedforward) models such as multilayer perceptron (MLP). The investigated sample with experimental data includes 300 observations of alloys with different compositions and corresponding values of the parameters Rp 0,2 and E.
b. The study was conducted with the specialized software StatSoft Statistica 10, module Artificial Neural Networks [8].

For each of the neural models in the research the output experimental data are divided into three sets: Training, Test and Validation, in which the numbers of the included observations are in the ratio 70%: 15%: 15%. Observations included in these sets are chosen randomly.

For modeling the relation between the composition of the alloy, and each of the parameters $Rp_{0,2}$ and E there were tested in each case 300 separate neural model, differing in their configuration (the number of internal neurons) and the activation functions of the neurons in the internal layer and output layer.

When designing MLP neural model, the following activation functions were used:

- Identity: $f(x) = x$,
- Logistic (sigmoid) function: $f(x) = \frac{1}{1-e^{-x}}$,
- Hyperbolic tangent (Tanh): $f(x) = \frac{e^{x} - e^{-x}}{e^{x} + e^{-x}}$,
- exponential function (Exponent): $f(x) = e^{-x}$.

The quality assessment of the examined neural models is based on the following indicators:

- Correlation coefficient between observed and modeled output values of the network:

$$R = \frac{\sum_{i=1}^{N}(y_i - \bar{y})(t_i - \bar{t})}{\sqrt{\sum_{i=1}^{N}(y_i - \bar{y})^2 . \sum_{i=1}^{N}(t_i - \bar{t})^2}},$$

where $N$ is the number of elements (observations) per set (training, test or validation), $y_i$ is the calculated output of the network, and $t_i$ is the observed value of the approximated parameter, $\bar{y}$ and $\bar{t}$ are statistical means for modeled and observed output values (for the respective set),

- Error function - the sum of the squares of the differences (SumOfSquaRp0, 2s) between observed and modeled values at the output of the network:

$E_{SOS} = \sum_{i=1}^{N}(y_i - t_i)^2$, where the denotations are as above.

### 3.Results of the research

Based on the survey for each of the parameters $Rp_{0,2}$ and E there were selected for comparison four neural models having the best indicators of quality (R and $E_{SOS}$).

The data for the selected neural models of type MLP are shown in Table 2 for parameter $R_{p0,2}$ and Table 3, respectively, for the parameter *E*. The tables contain the values of the correlation coefficient *R* and the error $E_{SOS}$ respectively for the training, test and validation sets, and also the type of the activation function in the internal (hidden) and output layers of the neural model.

**Table 2. Neural networks of type MLP approximating parameter $Rp_{0,2}$.**

| Type of network (model) | R Learning | R Test | R Validation | Esos Learning | Esos Test | Esos Validation | Hidden layer | outputs |
|---|---|---|---|---|---|---|---|---|
| MLP 18-12-1 | 0.83395 | 0.74753 | 0.657366 | 9317.23 | 14438.07 | 18852.15 | Logist. | Logist. |
| **MLP 18-17-1** | **0.83001** | **0.76056** | **0.690320** | **9502.65** | **13157.55** | **15642.37** | **Tanh** | **Exp** |
| MLP 18-4-1 | 0.82326 | 0.77670 | 0.691622 | 9035.31 | 12147.37 | 15094.05 | Exp | Identity |
| MLP 18-13-1 | 0.77847 | 0.75439 | 0.686471 | 12061.65 | 13378.37 | 16388.66 | Tanh | Tanh |

**Table 3. Neural networks of type MLP approximating parameter E**

| Type of network (model) | R Learning | R Test | R Vali-dation | Esos Learning | Esos Test | Esos Validation | Hidden layer | outputs |
|---|---|---|---|---|---|---|---|---|
| **MLP 18-11-1** | **0.782609** | **0.510805** | **0.498148** | **9.025336** | **18.79139** | **47.50873** | **Tanh** | **Exp** |
| MLP 18-16-1 | 0.559748 | 0.610145 | 0.421234 | 17.61457 | 16.00133 | 11.37933 | Identity | Exp |
| MLP 18-8-1 | 0.541575 | 0.508431 | 0.336787 | 16.72096 | 22.46308 | 16.04996 | Tanh | Identity |
| MLP 18-4-1 | 0.543187 | 0.528061 | 0.334364 | 16.71263 | 21.79676 | 16.47646 | Idetity | Tanh |

Figure 1 and Figure 2 are two-dimensional diagrams comparing the observed and modeled values for $Rp_{0,2}$ and E for type networks MLP 18-17-1 (approximating parameters Rp0, 2) and MLP 18-11-1 (approximating parameter E ).

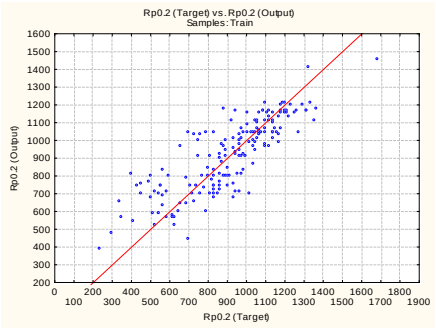


**Fig.1 Network type MLP18- 17- 1, approximating parameter $Rp_{0,2}$, comparing observed and modeled**

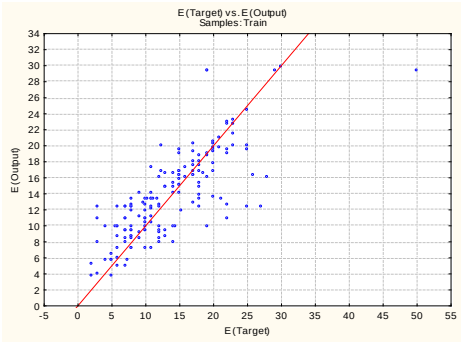


**Fig.2 Network MLP 18-11-1 approximating parameter E, comparing the observed and modeled**

The results of the predicted values of the parameters $Rp_{0,2}$ and E, calculated on the basis of the data (2 experimented compositions)

| Grade/Composition | Al | V | Mo |
|---|---|---|---|
| BT16 | 2.7 | 4.5 | 5.0 |
| outputs | **$Rp_{0.2}$ [MPa]** | **E [%]** | |
| Model | 768.87 | 15.044 | |
| Catalogue data | 850-950 | 14 | |

| Grade/Composition | Al | V | Mo | Cr | Fe |
|---|---|---|---|---|---|
| ВТ22И | 5.15 | 4.75 | 4.75 | 1.35 | 1.0 |
| outputs | **$Rp_{0.2}$ [MPa]** | | **E [%]** | | |
| Model | 821.27 | | 13.52 | | |
| Catalogue data | 900-950 | | 12 | | |

**Conclusion.**

Relying on extensive knowledge from companies, on various databases in the research of the relationships between them, it is possible to make valuable suggestions improving the parameters of the created products and technologies. 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, using prior information of data linking composition, processing and properties. This methodology is the way to design alloys at a redetermined database.Its main advantage is the possibility to create and design alloys of predetemined user requirements about the set of properties, providing the specific application. Conceptually, this approach is applicable to design and optimization of random alloys, since in practice it is independent of the used database. The approach extends our revious research and ir covers additional objectives, such as the impact of various types of heat treatment.

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# МОДЕЛИРАНЕ СЪСТАВА И ПРЕДСКАЗВАНЕ НА СВОЙСТВАТА НА СПЛАВИ НА ТИТАНОВА ОСНОВА С ПОМОЩТА НА ИЗКУСТВЕНИ НЕВРОННИ МРЕЖИ

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***Ключови думи:*** *металургично проектиране, ANN моделиране, оптимизация, титанови сплави*

***Резюме:*** *В съобщението е предложен подход за прогнозиране на механичните свойства на сплави на титанова основа при зададен състав и режим на термично обработване. По предварително определени оптимални експериментирани състави, извън използваната за апроксимация база от данни, се определя апроксимация най-точно отговаряща на определените условия. Апроксимацията се извършва посредством невронни модели. Подходът дава възможност за по-точно автоматизирано прогнозиране на свойствата на сплавите в зависимост от състава и термичното обработване на сплавта.*