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Hybrid modelling methods in materials science - selected examples

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Analysis and modelling

ABSTRACT

Purpose: The paper presents selected examples of application of computational tools, including artificial intelligence methods to solve examples of tasks in the area of materials science. (i) Selection method of steel grade with required hardenability; (ii) Modelling of CCT diagrams for engineering and constructional steels; (iii) Application of neural networks for selection of steel with the assumed hardness after cooling from the austenitising temperature; (iv) Designing of high-speed steels chemical composition
Design/methodology/approach: In the paper been applied a hybrid approach that combined application of various mathematical tools including artificial neural networks, linear regression and genetic algorithms to solve selected tasks from the area of materials science.
Findings: Computer modelling and simulation make improvement of engineering materials properties possible, as well as prediction of their properties, even before the materials are fabricated, with the significant reduction of expenditures and time necessary for their investigation and application. Methods used in hybrid systems are complementary and disadvantages of one method are compensated by the advantages of another method.
Practical implications: Solutions presented in the work, based on using the adequate material models may feature an interesting alternative in designing of the new materials with the required properties. The practical aspect has to be noted, resulting form the developed models, which may successfully replace the above mentioned technological investigations, consisting in one time selection of the chemical composition and heat treatment parameters and experimental verification of the newly developed materials to check of its properties meet the requirements.
Originality/value: The presented approach to new materials design assumes the maximum possible limitation of carrying out the indispensable experiments, to take advantage of the existing experimental knowledge resources in the form of databases and most effective computer science tools, including neural networks and evolutionary algorithms.
Keywords: Steels; Artificial intelligence methods; Modelling; Simulation

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1. Introduction

In recent years significant progress has been made in methods and tools for modeling and simulation the technological processes of manufacturing and processing of materials and forming the micro-structure, functional and service properties of materials as well. Computer-aided modeling is becoming increasingly present in both research and in industrial practice. Progress in the area of materials engineering is connected inseparably with employment and development of numerical methods and mathematical modelling in particular. Computer modelling and simulation make improvement of engineering materials properties possible, as well as prediction of their properties, even before the materials are fabricated, with the significant reduction of expenditures and time necessary for their investigation and application. Research in the area of mathematical modelling, computational intelligence, and artificial intelligence indicate to the big potential connected with using the hybrid models [1], [2], [3].

Merging methods in one model makes analysis possible of a broader problem space, and - which is even more important - benefiting from advantages of every method and achieving the synergetic effect. Assumption that these methods are complementary is the base for development of such solutions. Methods used in hybrid systems are complementary and disadvantages of one method are compensated by the advantages of another method [3].

An example of hybrid systems can be the combination of symbolic methods of knowledge representation and processing specific to expert systems with numerical methods of data representation and processing, that are specific to artificial neural networks. One of the difficulties related to the design of expert systems is the acquisition of knowledge from experts and its verification. Experts are not always able to justify their intuitive way of reasoning. Artificial neural networks can be used to automatically acquire knowledge by learning from examples and gathering knowledge in the numerical values of weights of connections between neurons. In the case of a complex neural network interpretation of the knowledge contained in its structure is difficult or simply impossible. This makes it difficult explanation provided by neural network solutions, which is often indicated as a significant disadvantage of this solution.

Artificial neural networks are also often combined with other methods of computational intelligence and statistical methods. The examples of this approach are genetic algorithms and their modifications. Evaluation of adaptation of individual chromosomes, which are set of possible solutions, is based on the value calculated by artificial neural network. In the case of multi-criteria optimization is possible to create a complex objective function. The value of this function can be calculated by a number of neural networks and / or statistical regression equations. Interesting opportunities also provides a connection in one model, two classes of tasks that can be solved by artificial neural networks - classification and regression..

The paper presents selected examples of the use of hybrid methods to solve selected tasks in the area of materials science.

2. Selection method of steel grade with required hardenability

Hardenability assessment, being one of the main criteria for the selection of steel for constructional elements, makes it possible to accomplish the expected properties' distribution in the element transverse section. [4],[5]. The purpose of this study is to work out the computer aided method for selecting grades of steel with a required hardenability. Moreover in the initial stage, a neural network model for calculating the Jominy curve on the basis of the chemical composition has been worked out.

The aim of this study [6] is to work out the system that would help to select the steel grade with the required course of the hardenability curve. It has been assumed that the steel will fulfill this criterion if the curve, defined by the user, is contained in the hardenability band characteristic for a given steel grade. The hardenability band for the given steel grade has been defined as the lowest and highest hardness calculated for the consecutive 13 distances from the quenched end.

Determining the hardenability bands requires working out the appropriate calculating model for the range of mass concentrations of elements presented in Table 1.

Table 1.
Ranges of mass concentrations of elements

Range	Mass fractions of elements, %						
	C	Mn	Si	Cr	Ni	Mo	V
min	0.22	0.30	0.05	0	0	0	0
max	0.60	1.60	1.37	2.20	2.20	0.50	0.25

Next, the neural network has been designed and numerically verified that made possible to calculate the hardness of the steel on the basis of the chemical composition for the assumed distance from the quenched end. It has initially been assumed that the designed system will include the information about 20 steel grades for carburizing and quenching and tempering. For each steel grade 150 chemical compositions have been randomly generated, and the hardness for the assumed 13 distances from the quenched end has been calculated. This way a training set for the neural classifier has been created whose task was to propose the grade of steel after defining the required Jominy curve by the user.

The neural network designing enabling the calculation of the hardening curve has been carried out in two variants. In the first variant the mass concentrations of the elements and the distance from the quenched end have been used as the input data. The activation level of a single output neuron determined the hardness of the steel. In the second variant, the response coding of the neural network in the form of 13 neurons has been applied, each of them determining the hardness of the steel in the consecutive distance from the quenched end.

The following quantities determined for the data sets were used as the basic coefficients for evaluation of the neural network model performance: average network prediction error, ratio of standard deviations of errors and data, Pearson correlation coefficient. These coefficients have been calculated for the consecutive distances from the quenched end. In both analysed variants, the best quality coefficients have been obtained for the MLP (multilayer perceptron) network. The analysis of the quality coefficients in the consecutive distances from the quenched end calculated for the training, validating, test and verifying sets has proved that the smallest error occurs in the network with one neuron in the output layer.

In Figure 1 the Jominy curve has been compared, that has been calculated with the help of the neural network and determined experimentally.

For calculations of steel grade the feed-forward neural networks have been applied. Two options of network response coding have been analysed. In the first option, there has been used one output variable equal to the number of steel grades. In the other, the number of output variables equal to the number of classes have been applied on the assumption that each variable can have two (yes or no) values to state whether certain steel meets the user's requirements.

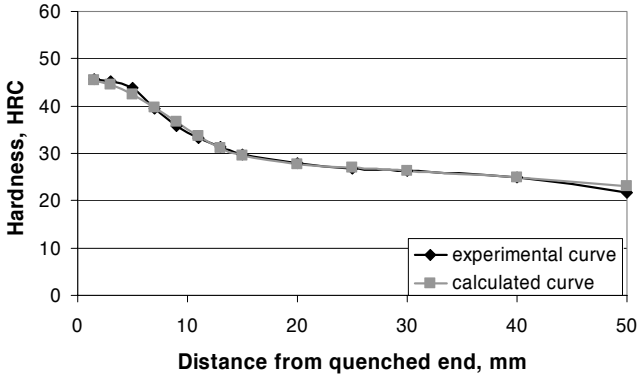

Fig. 1. The comparison of the experimental and calculated curves for the steels with a mass concentration of elements: 0.19% C, 0.94% Mn, 0.28% Si, 0.94% Cr, 0.17% Ni, 0.23% Mo

For neural network response code by means of one dependent the number of neurons in the output layer variable has been used that is equal to the number of nominal-value variables, so eventually equal to the number of classes. The one-with-N conversion type has been applied. The class attribution of the investigated case requires stimulation of one neuron and simultaneous disconnection of the others. It is the level of activation of the winning neuron that decides on the class attribution. Each training vector consisted of 13 calculated values of steel hardness and a nominal output variable in the form of steel grade marking.

Figure 2 show the examples of hardness curve in function of distance from quenched end against a background of the range of hardness change for steel grades accepted as a model and suggested by the network.

The other option of neural network response coding has been the application of the number of output variables equal to the number of steel grades (classes). In that case, the number of neurons in the network output layer has been assumed according to the number of steel grades. The double conversion has been applied, which means that each variable could have one of the two nominal values indicating either class affiliation or the lack of a certain class affiliation. For neurons in the output layer the values of acceptance and rejection level have been established. The value of the activation of output layer neuron that is higher than the acceptance level has been interpreted as the selection of steel grade that meets the predetermined requirements. The activation level of the output layer neuron that is lower than the rejection level has excluded the steel grade from the accepted selection.

Figure 3 show the example of predetermined Jominy curve in function of distance from quenched end against the background of hardness ranges for steel grades: the one assumed as a model and the one suggested by the neural network. In this case the network response should be considered as a set of potential solutions with the final decision to be taken by the user of the system.

The presented in the paper model of interrelation between the chemical composition and the distance from the quenched end and the hardness of steel may be used when estimating the difference between the assumed hardness and the possible hardness to obtain for the cast with a specific chemical composition. The presented in the paper project may be supplemented with other steel grades.

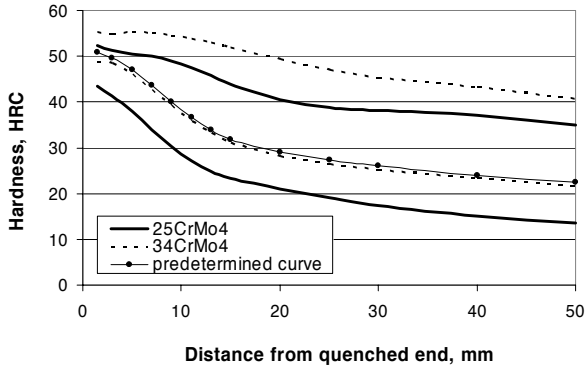

Fig. 2. Comparison of the predetermined Jominy curve and range of hardness change accepted as a model (34CrMo4) and suggested by the neural network (25CrMo4)

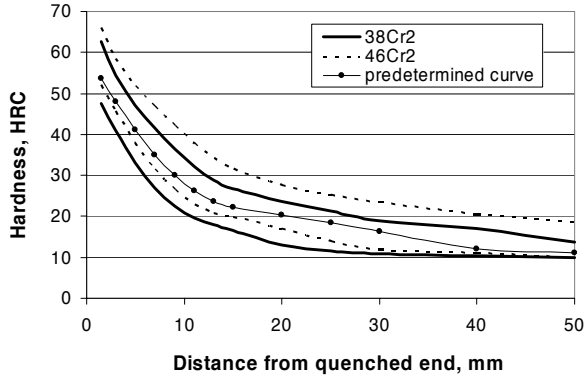

Fig. 3. Comparison of the predetermined Jominy curve and hardness ranges for steel grades suggested by the neural network: variant 1-38Cr2; variant 2 - 46Cr2

3. Modelling of CCT diagrams for engineering and constructional steels

The CCT diagrams containing the quantitative data pertaining to the dependence of steel structure and hardness on temperature and time of the supercooled austenite transformations are used for determination of the structure and hardness of the quenched,

normalised, or fully annealed steels. In papers [7],[8],[9] the authors' method of CCT diagrams calculation has been described.

In this example there has been presented a hybrid method of calculating of the continuously cooled austenite transformations from the austenitizing temperature in which the regression analysis, artificial neural networks and a comprehensive collection of empirical data have been used. [10] The preparation of a representative set of empirical data has had a fundamental significance for preparing a hybrid method of calculating CCT diagrams. The data set, made on the basis of available publications, included the chemical composition, austenitizing temperature and CCT diagrams for constructional and engineering steels. The obtained diagrams have been subjected to a selection, taking the mass concentration of alloy elements as a criterion. A range of the accepted mass concentrations of the elements has been presented in Table 2

Table 2.
Ranges of mass fractions of elements for the analysed steels

Range	Mass fractions of elements, %							
	C	Mn	Si	Cr	Ni	Mo	V	Cu
min	0.11	0.2	0.14	0	0	0	0	0
max.	0.77	1.53	1.37	1.54	1.72	0.72	0.31	0.26
%Mn+%Cr+%Ni+%Mo≤5								

According to the suggested method, the calculation of CCT diagrams proceeds in two stages.

The first consists in determining the characteristic values of transformations' temperature and the time for starting the transformations. To this end the interrelations including the influence of the chemical composition as well as optionally austenitizing temperatures and the cooling rate on the modeling dependencies have been worked out. The method of multiple regression has been used. The received calculations do not allow for determining the range of the cooling rate for which bainitic and martensite transformations proceed. To solve this problem, classifiers based on neural networks have been prepared.

The independent models were developed making it possible to calculate the following quantities:

- temperature of the eutectoidal transformation during heating - A_{c1},
- temperature of the ferrite to austenite transformation during heating - A_{c3},
- temperature of the bainitic transformation start - B_{smax},
- temperature of the martensitic transformation start - M_s,
- time referring to the lowest austenite life in the temperature range characteristic for the ferrite occurrence zone - t_F,
- time referring to the lowest austenite life in the temperature range characteristic for the pearlite occurrence zone - t_P,
- time to the start of the bainitic transformation, referring to the point of the shortest supercooled austenite life in the bainitic occurrence zone - t_B.
- temperature of start of ferrite occurrence at a particular cooling rate - F_s,
- temperature of start of pearlite occurrence at a particular cooling rate - P_s,
- temperature of start of bainite occurrence at a particular cooling rate- B_s.

On the basis of the analysis of different forms, general interrelations embracing the influence of the chemical composition and optionally, the austenitizing temperature as well as the cooling rate on the temperature value and the time of transformations including the interrelations accounting for synergy of alloy elements' interactions, the general forms of equations have been accepted. The judgment of the worked out empirical interrelations has been made on the basis of the analysis of the mean error value, the deviation of the standard error and Pearsons' correlation coefficient. The interrelations describing the influence of the chemical composition on the critical temperature values and the time of transformations as well as the temperature of the beginning of transformations in the function of the cooling rate, worked out using the multiple regression, are presented in equations 1-9.

$$A_{c1}=739.3-22.8\cdot C-6.8\cdot Mn+18.2\cdot Si+11.7\cdot Cr-15\cdot Ni-6.4\cdot Mo-5\cdot V-28\cdot Cu \quad (1)$$

$$A_{c3}=937.3-224.5\cdot C^{0.5}-17\cdot Mn+34\cdot Si-14\cdot Ni+21.6\cdot Mo+41.8\cdot V-20\cdot Cu \quad (2)$$

$$B_{smax}=752-223.5\cdot C-55\cdot Mn-21.6\cdot Si-46.8\cdot Cr-36.9\cdot Ni-47.4\cdot Mo-70\cdot V-11\cdot Cu \quad (3)$$

$$M_s=532.6-396.7\cdot C-33\cdot Mn-1.4\cdot Si-14\cdot Cr-18\cdot Ni\ 11\cdot Mo+49.7\cdot V+31\cdot Cu \quad (4)$$

$$logt_B=-1.52+2.93\cdot C+0.68\cdot Mn+0.25\cdot Si+0.73\cdot Cr+0.31\cdot Ni+0.69\cdot Mo-0.23\cdot V \quad (4)$$

$$logt_F=-1.56+2.67\cdot C+0.95\cdot Mn-0.1\cdot Si+1.27\cdot Cr+0.22\cdot Ni+2.27\cdot Mo-1.06\cdot V-0.47\cdot Cu \quad (5)$$

$$logt_P=0.19-0.3\cdot C+0.64\cdot Mn+0.06\cdot Si+1.02\cdot Cr+0.4\cdot Ni+4.9\cdot Mo+0.38\cdot V-0.42\cdot Cu \quad (6)$$

$$Fs=968.7-254\cdot C-71\cdot Mn+27.6\cdot Si-30\cdot Cr-44\cdot Ni-54\cdot Mo+95,8\cdot V-0.02\cdot T_A-62.8\cdot v_r^{0.25} \quad (7)$$

$$Ps=789.8-12.7\cdot C-61\cdot Mn+13.7\cdot Si-5\cdot Cr-30.4\cdot Ni-70.7\cdot Mo-1.4\cdot V-0.016\cdot T_A-47.3\cdot v_r^{0.25} \quad (8)$$

$$Bs=678.9-239.6\cdot C-35.2\cdot Mn-1.6\cdot Si-19.8\cdot Cr-27.9\cdot Ni-18\cdot Mo-171\cdot V-0.03\cdot T_A-15.5\cdot v_r^{0.25} \quad (9)$$

The presentation of anisothermal transformations of the supercooled austenite requires not only calculating the transformations' temperature in the function of the cooling rate but also determining the range of the cooling rate in which the transformation occurs. The problem amounts to the calculation of the lowest time value for which a ferrite, pearlite and bainite occur and the highest time value for which bainite and martensite occur in the structure of the steel. In case of the ferrite and pearlite ranges as well as the point of the bainite range, the interrelations (1-9) have been applied, whereas for the end of the bainite and

martensite ranges, the neural networks have been applied. A classifier had to be developed, to obtain this information, using as input data the mass concentrations of the particular alloying elements, austenitizing temperature, and cooling rate.

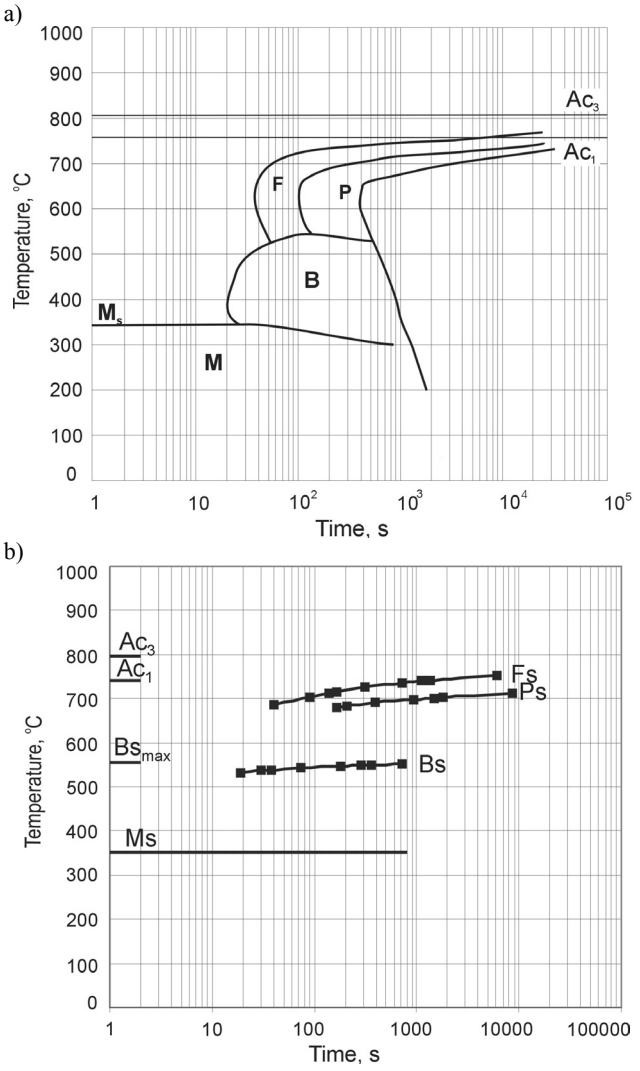

Fig. 4. CCT diagram for steel with concentrations: 0.36% C, 0.49% Mn, 0.25% Si, 1.54% Cr, 0.21% Ni, austenitised at temperature of 860°C: a) experimental, b) calculated

In this study possibility of employing the modular neural networks was analysed. Multi-network structures are used more and more often in designing the classifiers employing the artificial neural networks. This solution, called most often modular neural network, consists in employing many neural networks independently developed and in determining the response of the entire system using the supervisor module. In many complex issues a network mapping its specific fragment only of the modelled problem fulfills its task much better. Using the modular networks of less complex structure prevents many a time from the excessive matching the network to the data from the training set, which leads to losing by the network its capability to generalise the acquired knowledge. However, employment of the collective decision of the modular neural network gives hope that it will be subjected to a smaller error than the response of a single network. A very important issue in case of the modular neural networks is the method of reaching the classifier's final decision. The particular classifiers were developed using the unidirectional neural networks of the MLP type (multilayer perceptron) with one or two hidden layers. The voting method based on the absolute majority of votes was chosen.

In Figure 4 the calculated values of the transformations' temperature were compared with the empirically determined CCT diagrams.

The applied in the paper numerical verification of the worked out interrelations allows to state that in the range of the assumed mass concentrations of the alloy elements, the proposed method makes it also possible to make CCT diagrams for the newly worked out types of steel. The presented model facilitates the analysis of the interaction of the particular elements on the characteristic points and the curves of the supercooled austenite transformations. This model delivers crucial information for the reasonable choice of steel for those parts of the machines that are subjected to the heat treatment.

4. Application of neural networks for selection of steel with the assumed hardness after cooling from the austenitising temperature

The aim of the study is to establish a system that supports the choice of steel grade for quenching and tempering at a required hardness curve as function of cooling rate from the austenitising temperature [11]. It has been assumed that the steel will meet the criterion provided that the hardness curve, defined by the user, is included within the range of hardness change that is characteristic of a certain steel grade. The hardness range for the certain steel grade has been defined by the highest and lowest hardness calculated for ten predetermined successive time units until the end of steel cooling from the austenitising temperature.

In order to determine the steel hardness ranges it has been necessary to work out a suitable calculation model. Therefore, a neural network has been designed and verified numerically to calculate the steel hardness on the basis of chemical content for the predetermined cooling rate. Basing on the literature information, the data set was worked out containing chemical compositions, austenitising temperatures, as well as hardness as functions of the cooling rate of the steels for quenching and tempering. The ranges of the assumed mass fractions of elements are included in Table 3.

To develop the relationship between the chemical composition, austenitising temperature, cooling rate, and hardness of the steel the feedforward neural network (MLP) was used. The activation level of the successive 13 network input nodes depended on: mass concentration of elements (C, Mn, Si, Cr, Ni, Mo, V), austenitising temperature, cooling rate, and structure type. The average cooling rate has been calculated on the basis of

the time until the end of steel cooling from the austenitising temperature. The types of the structural constituents were determined using four bivalued nominal variables containing the information if the following constituents are present in the structure: ferrite, pearlite, bainite, martensite. A classifier had to be developed, to obtain this information, using as input data the mass concentrations of the particular alloying elements, austenitising temperature, and cooling rate. The detailed problem description was presented in [8,13].

Table 3.
Ranges of mass concentrations of elements

Range	Mass fractions of elements, %						
	C	Mn	Si	Cr	Ni	Mo	V
min	0.22	0.30	0.05	0	0	0	0
max	0.60	1.60	1.37	2.20	2.20	0.50	0.25

It has been required to prepare a representative training database in order to design a neural network as a classifier that on the basis of the hardness curve defined by the user is able to select the optimal steel grade. Then for each steel grade (according to EN-10083-1) 150 chemical contents have been made at random and the hardness for ten predetermined cooling rates has been calculated. As a result, there has been made a training set for artificial neural network whose task is to suggest the steel grade after the hardness for 10 average cooling rates have been defined by the user.

Two options of network response coding have been analysed. In the first option, there has been used one output variable equal to the number of steel grades. In the other, the number of output variables equal to the number of classes have been applied on the assumption that each variable can have two (yes or no) values to state whether certain steel meets the user's requirements. For calculations the feedforward neural networks have been applied. Mutual entropy has been applied as error function. In that case, the error is calculated as a product-sum of assumed values and error algorithms for each output neuron. This version of error function, designed especially for classifying problems, is used with output layer activation function of the softmax type. The softmax function is an exponential function of additionally normalized value so as the activation sum for the whole layer is 1. The application of the softmax function in the output layer of multilayer perceptron designed for classifying problem solutions, allows to interpret the neuron's activation level of the output layer as the estimated probability of a certain class affiliation.

Figure 5 show the examples of hardness curve in function of time necessary for sample cooling from the austenitising temperature against a background of the range of hardness change for steel grades accepted as a model and suggested by the network.

The system presented can be applied to selection of steel grade intended for machine parts of predetermined hardness in the section of a hardened or normalized element. Differences of chemical content acceptable within the same steel grade and also altering of austenitising conditions are the reason that it is difficult to evaluate possible hardness in the section of the element only on the basis of steel grade and it must produce great error. It has been confirmed by ranges of hardness change in function of cooling rate calculated for different steel grades for quenching and tempering. As it has been shown in the study, the model of relationship between chemical composition, the austenitising temperature, cooling rate and steel hardness can be applied to determine a difference between the predetermined hardness and the hardness feasible in the casting of certain chemical content.[12],[13] The project of advisory system presented in the study can be supplemented with other steel grades.

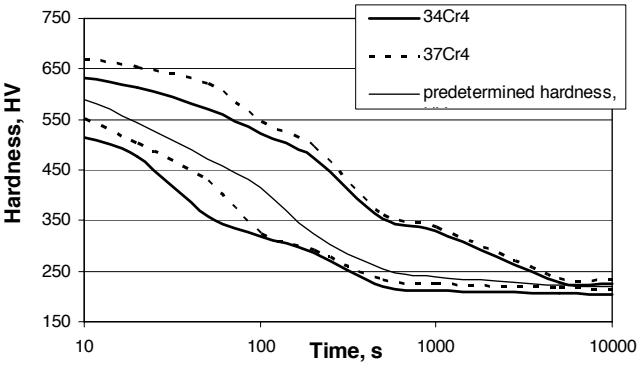

Fig. 5. Comparison of the predetermined hardness curve and range of hardness change accepted as a model (34Cr4) and suggested by the neural network (37Cr4)

5. Designing of high-speed steels chemical composition

The goal of the research carried out was developing the design methodology for the new high-speed steels with the required properties, including hardness and fracture toughness, as the main properties guaranteeing the high durability and quality of tools made from them [14]. For the high-speed steels design, as a task which is the optimization one because of the computational method employed, it was assumed that the criterial properties are hardness and fracture toughness expressed by the fracture toughness K_{Ic}. Moreover, the heat treatment technological parameters are optimised also, i.e., austenitizing-, and tempering temperatures.

Achieving the main goal required carrying out the following partial tasks, consisting in:

- development of the high-speed steels hardness model making it possible to compute hardness based on the steel chemical composition and its heat treatment parameters (austenitizing and tempering temperatures).
- development of the model making it possible to determine the high-speed steels fracture toughness, based on the steel chemical composition and its heat treatment parameters (austenitizing and tempering temperatures).

The neural network models were developed making computation possible of the high-speed steel hardness and the K_{Ic} The developed material models were used for designing the chemical compositions if the new high-speed steel, demonstrating the desired properties, i.e., hardness and fracture toughness.

The following data feature the base for development of models making it possible to compute the high-speed steels properties based on their chemical composition and austenitizing- and tempering temperatures only:

- investigation results of the newly developed high-speed steels [15,16],
- data contained in the relevant standard [17],
- data from the high-speed steels manufacturers' catalogues [18],
- results of the own supplementary investigations of the selected high-speed steels grades.

Ranges of alloying elements concentrations for the newly developed steels, collected from standards, and from catalogues of steel manufacturers are presented in Table 4. The austenitizing temperature range for which the data was processed is 1120°C-1280°C, and the tempering temperature range is 480°C-630°C.

Table 4.
Ranges of the alloying elements occurring in analyzed steels

Range	Mass fractions of elements, %					
	C	Cr	W	Mo	V	Co
min	0.72	3.7	0	0	1	0
max	1.41	4.7	18	9.5	4.5	11

The adequacy of the developed models was checked by analysing the error between the calculated hardness and its corresponding hardness tested experimentally. The average error for the tested data file was assumed as the criterion:

$$R = \frac{\sum_{i=1}^{N} (HRC_{ci} - HRC_{mi})}{N} \tag{10}$$

where: N - test file size, HRC_{ci} - calculated hardness (ith), HRC_{mi} - measured hardness (i-th).

The assumption was made that the model that would make it possible to obtain the calculation error ca. 1 HRC will be a valid one.

5.1. High-speed steels hardness model

For the secondary hardness modelling results of the experimental research, containing information about the chemical compositions and the steel hardness test results, taken from [14-17] feature the base for the neural networks design. Were available in more than 2100 data patterns, which may be considered as the sufficient number to develop the fully adequate neural networks model.

It was assumed, referring to the developed neural networks structure, that the network has 8 inputs, corresponding to concentration values of the six main alloy elements occurring in this steel group and to the austenitizing- and tempering temperatures, and one output, corresponding to hardness. The StatSoft STATISTICA Neural Networks v. 4.0 program was used for development, training, and testing of the neural networks.

Several hundred neural networks were generated using the Statistica Neural Network program with the various numbers of neurons in the hidden layers. The average absolute error, quotient of standard deviations, and correlation coefficient were assumed as the network quality coefficients. Finally one network was selected, from the entire set of the developed networks -the multilayer perceptron with the 8-7-1 structure (i.e., 8 inputs, 7 neurons in the hidden layer, and 1 output), with the average calculation error of 1.01 HRC. In Fig. 6 comparison of the calculated and experimental tempering curves are shown for selected steels, from all included in the data set used to develop the models.

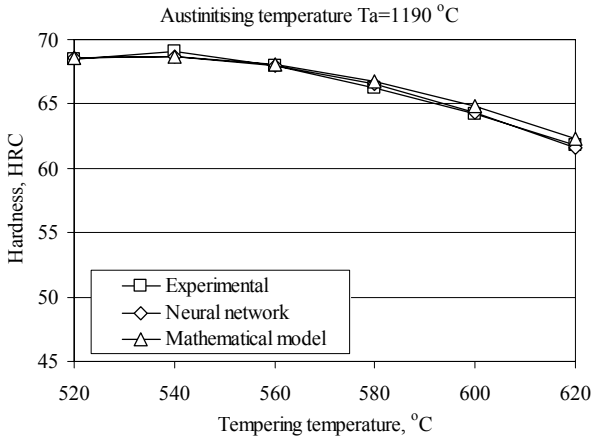

Fig. 6. Comparison of experimental results and hardness calculations for HS2-9-1-8 steel

5.2. High-speed steels fracture toughness model

The further works were focused on development the model making it possible to determine the high-speed steel fracture toughness solely based on the steel chemical composition and heat treatment parameters.

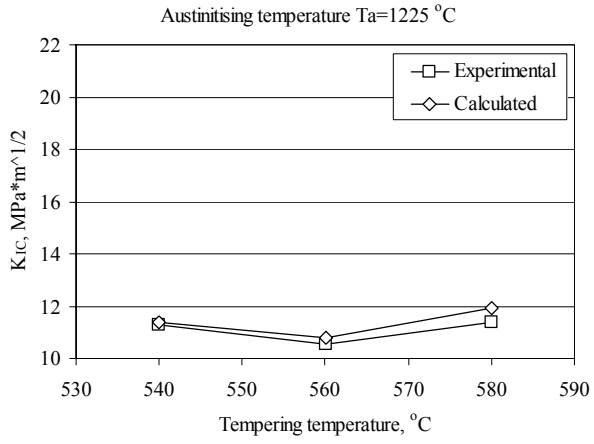

Fig. 7. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS6-5-2 steel

The StatSoft STATISTICA Neural Networks v. 4.0 program was used for development, training, and testing of the neural networks. After entering the training data to the program, the neural network design process was started. Several dozen neural networks were generated using the program, with the various numbers of neurons in the hidden layer. Finally one network was selected, from the entire set of the developed networks -the multilayer perceptron with the 8-6-1 structure (i.e., 8 inputs, 6 neurons in the hidden layer, and 1 output), with the average calculation error of 0.39 MPa·m$^{1/2}$. Comparison of the calculated K_{Ic} coefficient values with the experimental data is shown in Fig. 7.

5.3. Optimisation of the chemical composition of high-speed steels

For the high-speed steels chemical compositions design, which is the optimisation problem, the evolutionary algorithms were used. The object function is the index defining the set of the optimised properties, in this case hardness and fracture toughness. It was assumed that it will be possible to determine weights for each property, which will make it possible to make a decision which of the properties in the optimisation procedure actually carried out is the most important one. The optimisation result, with the maximum secondary hardness as the goal, are the chemical compositions high-speed steels with the highest hardness, and with the fracture toughness as a goal, the chemical compositions of steels demonstrating the highest fracture toughness K_{Ic}. Moreover, the possibility was assumed to limit the search area for the optimum chemical composition meeting the assumed criteria. Because of the form of the developed material models employed for design of the chemical composition, not only the alloy elements concentrations are optimised, but also the heat treatment parameters, i.e., the austenitizing- and tempering temperatures.

The assumptions made were used in optimisation, pertaining to relationships among the particular concentrations of the alloy elements occurring in the high-speed steel and its hardening- and tempering temperatures - and its properties. The own computer program was developed to carry out the high-speed steel chemical composition optimisation task, with the maximum hardness and fracture toughness as the goal, in which the genetic algorithm was employed with the hardness- and fracture toughness functions as the neural network models.

The object function was optimised expressing the high-speed steel hardness and its fracture toughness in the following form:

$$Z = a \cdot HRC(x) + b \cdot K_{IC}(x) \tag{11}$$

where: HRC(x) - hardness function (neural network model), $K_{Ic}(x)$ - fracture toughness function (neural network model), x_i, - vector of parameters (mass concentrations of alloying elements, austenitizing- and tempering temperatures), a, b - weight coefficients for both of the object function components, assuming values from the <0;1> range.

The chemical composition optimisation procedure calls for specifying the limits the optimised function parameters, i.e., alloy elements concentrations ranges and the austenitizing and tempering temperatures. Based on analysis of concentrations of chemical compositions of steels, optimisation limits used in the genetic algorithm are presented in Table 5; whereas, the additional limitations are listed in Table 6. The roulette method was used in this algorithm for selection.

Parameters of the algorithm defined by the user in the developed program are:

- **Number of generations** - determines the number of algorithm repetitions;
- **Population size** - number of indivduals
- **Crossing coefficient** - value from the range from 0 to 1 (0 denotes the probability of crossing equal to 0, 1 denotes the probability of 0.2), specifying probability of the selection of the relevant pair of specimens to transform the population (default value of 1);
- **Mutation coefficient** - value from the range from 0 to 1 (0 denotes the probability of mutation equal to 0, and 1 denotes the probability of 0.2), specifying probability of the selection of the particular specimen for mutation operation (default value of 0.5);
- **Accuracy of calculations** - specifies precision of the environment search
- **Weights a and b** - specifying weights attributed to each object function component

The optimisation algorithm functioning consists in such selection of the alloying elements and hardening- and tempering temperatures so that the chemical composition of the steel is obtained with the possibly highest hardness and fracture toughness, while maintaining proportions for these properties specified by their weights (Eq. 11). The developed own computer program makes investigations possible pertaining to designing the chemical composition of steel with the required hardness and fracture toughness. Arbitrary defining is possible, within the optimisation limits, of the search space of the optimum chemical composition of the high-speed steel. Moreover, provision is made in the program for adjustment of the optimisation parameters, which can also affect the calculations results, i.e., the arbitrary selection of the set of parameters connected with managing the population. One should clearly stress that computations yield different results each time which results from drawing the initial population. As an illustration of research carried out using the developed program two selected examples are presented of the chemical composition optimisation results, obtained for various genetic algorithm parameters and for various limits imposed on the search space of the optimum chemical composition.

Table 5.
Boundary of the optimisation procedure

Parameter	C	Cr	W	Mo	V	Co	Ta	Tt
min	0.72	3.7	0	0	1	0	1150	500
max	1.41	4.7	18	9.5	4.5	11	1280	630

Table 6.
Optimisation procedure constrains used in calculation

Constrain	Cr+W+Mo+ V+Co	(Cr+W+Mo+ V+Co)/C	Mo+V +Co	W+Mo +V
min	9.3	11.1	1.1	5.3
max	31	30.9	18.7	19.2

Example 1

Algorithm parameters

Number of generations	100	Coding precision	8 bits
Number of individuals	50	HRC Weight	1
Crossing coefficient	1	K_{Ic} Weight	1
Mutation coefficient	0.5	Number of the best individuals	2

Optimisation limitations

Parameter	C,%	Cr, %	W, %	Mo, %	V, %	Co, %	Ta,°C	Tt, °C
Minimum value	0.72	3.7	2	2	1	0	1150	500
Maximum value	1.41	4.7	18	9.5	4.5	11	1280	630

Calculation results

Solution	% C	% Cr	% W	% Mo	% V	% Co	Ta, °C	Tt,°C	Fbest	Fpopul	HRC	K_{IC}
1	1.22	4.67	10.53	2.12	1.98	1.12	1253	512	84.3	81.5	66.4	17.9
2	1.16	4.65	2.13	4.24	1.06	10.01	1254	589	86.9	80.3	68.5	18.5
3	0.99	4.59	3.51	2.24	1.00	7.72	1264	533	87.5	82.7	68.8	18.6
4	1.18	4.61	2.13	3.35	1.37	3.62	1253	585	86.0	78.2	67.0	19.0
5	1.34	4.68	9.03	3.62	1.00	0.69	1267	501	85.3	79.5	67.1	18.1

Example 2

Algorithm parameters

Number of generations	100	Coding precision	8 bits
Number of individuals	50	HRC Weight	0.95
Crossing coefficient	1	K_{Ic} Weight	1
Mutation coefficient	0.5	Number of the best individuals	2

Optimisation limitations

Parameter	C,%	Cr, %	W, %	Mo, %	V, %	Co, %	Ta,°C	Tt, °C
Minimum value	0.72	3.7	2	2	1	0	1190	520
Maximum value	1.41	4.7	18	9.5	4.5	11	1240	590

Calculation results

Solution	% C	% Cr	% W	% Mo	% V	% Co	Ta, °C	Tt,°C	Fbest	Fpopul	HRC	K_{IC}
1	0.86	4.20	3.00	2.71	1.17	10.53	1215	572	82.1	74.3	67.1	18.3
2	0.98	4.40	5.51	2.44	1.12	6.51	1212	520	80.9	74.3	67.2	17.0
3	1.09	4.68	3.95	2.00	2.25	0.04	1205	584	84.7	83.2	64.0	23.9
4	0.83	4.45	4.01	3.35	1.62	1.81	1226	578	81.4	80.3	64.4	20.2
5	1.16	4.61	5.77	2.35	2.22	0.00	1235	577	80.8	75.7	65.9	18.2

6. Final remarks

The presented approach to selection or new materials design, being the new materials design philosophy, assumes the maximum possible limitation of carrying out the indispensable experiments, to take advantage of the existing experimental knowledge resources in the form of databases and most effective computer science tools, including neural networks and evolutionary algorithms. It should be indicated that the materials science knowledge, pertaining oftentimes to the multi-aspect classic problems and described, or - rather - saved in the existing, broadly speaking, databases, features the invaluable source of information which may be used for discovery of the unknown so far relationships describing the material structure - properties

relations. The main task is integration of the materials science knowledge and computer science tools to find the new, undiscovered yet relationships and development of materials models based on the knowledge, which was acquired in experimental research over many years. Using the adequate material models makes carrying computer simulations out, which let forecasting possible of materials properties in various configurations of, say, chemical composition, processing stage (e.g., heat treatment) or product type.

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