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CONTRIBUTION TO THE 'MATERIALS GENOME INITIATIVE'WITH NUMERICAL METHODS FOR METALLURGICAL DESIGN

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Abstract:*This generalized research is devoted to numerical approaches to identify effective solutions in the field of metallurgy. Approaches to obtain the optimal combination of chemical composition and heat treatment to achieve certain properties are of fundamental importance for the realization of an effective project. They are at the basis to design or improve new alloys and the associated with them costs.*

Effective solutions for rational alloying alloys are able to increase the strength / to reduce the weight while maintaining or reducing the cost of the alloy. The determination of these solutions, however, goes through numerical methods, algorithms and procedures that do not depend on the used databases.

The research of the genome of the material in this generalization of publications, relies entirely on statistical processing and it is aimed at creating opportunities for predicting the mechanical parameters as a function of the chemical composition and the heat treatment parameters taking into account the relevant boundary conditions.

1. INTRODUCTION

An overview of innovative solutions to choose and synthesize iron-based materials is available in [1]. The cited therein databases select the material only from the previously created databases. These databases cannot be used directly in the optimization of the composition. They can only provide the necessary information for the class of materials at the specified heat treatment.

To determine how to deal with the issue of improving the properties of the chemical composition and processing through the methods of modeling and optimization, in [1] there were considered methods for preparation of alloys. Multi-parametric regression analysis is one of the most popular methods for data processing. It has been applied successfully in the research of a set of relations in the metallurgical industry. Due to the nature of each statistical analysis, the coefficients of the restrictions caused by the regression analysis are known only approximately.

In this respect, competing metallurgical companies develop software tools and approaches, supporting their work in finding rational solutions on the final properties of the products. It is impressive in the analysis of the bibliography about the simultaneous improvement of the strength and the ductility that alloying or processing parameters do not guarantee much data. This fact in the subsequent studies should be considered for the creation of mathematical models to analyze the objects for the observed metallurgical process. This is an important motive in the implementation of future targets for research relevant to a new generation of steels.

The author of the present research has reported [2,3], related to the requirements of the steel of the martensitic class related to a specific application.

Automated design of the composition and the procedures of processing ferritic steels of all generations is possible to realize with modern computing resources. The innovation of these technologies for the production of new generations of steel and also the widespread use of modern materials, are important for the economic development and for the ways to increase security, too.

The approbated approach is realized at the methodical level.

The purpose of the cited authors' works is to cover the following two problems :

- Creation of nonlinear analytical models for control of the properties of steels, depending on the chemical composition in the heat-treated condition. For this purpose there has been developed a procedure and software for analysis of the research parameters;
- Theoretical research by means of modern computer technology and software, of the influence of individual elements on the value of the final properties via artificial neural networks for approximation and also by a genetic algorithm for optimization.

It is expected that the defined problem will produce a solution joining control parameters together with the quality parameters that will provide exceeding certain thresholds and also obtaining certain properties thus satisfying user requirements. Multi-criteria optimization realizes the possibility to achieve a compromise between characteristics of contradictory trends.

2. ANALYSIS AND OPTIMIZATION OF SELECTED QUALITY INDICATORS БЩО

The first contribution to the 'MGI' is adaptation of the method of shifting constraints for the purpose of multicriteria optimization [4,5,6].

Fig.1. presents a sample surface of the response for changing the quality indicator due to depending on the values of the technological inputs .

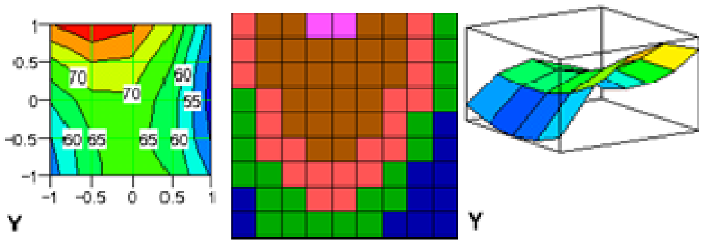

Fig.1. Graphical interpretation of single-criteria optimization problem with two factors of change.

The usual practice analyses such surfaces graphically via contour diagrams determined by equilevel lines. Thus it is possible to determine graphically coordinates of values for technological parameters with local or global maxima or minima of the goal parameter.

The scalarization of the problem for MKVR passes through two stages:

Making criteria dimensionless values (thus making them comparable);

Constructing a generalizing function /filter/.

The general scheme of the approach and the algorithm of this a priori approach is presented in [4].

A single- criteria problem is solved unifying criteria according to a determined dependency on the basis of which a non-dominated solution is obtained.

It is proven in [5] that solutions for average, geometric-mean and minimax filters are effective points from the set of non-dominated solutions.

The presented numeric approach to solve single- and multicriteria problems is applied for solving a set of problems in the domain of material knowledge. The approach is applied after the formulation of regression models for the multicriteria problem.

A computer system is designed on the basis of the numeric approach which enables reliable solutions for welding, galvanic ironization and chemical-thermal processing [7]. This software automates calculations and extremely easy defines effective solutions with different scalarizing functions.

The proposed solution performing these requirements meets the min-max effective point. It is determined after discretization of variables with some precision and constructing a transform with the lowest value of the research criteria. Compiled function subsequently maximize, which determines the value of the control variables and the corresponding values of the individual target parameters. Constructed generalized function afterwards is maximized thus determining the values of the control quantities and the values of various different goal parameters.

Multicriteria approach is applied to select the material and the mode of ion nitriding for a given class of heat-resistant steels [7]. The solution lies in the choice of a steel from a given class and the mode of its processing, ensuring the highest operational durability, taking into account the energy consumption of the technology. A software solution for building tools for decision-making is valued at how friendly it is user-oriented.

The proposal to the user to work not in the plane of the criteria but in the plane of the variables and also the usage of different up to five-six color constraining intervals proved to be too unusual. These two prerequisites, however, are able to implement very useful analysis performed for different processes, at this stage, with up to four variables.

3. TAGUCHI METHODOLOGY APPLIED TO THE STEEL DESIGN

The second contribution [8] in the development of methods for metallurgical design is associated with the Taguchi methodology for analysis of the selected quality parameters.

In [9] there is optimization of steel compositions including all 5 strength and plastic characteristics that are ensured with experimental data; regression and neural models were identified.

Below is described the possibility to model and the results from modeling by regression analysis.

With respect to the objective problem, for each of the mechanical properties of the steels there are identified nonlinear regressions of the form:

$$f_i(x) = b_{00}^i + \sum_{j=1}^{8} b_{j0}^i x_j + \sum_{j=1}^{8} \sum_{l=j+1}^{8} b_{jl} x_j x_l + \sum_{j=1}^{8} b_{jj}^i x_j^2$$

Based on the Taguchi methodology, an experiment is being performed, modeled via developed by him orthogonal matrices. The experiment can be realized in two ways:

- Actual experiment implying results for processing;
- Numeric experiment in the presence of adequate regression models.

The adopted by us experiment is numeric and through it is possible to realize a numeric optimization with the obtained mathematical models, Xi is allowed to vary within the bounds set by the output data.

For this goal there has been selected a simplex method of Nelder and Mead with deformable polyhedron. This method was chosen because it is a method with a direct search for the extremum and it is suitable for the ravine surface of the target function.

The fact that some of the variables are not altered i.e. they retain their initial values, requires to proceed with the optimization individually for the chemical composition of each steel. There the specified above Xi maintain their initial level, and the optimization is carried out by modifying the rest of values.

In this way there are performed ninety different chemical optimizations with ninety different chemical compositions and in either case we obtain a different value of the extremum – the maximum. The number ninety is associated with the compositions from the database.

Then all the maxima are sorted in ascending order and we choose the ones satisfying the pledged desire to be bigger than the biggest in the source data. Such an approach is justified, because if the problem is examined in terms of the technology, the single optimization is the improvement of a single really existing alloy that has proved it's belonging to a given class. It is easier to upgrade anything existing, rather than create a new one. If the problem is examined from the point of view of optimization, then we have the case to search the extremum from many starting points, something recommended in search of global extremum.

4. METALLURGICAL DESIGN IN A SMALL DATABASE

The third contribution is related to the numerical procedure to determine the optimal composition using a limited-volume database with the same treatment [10]. The purpose of this trend is to propose a numeric procedure enabling the determination of the optimal composition of the alloy with a small-volume database of compositions and their properties for one and the same treatment. The multicriterial problem is solved via an algorithm described in [11] on the basis of which there are determined effective solutions for the yield strength greater than 680 MPa and the elongation A = 12%. The innovation of this approach is a significant reduction of the a priori information due to the reduction of variables from eight-ten up to one. This favors the experiment in metallurgy, which is expensive and the information from it is difficult to reproduce.

The procedure has been tested for a class of alloyed steels with application in power mechanical engineering. There has been obtained an optimal composition of the steel, ensuring the properties: yield strength Rp02 > 600 MPa and elongation values of A> 11%. The presented multicriteria decision of the established properties, needed for the design, are expressed via a generalized parameter of the chemical composition of the alloy. The research was carried out with different linear combinations of the generalized parameters of the chemical composition and it can be applied for alloys not only of ferrous materials .

5. METALLURGICAL DESIGN USING ANN APPROXIMATION

The fourth contribution to the metallurgical design is the optimization approach [11] based on the choice of neural models for approximation of the physical and mechanical parameters Rm, Rp02, A, Kcu and HB. There has been examined a significant number of (over 1000) various neural models with different number of nodes in the hidden layer and with different activation functions. There are selected those neural models that manifest the best quality of approximation, through multiple iterations defining activation functions and the number of neurons in the intermediate layer. A multicriteria approach is used taking into account the mutual dominance of criteria and the evaluation of the normalized weights with which they participate in the complex optimization criterion. The weights of private criteria may be changed according to the needs and the preferences of the designer, and also according to the intended purpose of the alloy. There has been used the described in [12] a universal and flexible optimization algorithm based on a genetic approach. In practice, the algorithm does not depend on the type of the approximating relations between the private criteria, it does not depend on the structure and the type of the complex optimization criterion. The algorithm may be used in a very wide range of conditions and requirements related to the properties of the material.

The discussed approach and the designed model can be widely used in the research, in the practical choice of the material and its composition, as well as for training professionals in the engineering field.

In [3, 13] trained neural models were used to find the Pareto front of two of the goal criteria and there has been selected a composition with the most economical use of alloying elements and compromising ratio of the two criteria.

In [3] it is proved that neural networks outperform non-linear regression models. It turned out, however, that the presence of eight alloying elements and six strength and plastic characteristics do not allow the creation of a simple neuron model with the required accuracy of all output variables and that the results of multicriteria optimization showed contradictory results between strength and ductility. Therefore there has been designed a single model of a neural network for each of the discussed output target parameters. The different requirements of every detail in operating conditions form a specific variation range of the target parameters. In [3] focuses on the production of alloys for crankshafts.

Finding a Pareto front of the optimal solutions in mul-ticriteria optimization.

In [2] there has been solved the bi-crireria optimization problem:

$$J_1 = \mathrm{Re}(C,\quad Si,\quad Mn,\quad Ni,\quad S,\quad Cr,\quad Mo) \rightarrow \max$$
$$J_2 = A(C,\quad Si,\quad Mn,\quad Ni,\quad S,\quad Cr,\quad Mo) \rightarrow \max$$

and finding a Pareto front of the optimal solutions. To generate potential solutions, which can be a Pareto front, the area of research was limited in the domain of well-known brands compositions suitable for a certain type of machine elements – shafts.

6.CONCLUTION

The design of algorithms and software for the Decision Maker (DM) is an actual problem in the field of science and technology, with the result determined by the relevant decisions. These solutions are evaluated for the effects of the achieved benefits in the area. The decisions are determined also by the method used for optimization of concrete models, the goal parameters of the study. A software solution for the construction of tools for decision-making is assessed by its friendliness to the DM analysis of the fitness functions.

The proposal of the paper to the DM to work not in the plane of the criteria but in the plane of the variables and the use of different / five-six / color restrictive intervals is rather untraditional. These two assumptions, however, are able to carry out a very useful analysis for various processes at this stage, with up to four variables.

It should be noted that one of the suggested approaches is able to significantly reduce the a priori information to generate an optimal composition. This facilitates the design of compositions to fill databases, to reduce the volume of experiments in metallurgy, which is expensive and the information it is difficult to reproduce.

Multi-linear analysis is valuable, but at this stage it is limited in terms of sampling made for different inputs. It establishes the effective status of a single parameter of the quality in terms of energy efficiency and saving materials. The importance of the study is subject to the universality of the approach developed for regression models and the apparatus of artificial neural networks. This results in the current research in a robust scientific style.

The proposal for a methodology and developed specialized software assisting to determine the optimal composition is necessary for the future development of the system of “composition-properties” in the development of new materials.

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ПРИНОС КЪМ ИНИЦИАТИВАТА ЗА ГЕНОМА НА МАТЕРИАЛА С МЕТОДИ ЗА МЕТАЛУРГИЧЕН ДИЗАЙН

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БЪЛГАРИЯ

Ключовидуми:*Сплави, Моделиране, Оптимизация,*

Резюме:*Обобщаващите тук изследвания са посветени на числени подходи за определяне на ефективни решения от областта на металургичното производство. Подходите за получаване на оптимално съчетание от химичния състав и термичното обработване за постигане на определени свойства са от фундаментално значение за осъществяване на един ефективен проект. Те са в основата на създаването или усъвършенстването на нови сплави и свързаните с тях разходи.*

Ефективните решения от рационалното легиране на сплавите са в състояние да повишат якостта/намалят теглото, при запазване или намаляване на себестойността на сплавта. За определянето на тези решения обаче са необходими числени методи, алгоритми и процедури, които да не зависят от използваните бази от данни.

Изследването на генома на материала в това обобщение на публикации, разчита изцяло на статистическата обработка и е насочено към създаване на възможности за прогнозиране на механичните показатели като функция от химичния състав и параметрите на термичното обработване с отчитане на съответни гранични условия.