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Numerical simulation of the alloying elements effect on steels' properties

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Analysis and modelling

ABSTRACT

Purpose: The goal of the research carried out was evaluation of alloying elements effect on high-speed steels hardness and fracture toughness and austenite transformations during continuous cooling of structural steels.
Design/methodology/approach: Multi-layer feedforward neural networks with learning rule based on the error backpropagation algorithm were employed for modelling the steels properties. Then the neural networks worked out were employed for the computer simulation of the effect of particular alloying elements on the steels' properties.
Findings: Obtained results show that neural network are useful in evaluation of synergic effect of alloying elements on selected materials properties when classical investigations' results do not provide evaluation of the effect of two or more alloying elements.
Practical implications: Numerical simulation presented in the work, based on using the adequate material models may feature an alternative for classical investigations on effect of alloying elements on steels' properties.
Originality/value: The use of the neural networks as an tool for evaluation of the chemical composition effect on steels' properties.
Keywords: Steels; Artificial Intelligence Methods; Modelling; Simulation

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1. Introduction

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. Modelling becomes, therefore, the indispensable tool in materials science and in materials engineering [1-10].

The artificial neural networks are a universal tool for a numerical modelling capable of mapping of complex functions. The adaptation of neural networks to fulfilling a definite assignment does not require the determination of an algorithm or recording it in the form of a computer program. This process replaces learning using a series of typical stimulations and corresponding to them desirable reactions. The basic feature of neural networks is their capability to a generalization of knowledge for the new data not presented in the learning process. The neural networks do not require collecting and direct access to the knowledge about the issue; they present a tolerance towards discontinuity, accidental disturbances or lacks in the learning set.

This fact allows applying them whenever there are problems with data processing and analysis, their classification, prediction or control. For several years, neural networks are more and more often used in the material engineering [11-15]. This growing popularity of neural networks results from the possibilities of creating relations between the examined quantities without any knowledge concerning a physical pattern of described phenomena. The results delivered by the neural network very often present bigger compatibility with the empirical data than with the results obtained thanks to the empirical interrelations or mathematic models of the analysed processes.

The paper presents the application of artificial neural network for evaluation of alloying elements effect on hardness and fracture toughness of high speed steels and austenite transformations during continuous cooling.

2. The effect of alloying elements on properties of HSS steels

Simulations of the alloying elements effect on steels properties has been made with use of suitable neural network models which make it possible calculation of the hardness and fracture toughness of high-speed steels.

For modelling of the high-speed steels secondary hardness basing only on steels chemical composition and austenitizing and tempering temperatures, the 8-7-1 multi-layer feedforward neural network with learning rule based on the error backpropagation algorithm and conjugate gradient were employed. There are eight nodes on the input of the network and 6 of them represent the values of the concentration of particular alloying element occurring in the analysed steels (C, Cr, Mo, V, W and Co). Next two inputs represent austenitising and tempering temperatures. The node on the output network layer represents the value of the secondary steel hardness.

The base of calculations are:

- results of investigations of newly developed high-speed steels [16-18],
- data included in standards [19],
- data included in suppliers catalogue [20] containing information about these steels.

Ranges of the alloying elements occurring in analysed steels and heat-treatment parameters are presented in Table 1.

Table 1.
Ranges of mass concentrations of the alloying elements occurring in the analysed high-speed steels

	Mass concentration of alloying element, %					
	C	Cr	W	Mo	V	Co
Minimum	0.72	3.7	0	0	1	0
Maximum	1.41	4.7	18	9.5	4.5	11

This way the appropriate set of data has been obtained which describes the secondary steel hardness' values depending on the chemical composition and heat–treatment parameters containing 2716 results. The model developed was experimentally verified. The verification procedure consists of the evaluation of the conformity of the computational results with the experimental data. As a criterion, an average error for a tested data set has been accepted:

$$R = \frac{1}{N}\sum_{i=1}^{N}\left(\left|H_{ci} - H_{mi}\right|\right) \tag{1}$$

where: N – testing set size, H_{ci} – calculated hardness, H_{mi} – measured hardness.

The calculation results obtained indicate good conformity of the secondary hardness calculations with the experimental data. The average value of the calculation error was R=0.59 HRC.

The methodology of modelling of the high-speed steels fracture toughness KIC is analogous to presented above. The 8-6-1 multi-layer feedforward neural network with learning rule based on the error backpropagation algorithm and conjugate gradient were employed. There are eight nodes on the input of the network and 6 of them represent the values of the concentration of particular alloying element occurring in the analysed steels (C, Cr, Mo, V, W and Co). Next two inputs represent austenitising and tempering temperatures. The node on the output network layer represents the value of the fracture toughness of steel. The average value of the calculation error was R=0.39 MPa $\sqrt{m}$).

The neural network models developed within the framework of the research make computer simulations possible pertaining, among others, to:

- effect of the selected element on steel properties or increase of this property value for the fixed concentrations of the other alloy elements and constant austenitizing- and tempering temperatures,
- analysis of the simultaneous effect of two selected elements on steel properties, for 6 fixed concentrations of the other alloy elements and constant austenitizing- and tempering temperatures.

Simulation investigations were carried out in the concentration ranges of the alloy elements occurring in the investigated steels, specified in Table 1.

2.1. Simulation of a single element effect on the high-speed steels hardness

In this example the developed neural network model was used for simulation of the effect of a single selected alloy element on hardness growth, with the fixed concentrations of the other elements. The exemplary analysis was carried out of the effect of the selected elements (tungsten and molybdenum) with and without the alloy addition of cobalt in steels.

It is also possible, apart from the presented examples, to carry out extended simulation analyses of the effect of the chemical composition on the secondary hardness effect within the range of concentrations of the alloy elements occurring in the analysed group of steels.

Examples of the analyses carried out of the effect of the selected alloy element with the fixed concentrations of the other alloy elements given in Table 2 are presented in Figures 1-6.

Table 2.
Fixed concentrations of alloy elements used in calculations

Mass concentration of alloying element, %					
C	Cr	W	Mo	V	Co
1.0	4.2	6.5	4	2	0

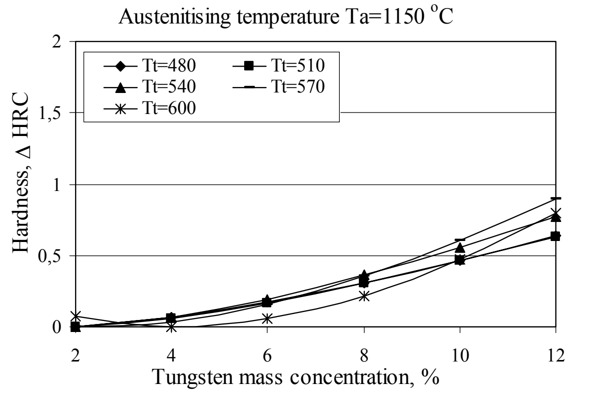

Fig. 1. Effect of tungsten on the high-speed steel hardness growth (Ta=1150°C)

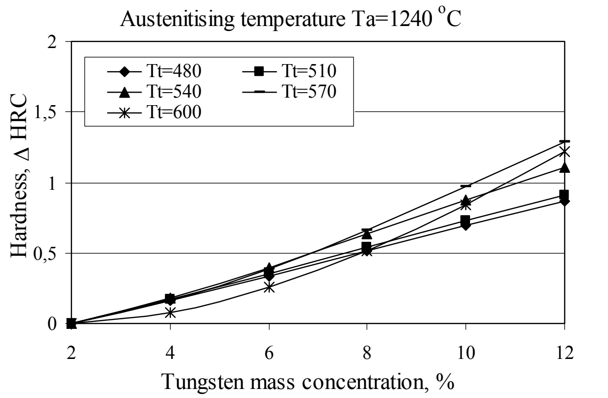

Fig. 2. Effect of tungsten on the high-speed steel hardness growth (Ta=1240°C)

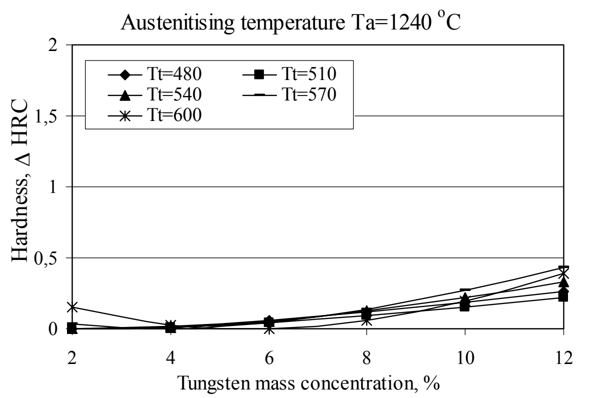

Fig. 3. Effect of tungsten on the high-speed steel hardness growth, Co=5.5% (Ta=1240°C)

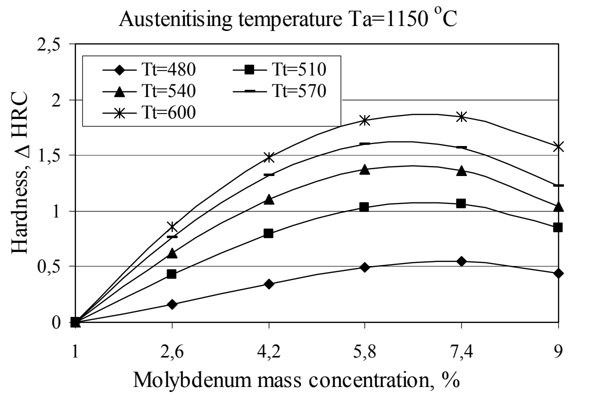

Fig. 4. Effect of molybdenum on the high-speed steel hardness growth (Ta=1150°C)

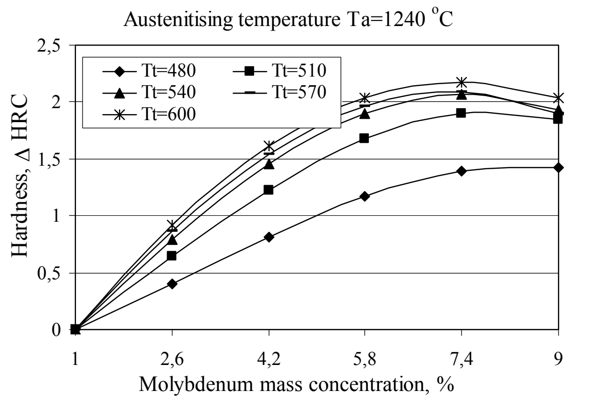

Fig. 5. Effect of molybdenum on the high-speed steel hardness (Ta=1240°C)

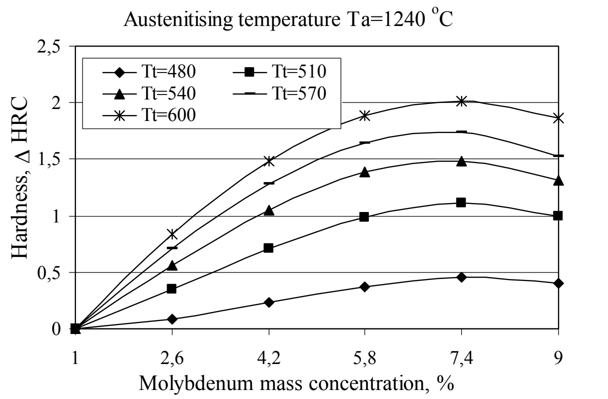

Fig. 6. Effect of molybdenum on the high-speed steel hardness growth, Co=5.5% (Ta=1240°C)

2.2. Simulation of two elements effect on the high-speed steels hardness and fracture toughness

The second simulation example presents the effect of two selected alloy elements on steel hardness with the fixed concentrations of the other elements and heat treatment parameters, as well as the fracture toughness. In case of fracture toughness, results of the effect of two elements are presented as well as of the heat treatment temperature. Fixed concentration was used and heat treatment parameters presented in Table 3.

Results of the simulation for various combinations of elements are presented in Figures 7-12.

Table 3.
Fixed concentrations of alloy elements used for simulation of the effect of two elements

Mass concentration of alloying element, %						Temperature, ^{o}C	
C	Cr	W	Mo	V	Co	Ta	Tt
0.95	4.1	6.5	4.5	1.8	0	1220	550

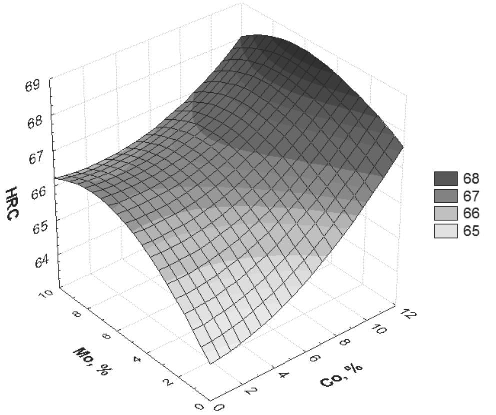

Fig. 7. Effect of molybdenum and cobalt on hardness of steel

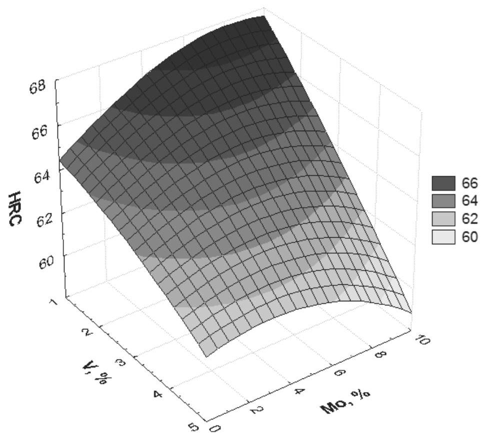

Fig. 8. Effect of vanadium and molybdenum on hardness of steel

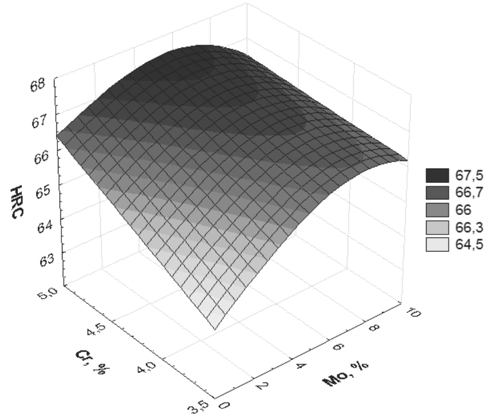

Fig. 9. Effect of chromium and molybdenum on hardness of steel

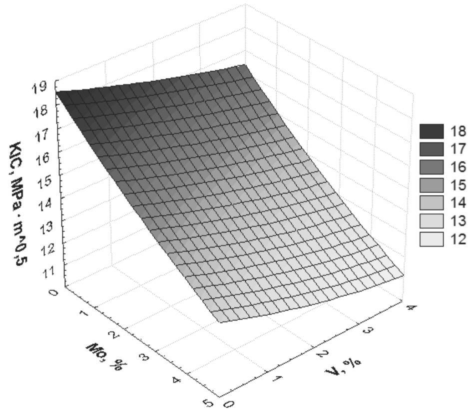

Fig. 10. Effect of molybdenum and vanadium on fracture toughness of steel

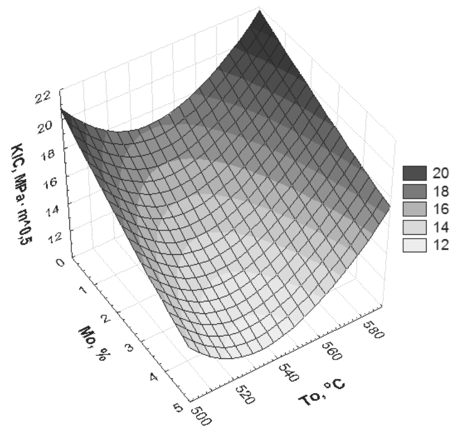

Fig. 11. Effect of molybdenum and tempering temperature on fracture toughness of steel

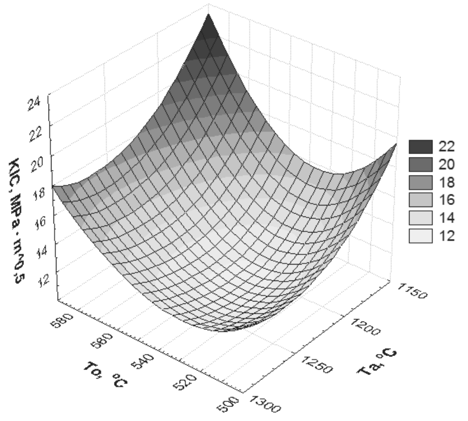

Fig. 12. Effect of austenitising and tempering temperature on fracture toughness of steel

3. The effect of chemical composition on CCT diagrams shape

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. Locations and shapes of the supercooled austenite transformations' curves, plotted on the CCT diagrams, depends mostly on the chemical composition of the steel, extent of austenite homogenising, austenite grain size, as well as on austenitizing temperature and time. Fluctuations of the chemical composition of steel, allowable even within the same steel grade, and also changes of the austenitizing conditions make that using the CCT diagrams published as catalogues does not provide reliable information on austenite transformations during cooling. In papers [21-23] the authors' method of CCT diagrams calculation has been described.

The data set was developed on the basis of on literature data, including chemical compositions, austenitising temperature (T_A) and the CCT diagrams of the constructional and engineering steels. The obtained curves were worked out, assuming mass fractions of the alloying elements as the criterion. Basing on the collected data it was assumed in addition that total of the mass fractions of manganese, chromium, nickel, and molybdenum does not exceed 5%. The ranges of the assumed mass fractions of elements and austenitising temperature are included in Table 4.

Table 4.
Ranges of mass fractions of elements for the analysed steels

	Mass concentration of alloying element, %						
	C	Mn	Si	Cr	Ni	Mo	V	Cu
Min	0.08	0.13	0.12	0	1	0	0	0
Max	0.77	2.04	1.90	2.08	3.65	1.24	0.36	0.3

The algorithm has been based on four modules. The task of the data entry module is receiving information like chemical composition and austenitizing temperature and linking them with the cooling rates. The classification module composed of classifiers based on the neural networks carries out the task of identification of the structural elements occurring in the steel after completing its continuous cooling at a pre-determined rate. The calculation module employs neural networks for determining the critical values of the time and temperature of transformations, temperatures of beginning and end of transformations, hardness, as well as concentrations of the structural elements. Some information from the classification and calculation modules is processed using rules included in the fourth module, safe-guarding from errors that may occur because of splitting the general task. The outputs from the particular modules feature the data that unequivocally defines the form of the CCT diagram and are the basis for its graphical representation. Total of 20 neural network models are used for calculating the CCT diagram for the assumed chemical composition, their task is to: determine the types of the occurring transformations at given cooling rates (classification), calculate the critical temperatures of transformations (Ac_1, Ac_3, M_s, B_s), calculate time to start and end of the particular transformations as functions of cooling rate, calculate hardness and volume fraction of the particular structural elements as functions of cooling rate. Computer program for forecasting anisothermic diagrams of supercooled austenite based on artificial neural networks model was presented in [23]. The developed neural network models make it possible to carry out computer simulation of the effect of chemical composition, austenitising temperature and/or cooling rate on a selected quantity describing austenite transformations in the CCT diagram i.e.: time to the start of the bainitic transformation, referring to the point of the shortest supercooled austenite life in the bainitic occurrence zone t_{Bs}, CCT diagrams shape.

Figures 13-22 present examples of diagrams illustrating the particular alloying elements' effects on the CCT diagrams shape and time to the bainitic transformation start.

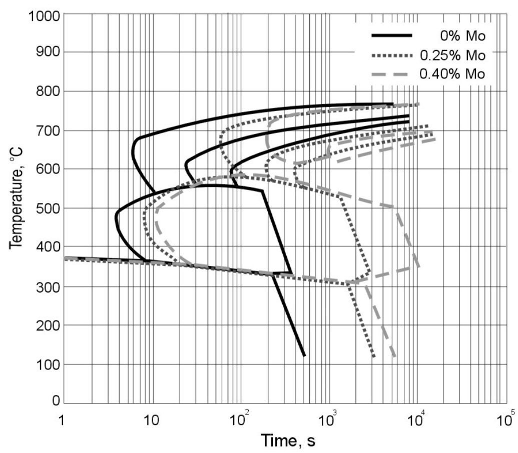

Fig. 13. Effect of molybdenum on CCT diagram shape of the steel austenitized at the temperature of 850°C with concentrations: 0.38%C, 0.64%Mn, 0.23%Si, 0.99%Cr, 0.08%Ni

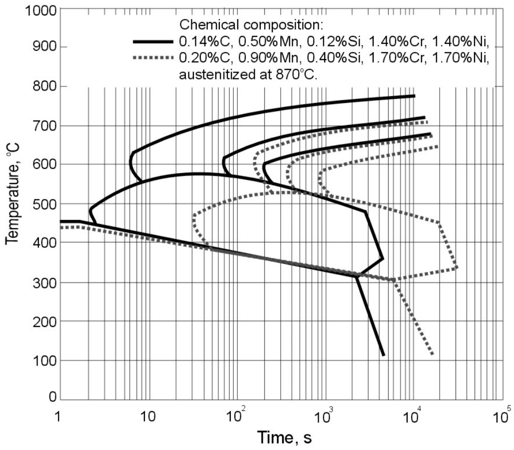

Fig. 14. Effect of alloying elements on CCT diagram shape of the 17CrNi6-6 steel grade

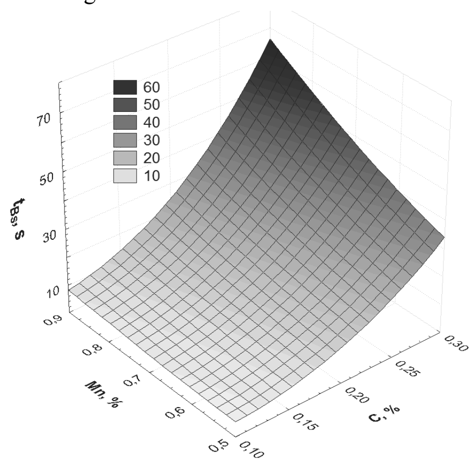

Fig. 15. Effect of carbon and manganese on t_{Bs} time of the steel austenitized at the temperature of 870°C with concentrations: 0.31% Si, 1.50% Cr, 1.55% Ni

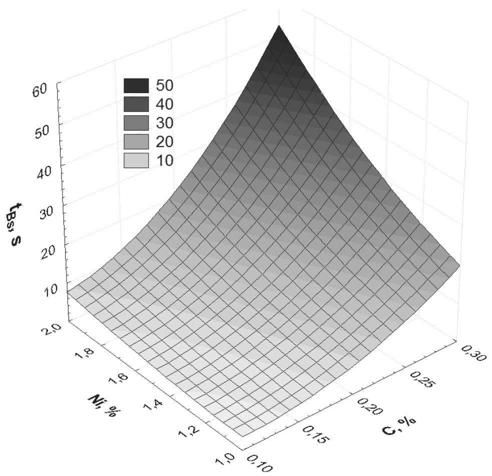

Fig. 16. Effect of carbon and nickel on t_{Bs} time of the steel austenitized at the temperature of 870°C with concentrations 0.51%Mn;0.31%Si;1.50%Cr

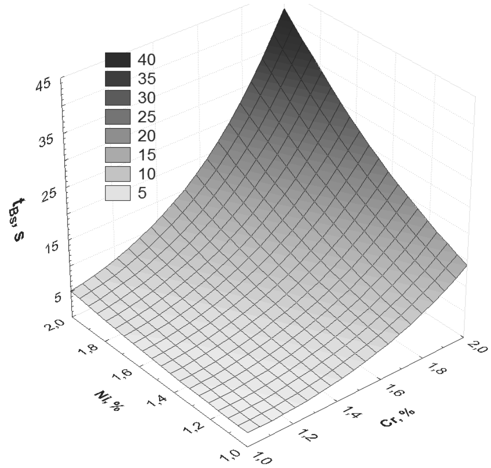

Fig. 17. Effect of chromium and nickel on t_{Bs} time of the steel austenitized at the temperature of 870°C with concentrations: 0.14%C, 0.51%Mn, 0.31% Si

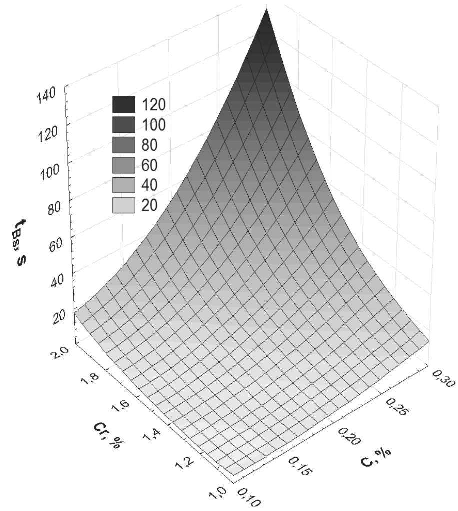

Fig. 18. Effect of carbon and chromium on t_{Bs} time of the steel austenitized at the temperature of 870°C with concentrations: 0.51%Mn, 0.31% Si, 1.55% Ni

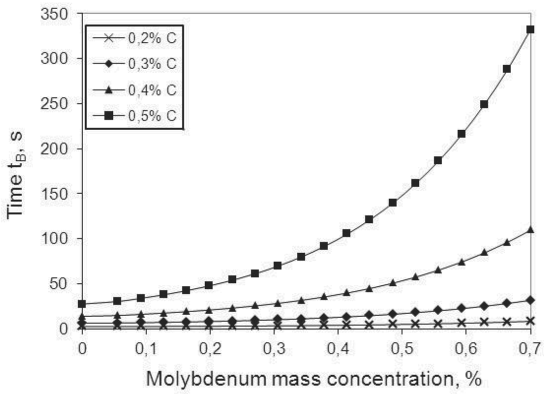

Fig. 19. Effect of carbon and molybdenum on t_{Bs} time of the steel with concentrations: 1.5%Mn, 0.15%Si, 0.02%Cr, 1.5%Ni

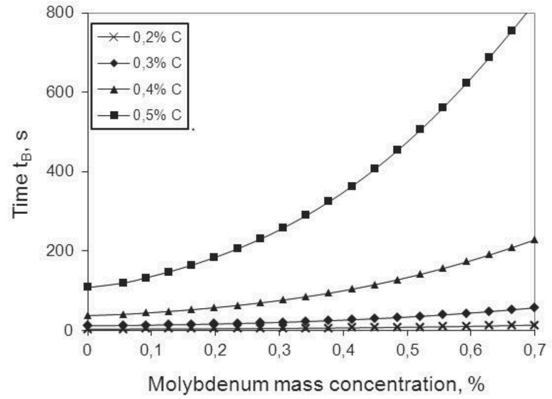

Fig. 20. Effect of carbon and molybdenum on t_{Bs} time of the steel with concentrations: 1.5%Mn, 0.15%Si, 1.5%Cr, 0.02%Ni

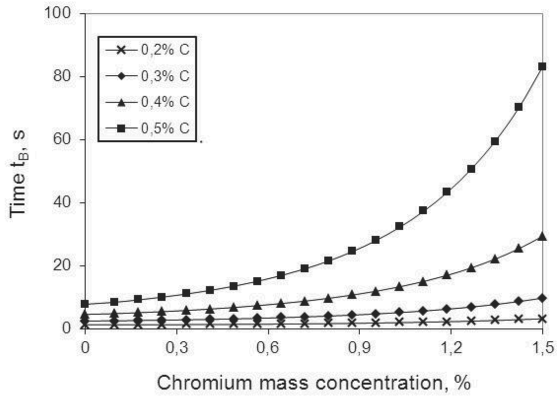

Fig. 21. Effect of carbon and chromium on t_{Bs} time of the steel with concentrations: 1.5%Mn, 1.3%Si, 0.02%Ni, 0.02%Mo

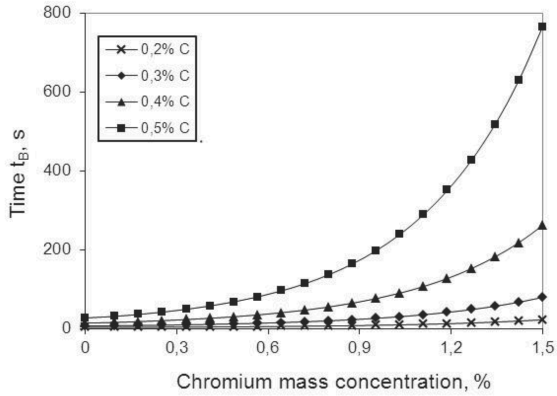

Fig. 22. Effect of carbon and chromium on t_{Bs} time of the steel with concentrations: 1.5%Mn, 0.15%Si, 1.5%Ni, 0.02%Mo

4. Final remarks

The paper presents the application of artificial neural network for evaluation of alloying elements effect on selected materials properties and austenite transformations during continuous cooling. Obtained results show that neural network are useful in evaluation of synergic effect of alloying elements on selected materials properties when classical investigations' results do not provide evaluation of the effect of two or more alloying elements.

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