Journal of Machine Engineering, Vol. 11, No. 1-2, 2011

tool steel, materials design,
artificial intelligence methods

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OPTIMISATION OF HIGH-SPEED STEELS CHEMICAL COMPOSITION USING THE ARTIFICIAL INTELLIGENCE METHODS

The main 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. It was decided that hardness and fracture toughness K_{Ic} are the criteria used during the high-speed steels design. In case of hardness, the statistical and neural network models were developed making computation possible of the high-speed steel hardness based solely on the steel chemical composition and its heat treatment parameters, i.e., austenitizing- and tempering temperatures. In the second case - high-speed steels fracture toughness, the neural network model was developed, making it possible to compute the K_{Ic} factor based on the steel chemical composition and its heat treatment parameters. 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. Methodology was developed to this end, employing the evolutionary algorithms, multicriteria optimisation of the high-speed steels chemical composition.

1. INTRODUCTION

The quick knowledge progress pace in many manufacturing engineering branches challenges the tool manufacturers and designers more and more. It is evident that reliability, durability, quality, and other properties of tools, ensuring comfort of their use, depend mostly on the deliberate, well studied materials selection, using the multicriteria optimisation. Economic- and ecological issues get more and more important amid many criteria, apart from the design-, engineering-, and service requirements. Hardness and ductility are the decisive properties in case of materials used for cutting tools. The task of the suitable material selection by the tool designer features the endless compromise between selection of the material with high hardness, yet with small ductility, or vice versa - selection of the material with good ductility, yet with the relatively lower hardness. High-speed steels are the

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materials with the best ductility and fracture toughness from all tool materials in use nowadays, which, as it seems, will remain irreplaceable in many applications for a long time.

The continuous intensive development of the tool materials and tool industry, e.g., in countries like Italy, Austria, Germany, Sweden, France, or Slovenia, is connected with changes in the tool- and advanced tool materials market. This is connected with the peculiar character of the contemporary manufacturing, which is compelled by the cheap competition from the Eastern markets, compared to the situation from several-, or a dozen or so years ago. It is still expected, concerning the tool materials, to provide their best feasible service- and use properties, and especially the tools' durability (service time), which extorts the need to carry out investigations of the new materials. Regrettably, the classic approach requires huge financial expenditures and a lot of time, and is connected with the need to carry out the complex fundamental research upon the newly designed tool materials, their manufacturing technologies, technologies improving their properties, and the applied research, consisting in the complex technological tests, making assessment possible of the service properties of tools. The requirements posed by the multi-aspect engineering design of tools, and also many world literature sources suggest the need of the complex approach to the materials selection problem, along with the technological processes for the contemporary tools, characteristic of the high quality, reliability, and being environment friendly [1-3].

Progress in the area of materials engineering is connected inseparably with employment and development of mathematical modelling, numerical methods, computational intelligence methods, and artificial intelligence. 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. Therefore, modelling becomes the indispensable tool in materials science and materials engineering ensuring the chemical and physical description of materials in a broad scale both of length and time. This is connected with the need to investigate behaviour of materials in various scales, from atomic, through the mezo- to macro scales, employing knowledge of physics and chemistry principles pertaining to the solid matter state and properties. In this way, the contemporary materials science, and especially materials design, whose essence is computer simulation for evaluation of materials properties in the virtual environment, makes adjustment possible of their chemical composition and structure to the set of properties required for the new materials and products, before fabrication of these materials [3-5].

One should differentiate two aspects of materials design. The first one, referring to selection of the material for the particular product from those developed and known to date [6-8], and the second one connected with development of new materials for applications undefined so far, or materials meeting the service requirements better [9-11]. Just in this second aspect it is especially important that the new materials solutions are reached not with the trial and error method, but with the mathematical or physical modelling, and the optimum solution is obtained with computer assistance without the need to carry out the time consuming and costly experiments. Knowledge of phenomena - electrical, magnetic,

mechanical, thermal, structural or others, and their further skilful exploration taking into account the theory pertaining to their fundamentals, using the contemporary modelling methods (e.g., artificial intelligence), analytical techniques and advanced investigation methods explaining behaviour of materials, makes design of new materials possible, with properties which meet best their practical application requirements.

2. MATERIAL FOR INVESTIGATIONS AND RESEARCH METHODOLOGY

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).

Moreover, the supplementary research was done of the structure and mechanical properties of the selected high-speed steel grades to complement the set of the relevant data collected so far, necessary for the experimental verification of the developed material models. Investigations of the mechanical properties included hardness tests of steel in the hardened state and after tempering and measurements of the fracture toughness K_{Ic}.

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 [12],[13],
- data contained in the relevant standard [14],
- data from the high-speed steels manufacturers' catalogues [15],
- results of the own supplementary investigations of the selected high-speed steels grades.

Alloy elements' concentrations for the newly developed steels, collected from standards, and from catalogues of steel manufacturers are presented in Tables 1-3 respectively. 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.

For development of models making it possible to compute the high-speed steels hardness based solely on their chemical composition, as well as on their austenitizing- and tempering temperatures, the multiple regression statistical method and the artificial neural networks were used. In case of the steel fracture toughness model the artificial neural networks were used.

The supplementary investigations carried out for verification of the developed models were made for the selected high-speed steels grades with chemical compositions shown in Table 4. Their heat treatment parameters which were determined individually for each steel grade are shown in Tables 5-7.

Table 1. Chemical composition of the newly developed high-speed steels used for development of the hardness models [12], [13].

Steel type	Average mass concentration of the alloying element, %					
	C	Cr	W	Mo	V	Co
9-2-2+Si	0.94	4.5	9.0	1.72	1.8	0.0
9-2-2+Si+Ti	0.93	4.5	9.0	1.88	1.7	0.0
9-2-2+Si+Ti (1)	0.93	4.7	8.9	2.0	1.5	0.0
9-2-2+Si+Nb	0.94	4.5	9.0	1.85	1.67	0.0
9-2-2+Si+Nb (1)	0.92	4.5	9.1	1.87	1.3	0.0
9-2-2-5	0.94	4.4	8.8	2.4	1.6	5.2
11-0-2+Si	0.93	4.5	11.2	0.0	1.8	0.0
11-0-2+Si+Ti	0.98	4.6	10.8	0.0	1.6	0.0
11-0-2+Si+Ti (1)	0.93	4.4	10.6	0.0	1.4	0.0
11-0-2+Si+Nb	0.94	4.5	11.4	0.0	1.6	0.0
11-0-2+Si+Nb (1)	0.93	4.5	11.5	0.0	1.3	0.0
11-0-2-5	0.91	4.5	10.9	0.0	1.8	5.2
11-2-2+Si	1.1	4.4	11.3	1.88	1.8	0.0
11-2-2+Si+Ti	1.05	4.5	11.2	1.9	1.7	0.0
11-2-2+Si+Ti (1)	1.04	4.2	11.1	1.8	1.5	0.0
11-2-2+Si+Nb	1.0	4.4	11.2	1.95	1.7	0.0
11-2-2+Si+Nb (1)	1.02	4.5	11.3	1.82	1.4	0.0
11-2-2-5	1.03	4.5	11.3	1.94	1.8	4.9

Table 2. Chemical compositions of high-speed steels specified in standard [14] used for development of the hardness models

Steel grade	Average mass concentration of the alloying element, %					
	C	Cr	W	Mo	V	Co
HS18-0-1	0.78	4.15	17.95	0	1.1	0.0
HS0-4-1	0.81	4.15	4.25	1.1	1	0.0
HS1-8-1	0.82	4.15	8.5	2.85	1.2	0.0
HS6-5-2	0.84	4.15	4.95	6.3	1.9	0.0
HS1-4-2	0.9	3.95	4.45	1.8	1.95	0.0
HS6-5-2C	0.9	4.15	4.95	6.3	1.9	0.0
HS6-5-2-5	0.91	4.15	4.95	6.3	1.9	4.75
HS3-3-2	0.99	4.15	2.7	6.3	2.35	0.0
HS2-9-2	1.0	4.15	8.7	1.7	1.95	0.0
HS6-6-2	1.05	4.15	6	6.3	2.45	0.0
HS2-9-1-8	1.1	4.15	9.5	1.55	1.1	8.0
HS6-5-3	1.2	4.15	4.95	6.3	2.95	0.0
HS10-4-3-10	1.28	4.15	3.55	9.5	3.25	10
HS6-5-3-8	1.28	4.15	5.0	6.3	2.95	8.4
HS6-5-3C	1.29	4.15	4.95	6.3	2.95	0.0
HS6-5-4	1.33	4.15	4.6	5.6	3.95	0.0

Table 3. Chemical compositions of high-speed steels specified in [15] used for development of the secondary hardness models

Steel type	Average mass concentration of the alloying element, %					
	C	Cr	W	Mo	V	Co
1-5-1-8	0.72	4.0	5.0	1.0	1.0	8.0
18-0-1	0.75	4.1	18	0	1.1	0
2-9-1	0.83	3.8	8.5	1.8	1.2	0
0-4-1	0.84	4.0	4.2	0	1.1	0
1-5-2	0.89	4.0	4.5	1.2	1.9	0
6-5-2	0.9	4.2	5.0	6.4	1.8	0
2-5-1-2	0.91	3.7	5.0	1.8	1.2	2.5
6-5-2-5	0.93	4.2	5.0	6.4	1.8	4.8
3-3-2	0.99	4.1	2.7	2.8	2.4	0
2-9-2	1.02	3.8	8.6	1.8	1.9	0
5-6-2-8	1.05	4.0	6.0	5.0	1.6	7.8
6-6-2	1.05	4.0	6.3	6.3	2.5	0
2-9-1-8	1.08	3.8	9.4	1.5	1.2	8.0
4-8-3	1.2	4.2	8.5	3.5	3.0	0
6-5-3	1.2	4.1	5.0	6.3	3.0	0
10-4-3-10	1.27	4.0	3.6	9.5	3.2	10.0
12-1-4	1.28	4.2	0.8	12	3.8	0
6-5-4	1.3	4.2	4.5	5.6	4.0	0
9-4-3-11	1.41	4.2	3.6	8.8	3.4	11.0

Table 4. Chemical compositions of high-speed steels used in supplementary investigations

Steel grade	Mass concentration of the alloying element, %					
	C	Cr	W	Mo	V	Co
HS 6-5-2	0.9	4.19	6.13	4.84	1.99	0.02
HS 18-0-1	0.85	4.08	17.57	0.56	1.3	0.07
HS 10-4-3-10	1.26	4.28	9.04	3.31	3.54	9.92

Table 5. Austenitizing- and tempering temperatures used for HS6-5-2 steel

Austenitizing temperture, °C	Tempering temperature, °C		
1150	500	550	580
1180			
1225			
Soft annealing temperature 860°C			

Table 6. Austenitizing- and tempering temperatures used for HS18-0-1 steel

Austenitizing temperture, °C	Tempering temperature, °C		
1180	520	550	580
1220			
1255			
1280			
Soft annealing temperature 860°C			

Table 7. Austenitizing- and tempering temperatures used for HS10-4-3-10 steel

Austenitizing temperture, °C	Tempering temperature, °C		
1180	540	560	580
1200	540	560	580
1225	540	560	580
1240	540	560	580
Soft annealing temperature 880°C			

Hardness tests with Rockwell method in scale C were carried out on the automatic ZWICK ZHR hardness tester. Each time 15 readings were made and their arithmetic average was assumed as the test result. Investigation of the K_{Ic} factor was carried out according to standard [16] using the three-point bending method.

3. MODELLING OF THE HIGH-SPEED STEELS PROPERTIES

For development of hardness models results were used of investigations carried out on the newly developed high-speed steels, relevant standards, and manufacturers' catalogues. The austenitizing temperature range for which the experimental data was processed is 1120°C-1280°C, and the tempering temperature range is 480°C-630°C.

Results of the supplementary investigations were not used for development of models and were used only for the final experimental verification of the developed models.

As tools for development of models making computation of the high-speed steels hardness possible based solely on their chemical composition, as well as on their austenitizing- and tempering temperatures the following were used:

- statistical method of multiple regression,
- artificial neural networks.

The main assumption made first was that steel hardness depends on concentrations of the main alloy elements occurring in these steels: carbon, chromium, tungsten, molybdenum, vanadium, and cobalt, as well as on their austenitizing- and tempering temperatures.

In the multiple regression method the general form of the equation - model was used:

$$HRC = \sum_{i=1}^{k} a_i f_i(X) \tag{1}$$

where: a_i – coefficients of the regression equation, HRC - steel hardness, f_i - functions of the equation variables, X - vector of the equation variables, (X = [% C, % Cr, ..., Ta, Tt]).

In the second high-speed steels hardness calculation method the artificial neural networks were used of the multilayer perceptron type, employing various learning methods. Use of a constant number of input neurons was decided (8) as a consequence of the main assumption that hardness depends on C, Cr, W, V, Co, and Co, as well as on the austenitizing- and tempering temperatures. The analysed networks had 1 output corresponding to the steel hardness. The numbers of hidden layers and neurons were modified in the investigations.

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:

$$R = \frac{\sum_{i=1}^{N} (HRC_{ci} - HRC_{mi})}{N} \tag{2}$$

where: N – test file size, HRC_{ci} – calculated hardness (i–th), 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.

3.1. STATISTICAL MODEL OF HARDNESS

Based on the prepared experimental data set several mathematical models were analysed for computation of steel hardness based on the alloy elements concentrations and heat treatment of the high-speed steels.

Results of these mathematical models analysis indicate that hardness calculations for the various forms of the mathematical equation tend to the computation error value of 0.7 HRC. Therefore, model (3) demonstrating the computation error of 0.71 was assumed to be the best one and used in the next analyses.

$$\begin{aligned} HRC = {} & 5.1 \cdot C - 0.13 \cdot Cr - 0.06 \cdot W + 0.11 \cdot Mo - 0.81 \cdot V + 0.17 \cdot Co - 21.4 \cdot Ta \\ & - 1.63 \cdot To + 0.37 \cdot Ta^2 - 4.86 \cdot To^2 + 58.23 \sqrt{(ToTa)} - 23.46 \cdot (Ta/To) \end{aligned} \tag{3}$$

It should be noted that in case of the austenitizing- and tempering temperatures their readings were divided by 100. Therefore, using the developed mathematical models, the real

temperature should be presented in this way as a variable in the model. So, e.g., if the real austenitizing temperature is 1200°C, then its value after normalising should be entered to the model, i.e., 12.

3.2. NEURAL NETWORK MODEL OF HARDNESS

Next, the artificial neural networks were used for the secondary hardness modelling. Results of the experimental research, containing information about the chemical compositions and the steel hardness test results, shown in Tables 1-3, feature the base for the neural networks design. A set of 2714 reference standards was available, 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. Some of them were eliminated at the initial design stage due to the excessive error or the excessive number of neurons in the hidden layers. Training error graph for every network was studied after completing the training process or in its course. Based on that the networks were checked if the overtraining did not take place and the overtrained ones were eliminated from the subsequent analysis. 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 0.59 HRC. Quality coefficients of the developed network are shown in Table 8. The developed models were subjected to additional verification based on the supplementary investigation results. Hardness calculations were made using the developed models for steels with chemical compositions presented in Table 4. The calculation errors were estimated next

Table 8.Quality coefficients of the neural network developed for the steel hardness calculation

Network structure	Training method/number of training epochs	Data set		
		Training	Validating	Testing
MLP 8-7-1	BP/50 CG/462	Average absolute error, HRC		
		0.53	0.57	0.59
		Quotient of standard deviations		
		0.23	0.25	0.27
		Correlation coefficient		
		0.97	0.97	0.96
BP – error back-propagation learning method, CG – conjugate gradients learning method				

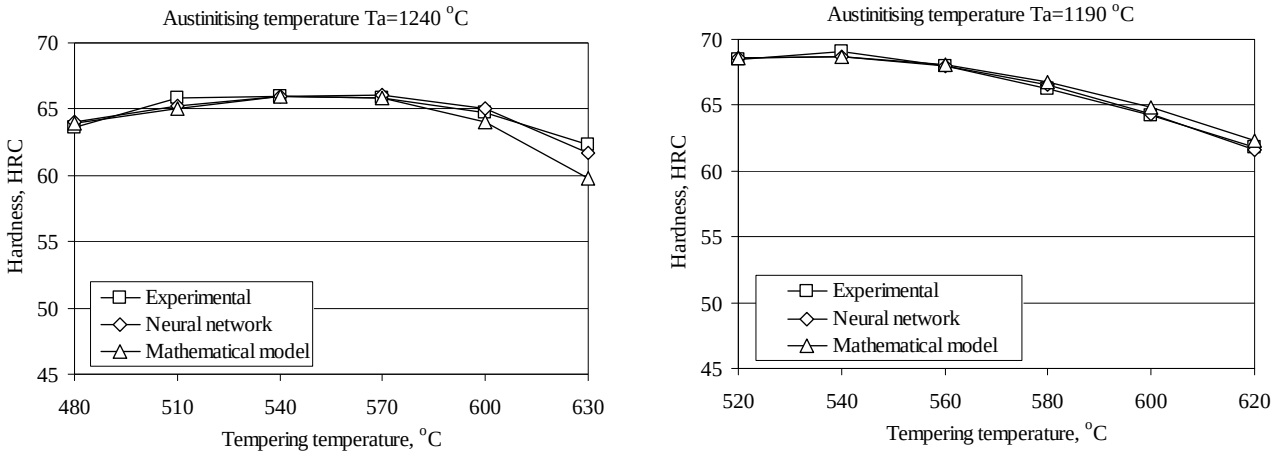

Fig. 1. Comparison of experimental results and hardness calculations for 9-2-2+Si steel (left) and 2-9-1-8 steel (right)

according to Eq. 2, which for the statistical model and neural network are 0.99 HRC and 1.01 HRC respectively. Therefore, one can state that the developed models meet fully the calculation accuracy assumptions. In Fig. 1 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.

3.3. 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. The artificial neural networks were used as a modelling tool. It was assumed, referring to the developed neural networks structure, as in case of hardness modelling, 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 the value of the fracture toughness K_{Ic}.

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. About half of them were eliminated immediately due to the excessive error or the excessive number of neurons in the hidden layers. Training error graph for every network was studied after completing the training process or in its course. Based on that the networks were checked if the overtraining did not take place and the overtrained ones were eliminated from the subsequent analysis. 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 8-6-1 structure (i.e., 8 inputs, 6 neurons in the hidden layer, and 1 output), with the average calculation error of 0.39 MPa·m$^{1/2}$. Quality coefficients of the developed network are shown in Table 9. Comparison of the calculated K_{Ic} coefficient values with the experimental data is shown in Fig. 2.

Table 9. Quality coefficients of the neural network developed for the fracture toughness K_{Ic} calculation

Network structure	Training method/ number of training epochs	Data set	
		learning	validating
MLP 8-6-1	BP/50 CG/56	Average absolute error, MPa·m$^{1/2}$	
		0.39	0.39
		Quotient of standard deviations	
		0.15	0.22
		Correlation coefficient	
		0.99	0.98
BP – error back-propagation learning method, CG – conjugate gradients learning method			

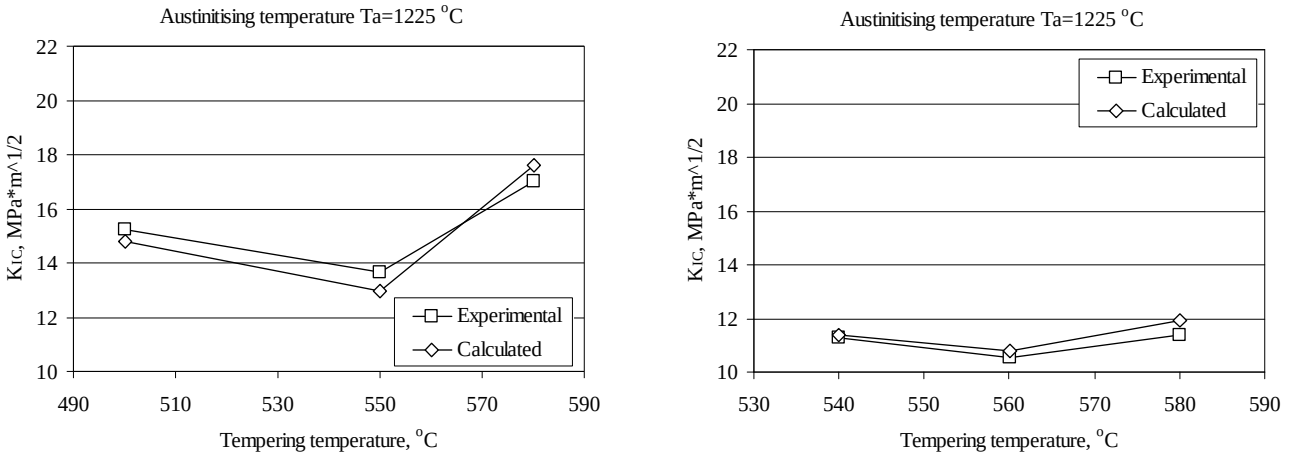

Fig. 2. Comparison of the calculated K_{Ic} coefficient with the experimental data for HS6-5-2 steel (left) and 10-4-3-10 (right)

4. OPTIMISATION OF 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:

$$Z = a \cdot HRC\,(x) + b \cdot K_{IC}\,(x) \tag{4}$$

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 shown in Tables 1-3, optimisation limits used in the genetic algorithm are presented in Table 8; whereas, the additional limitations are listed in Table 9. 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 individuals.
- **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. 4). 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 10. 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 11. 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

Solu-tion	% C	% Cr	% W	% Mo	% V	% Co	Ta, °C	Tt,°C	F_{best}	F_{pop}	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

Solu-tion	% C	% Cr	% W	% Mo	% V	% Co	Ta, °C	Tt,°C	F_{best}	F_{pop}	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

5. SUMMARY

The main 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. It was decided that hardness and fracture toughness K_{Ic} are the criteria used during the high-speed steels design. To this end the relevant models were developed - for hardness and for fracture toughness expressed with the K_{Ic} coefficient. 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. Methodology was developed to this end, employing the evolutionary algorithms, multicriteria optimisation of the high-speed steels chemical composition. 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. 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.

The presented approach to 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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