SOFWARE MODEL FOR SELECTION OF THE APPROPRIATE CHEMICAL COMPOSITION OF TITANIUM ALLOYS UNDER DEFINES REQUIREMENTS FOR MECHANICAL CHARACTERISTICS

СОФТУЕРЕН МОДЕЛ ЗА ИЗБОР НА ЦЕЛЕСЪОБРАЗЕН ХИМИЧЕСКИ СЪСТАВ НА ТИТАНОВИ СПЛАВИ ПРИ ЗАДАДЕНИ ИЗИСКВАНИЯ КЪМ МЕХАНИЧНИТЕ ХАРАКТЕИСТИКИ

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Abstract: *The paper presents the application of modern computational approaches in determining the appropriate chemical composition of titanium alloys . Discusses three types of problems for the selection of the chemical composition of alloy at set requirements for mechanical properties . Tasks are solved in a different formulation of the target criteria . The proposed solutions are based on software model using approximation with artificial neural networks and genetic optimization algorithm.*

Keywords: ….

1. Introduction

The numeric design of the composition and the operative mode in metallurgy is a problem of particular complexity due to its multivariate nature. There is a need for continuous improvement of the whole industry in order to improve the properties of alloys with broad application.

Very small amounts 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 [1].

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. That is why in science, probably the biggest asset comprises the rational ideas that jointly with the appropriate scientific infrastructure is implemented to specific technologies. The criteria evaluating various parameters of technology and products, as well as the methods for targeted search, refine initial ideas, and therein lies the essence of design with optimization.

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 [2] [3], 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.

The traditional alloy-development strategy consists of producing numerous samples with varying composition and set of the elements, the processing mode included, to { determine | define } an alloy with optimal properties [Campbell and Olson, 2001].

The approach resulted in high costs of experimentation [4].

This is the reason that the methods of directed search and the 'trial and error' method reside on, the highest 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.

Compared to physical models, the advantage of statistical models lies in their ability to survey complex, multi-scale information in a timely and effective manner, even when well-established physic theories and models do not exist.

The results from the analysis of the models and the optimization can provide a guideline for further experimental and computational investigation [8].

The present paper aims at exploring and illustrating the possibility of using modern computational tools to solve specific engineering problems in the processing of titanium alloys.

The presented problem is formulated in the following way - determine an appropriate chemical composition of a titanium alloy from the elements Al, Mo, Sn, Zr, Cr, Fe, V, Si and O.

The percentage of elements in the alloy is represented by the arguments of the target function $X=(x_1, x_2,.., x_n)$. Three specific subproblems are formulated and examined with respect to the appropriateness of the decision of the most common problem:

- Define the requirements for the mechanical properties of titanium alloys as specific ("precise", "point") target values g_i (i = 1, ..., m);
- Define the requirements by the boundary (minimal or maximal) values (as unilateral restrictions);
- Define the requirements for the mechanical parameters in the closed interval (as bilateral restrictions on the parameters).

In the **first** case is solved an optimization problem of the form:

$$\min Z_1(X) = \sum_{i=1}^{m} (g_i - f_i(X))^2 , \quad (1)$$

where:

q_i – is the target value of the i-th mechanical parameter: i = 1, .., m;

$X = (x_1, x_2, ..., x_n)$ – is a vector of the decision (with the values of the arguments for the percentage of the elements in the alloy);

$f_i(X)$ – are links between the values of the arguments ($X = (x_1, x_2, ..., x_n)$) and the mechanical parameters of the alloy (obtained by approximation of the experimental data).

The problem domain is formulated by a set of bilateral restrictions:

$$D: x_i \in [l_i, h_i], i = 1,...,n , \quad (2)$$

where l_i and h_i (i = 1, ..., n) are the lower and upper limits of the range, wherein is defined the i-th argument (the percentage of relevant chemical element).

The **second** problem is solved with the following formulation:

(3) $\min Z_2(X) = \sum_{i=1}^{m} w_i.\varphi_i(X),$

where:

(4) $\varphi_i(X) = \begin{cases} 0, & f_i(X) \text{ comply with the requirements} \\ |g_i - f_i(X)| & \text{otherwise} \end{cases}$

w_i – are assessments for violation of the requirements ("penalties"), which are determined separately for each of the mechanical parameters (criteria).

$f_i(X)$ - are approximations of the mechanical properties (as in problem (1)).

The problem domain is as above (2).

The third task is essentially a variant of the second, which limits the mechanical parameters are bilateral.

2. Methodology for solving the problem.

The considered tasks are based on research and results published in [1]. The methodology for solving problems is similar. It includes two basic approaches:

- Approximation of the relationships between the chemical composition of the alloy, and the mechanical characteristics based on neural models of the type of multi-layer perceptron (a method presented in [3]).
- Applying a genetic optimization algorithm ([6][7]) for determining an appropriate composition of the alloy - for each of the above-mentioned problems. The genetic algorithm is composed by the procedure described in [3].

The proposed methodology overcomes the difficulties with the usage of relations between the problematic parameters in an explicit analytical form and the classic optimization methods. The methodology is implemented in software code written in the language C, as an experimental software model (the scheme in Fig. 1).

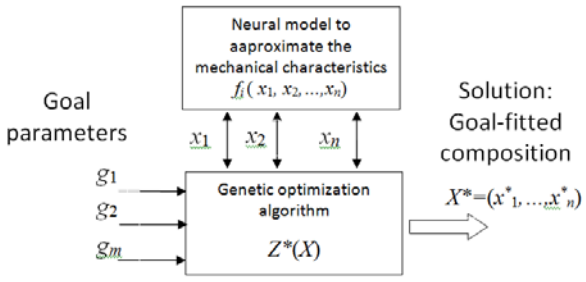

Figure 1. *Scheme of the software model.*

3. Experimental results.

Here are given some of the results obtained after series of experimental applications of the software model. The problems are applied to select the mechanical parameters $Rp_{0.2}$, E, IS and HRC, where the approximation relations give the most reliable results. Data for constructing the studied relationships in the software model are taken from [3].

Table 1 and Table 2 consistently present the mechanical parameters and the alloy composition according to Problem (1); Table 3 and Table 4 – the mechanical parameters and the alloy composition under requirements in the form of unilateral constraints; Table 5 and Table 6 – the mechanical parameters and the alloy obtained by imposing minimal and maximal constraints on the mechanical parameters.

The table shows the values of the target conditions (requirements) generated by the model values, the value of the goal function and the chemical composition of the alloy.

Table 1. *Target values of physical and mechanical parameters Rp02, E, IS and HRC and results from the optimization of Problem (1).*

Solution No	Initial requirements	Results	Deviation (Goal function)
1.	Rp0.2 = 950 E = 35 HT =2	Rp02 = 9.49 85315417 E = 35.000895290	1.076700256161e-008
2.	Rp02 = 800 IS = 35 HT = 2	Rp02 = 8.04.08046962 IS = 32.330481643	7.1137050227e-004
3.	HPC = 25 IS = 35 HT = 2	HPC = 25.001246681 IS = 35.000952059	8.5996124444e-010

Table 2. *Chemical composition of the alloy related to the decisions in Table 1.*

Sol. No	Chemical composition [%]								
	Al	Mn	Sn	Cr	Zr	Fe	V	Si	O
1.	0.12280648	1.40079958	5.51292458	3.1035798	4.093234	1.872463	7.493835	4.513992	2.0005951
2.	0.02685628	8.51100192	0.06378368	0.0067140	1.099127	4.991254	1.406257	0.016751	0.24967650
3.	0.68263801	9.66414380	8.45167394	3.3211157	2.652058	4.965371	0.145275	0.082504	0.2307855

Table 3. *Target values of physical and mechanical parameters Rp02, E, IS and HRC, and results from the choice of Problem (2).*

Solution No	**Initial requirements**	**Results**	**Deviation (Goal function)**
1.	Rp02 > 950 E > 35 HT = 2	Rp02 = 1.2803199668e+003 E= 4.8938539044e+001 Ht=2	0.0
2.	Rp02 > 1050 IS > 35 HT = 2	Rp02 = 1341.6185481e+003 IS = 33.139429441e+001 HT = 2	1.8605705586
3.	HRC > 40 IS > 35 HT = 2	HRC = 43.428584903 IS = 35.831069211 HT = 2	0.0

Table 4. *Chemical composition of the alloy related to the results in Table 3.*

Sol. No	Chemical composition [%]								
	Al	Mn	Sn	Cr	Zr	Fe	V	Si	O
1.	1.8936124	0.01556443	0.504898220	9.76595355	7.33109530	3.902914	0.105746	0.40852	0.112495
2.	0.0236823	14.948728	0.018799401	0.0701623	10.979522	3.99333	3.81054	4.99223	0.248327
3.	1.4412060	12.174138	5.046632282	3.5812860	9.5890377	4.81956	7.10196	0.44746	0.246832

Table 5. *Target values of the physical and mechanical parameters Rp02, E, IS and HRC and results from the choice of setting bilateral requirements.*

Solution No	**Initial requirements**	**Results**	**Deviation (Goal function)**
1.	Rp02 = [950,1200] E = [35,40] HT = 2	Rp02 = 1.171.3229999 E = 36.359591800e+001 HT = 2	0.0
2.	Rp02 = [950,1200] IS =[30,35] HT = 2	Rp02 = 1199.6942091 IS = 32.738526176	0.0
3.	HPC= [35,40] IS = [25,30] HT = 2	HPC = 39.353021119 IS = 29.626693242	0.0

Table 6. *Chemical composition of the alloy related to the decisions of Table 5.*

Sol. No	Chemical composition [%]								
	Al	Mn	Sn	Cr	Zr	Fe	V	Si	O
1.	6.30463576	10.0985747	0.21820734	7.7806024	1.1971194	1.563393	7.493820	0.345164	0.084156315
2.	0.02002014	11.3794366	0.02014221	0.0647907	10.955353	4.957223	0.699942	0.321832	0.249633777
3.	0.42066713	10.6305124	0.76204718	6.7080294	3.4221621	2.516608	11.68614	0.043824	0.208696241

4. Conclusion.

This research is also an attempt to predict the concentrations of the majority of alloying elements, so as to create alloys with desired set of properties. This design concept was tested using experimental data. Thus it was shown that the approach has the potential to identify new compositions with significantly improved defined properties.

The new alloy-design concept uses a combination of a multicriteria algorithm and a stochastic optimization to predict mechanical properties of the explored alloys.

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