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Evaluation of chemical composition effect on materials properties using AI methods

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Analysis and modeling

ABSTRACT

Purpose: 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.
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.
Research limitations/implications: The results presented are valid in the ranges of mass concentrations of alloying elements presented in the paper.
Practical implications: The worked out relationships may be used in computer systems of steels' designing for the heat-treated machine parts.
Originality/value: The use of the neural networks as an tool for evaluation of the chemical composition effect on steels' properties.
Keywords: Computational material science; Artificial intelligence methods; Materials design; Mechanical properties; Metallic alloys

1. Introduction

The paper presents application the method for evaluation of the effect of the alloying elements on ssteels' properties, using neural networks. First the application of method of hardenability modelling for evaluation of the effect of the alloying elements on steels' hardenability, using neural networks is presented. The developed neural networks models can be employed for simulations of the relationship between hardness at a given distance from the Jominy specimen face and the chemical composition of steel. Next the possibility of employment of the supercooled austenite transformation anisothermic diagrams forecasting method for analysis of the chemical composition effect on the CCT diagrams shape is presented. The developed model makes it possible to substitute computer simulation for the costly and time consuming experiments. The information derived from calculations make it possible to plot diagrams illustrating the effects of the particular elements or pairs of elements, as well as cooling rate and/or austenitizing temperature, on any temperature or time describing transformations in steel during its continuous cooling. Evaluation is also possible of the effect of the aforementioned factors on hardness and fractions of the particular structural constituents. This can be done in the entire range of concentrations of the main alloying elements occurring in constructional and engineering steels.

There is a great interest in AI methods, which seems justified, since they can be applied both to solving novel problems and to dealing with the ones considered classical. For a couple of years, such trends have been present also in the domain of materials engineering [1-15].

2. Computer simulation of the effect of alloying elements on hardenability of steels

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. Hardenability depends mainly on the chemical composition. Therefore, frequent attempts to employ the numerical methods of evaluating of the steel hardenability, alternative to the experimental ones, were made. Employment of different calculation methods for steels with the same chemical composition often yields different hardenability estimation results. The incomplete pertinence of the mathematical model assumed, as well as errors committed in investigation of hardenability using a method of cooling from the specimen face, results often in discrepancy between the calculation results and the experimental data published in literature, standards, and steel catalogues. The authors' own works performed so far indicate to the necessity of developing a new method of Jominy curves calculation, more adequate to the curves obtained experimentally than the models published so far. The paper is continuation of these works and presents results of computer simulation of the effect of the alloying elements on hardenability of steels.

Multi-layer feedforward neural networks with learning rule based on the error backpropagation algorithm were employed for modelling of the hardenability curves. For designing, learning and testing the STATISTICA Neural Networks ver 4.0 software was employed. It was assumed that heat treatment has been done in optimal conditions for particular steel. All the neural networks considered had six input nodes and fifteen output nodes. The network architecture employed was the consequence of the assumption that the steel hardenability is mainly affected by six basic elements occurring in the alloy constructional steels, i.e. carbon, silicon, manganium, chromium, nickel and molybdenum. Six nodes of the neural network input layer correspond to the concentration of the elements mentioned. Hardness on the hardenability curve is calculated at fifteen points.

More than 500 neural networks with various number of the hidden layer and number of the hidden neurones were considered. The neural networks were trained and tested basing on the set of data consisted of information concerning the chemical compositions (concentrations of the main alloying elements occurring in theses steels' groups) and results of Jominy hardenability test of more than 1000 various heats of carburizing and heat-treatable alloy structural steel grades. During the learning procedure the number of iterations was changed in the range from 100 to 10000 and the learning coefficient in the range from 0.01 to 0.1.

The verifying calculations were made for 227 heats of carburizing and heat-treatable alloy constructional steels. Value of the error evaluating the calculation method adequacy was recorded during the procedure for each heat analysed. As the result of the error analysis the 3 neural networks with the architecture 6-5-8-15, 6-7-7-15 with the error of calculation of 1,64 HRC, and the 6-8-8-15 with the error of 1,63 HRC were accepted. The neural networks worked out were employed for the computer simulation of the effect of particular alloying elements on the steels' hardenability.

Table 1.
Mass concentration of the alloying elements for the maps presented in figure 1

Fig. 1	Mass concentration of the alloying element, %			
a-b	C	Mn	Si	Ni
	0.35	1.1	0.25	0.1
c-d	C	Si	Ni	Mo
	0.35	0.25	0.1	0.05

For the analyses the constant concentrations of the not-analysed elements were assumed as it is included in table 1. Hardness at a fixed criterial distance l from the specimen end-quench test was assumed as hardenability measure. As an example, the distances of 11, 25 and 40 mm from the specimen face were assumed. In such cases it is possible to make any two-dimensional maps and figure 1 presents the effect of selected elements on hardenability hardness at the assumed distances.

3. Analysis of chemical composition effect on CCT diagrams shape

In works [6-8] the original CCT diagrams forecasting method was presented for steels in which mass concentrations of elements are within the ranges shown in Table 2. The relationship between the chemical composition and austenitizing temperature, and the anisothermic diagrams of the supercooled austenite were developed using neural networks. The CCT diagrams calculation process may be divided into two stages. In the first stage it was determined if along the analyzed cooling rate path zones occur of: ferrite, pearlite, bainite, and if the martensitic transformation occurs. The range of the cooling duration time, characteristic for the particular transformations, and types of the structure constituents occurring in the steel after cooling were determined as a result of the classification process. Further, temperature values were calculated of start and end of the particular transformations for each of the analysed cooling rates. Information regarding the types of the structure constituents that originated in the steel as a result of its cooling at a particular rate was used to determine steel hardness and volume fraction of ferrite, pearlite, bainite, and martensite with the retained austenite The method consists of four modules: data entry module, classification module, calculation module, set of conditional statements. 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. 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

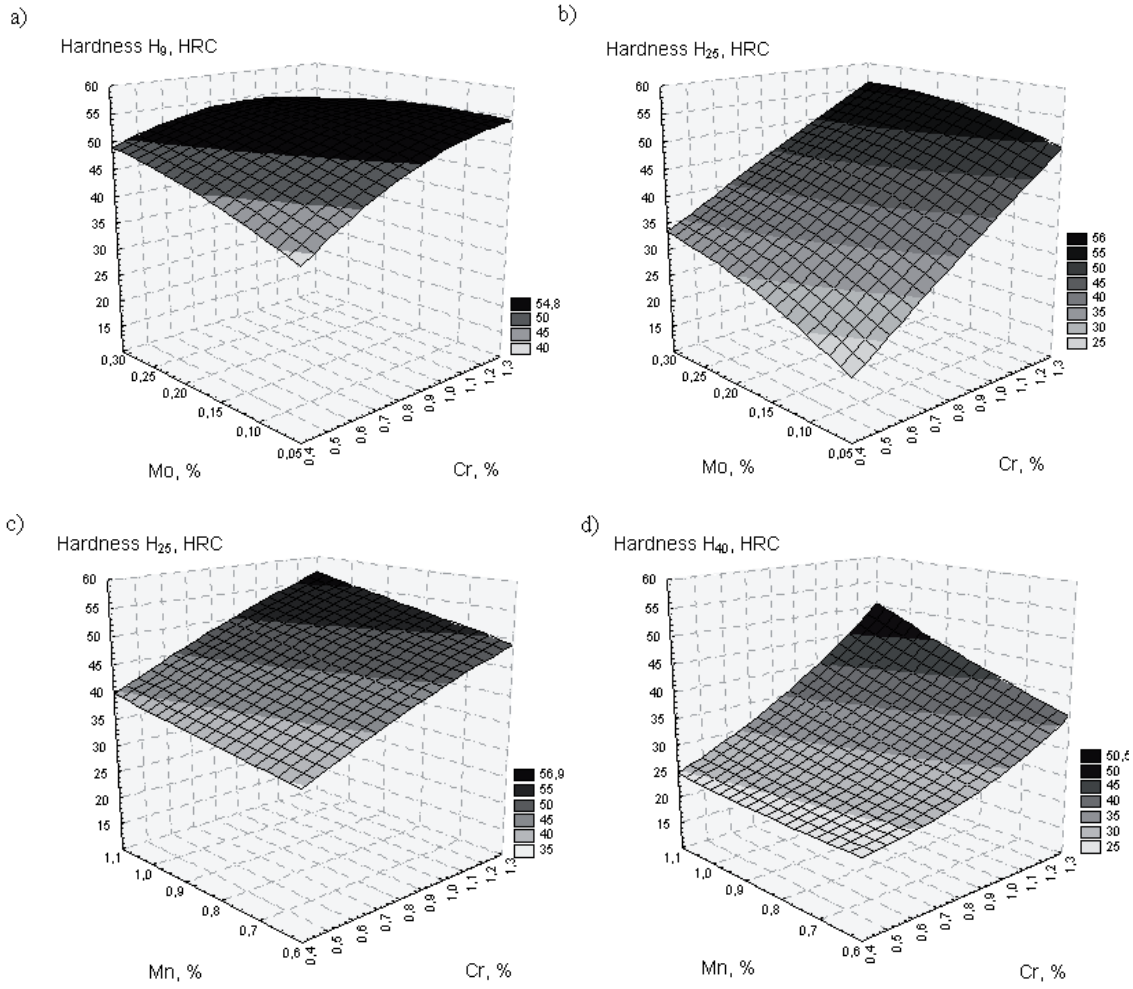

Fig. 1. Evaluation of the effect of selected elements on hardness at the criterial distances of 9, 25 and 40 mm from Jominy specimen face, for the set mass concentrations of the elements included in table 1

transformations in the CCT diagram i.e: 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_{smax}, temperatures of start and end of ferrite occurrence at a particular cooling rate F_s, F_f. The influence of a single factor, and also an arbitrary pair of factors on a selected quantity describing austenite transformations during the

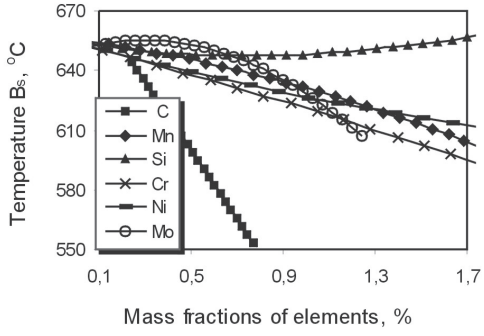

Fig. 2. Effect of the alloying elements on the A_{c3} temperature of the steel with the concentrations: 0.1%C, 0.2%Mn, 0.1%Si

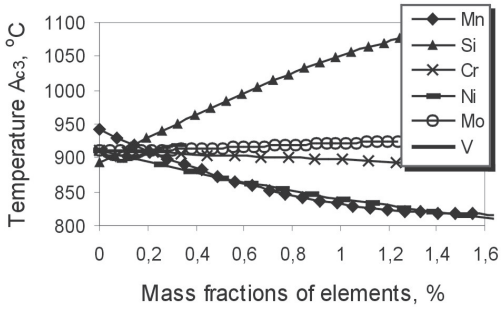

Fig. 3. Effect of the alloying elements on the B_s temperature of the steel of the remaining elements: 0.2%C, 0.2%Mn, 0.15%Si, 0.05%Cr, 0.05%Ni, 0.05%Mo

continuous cooling can be analysed in the steel chemical composition range presented in Table 2.

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

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

Figures 2-4 present examples of diagrams illustrating the particular alloying elements' effects on the A_{c3}, M_s, B_s temperatures and the time to the bainitic transformation start.

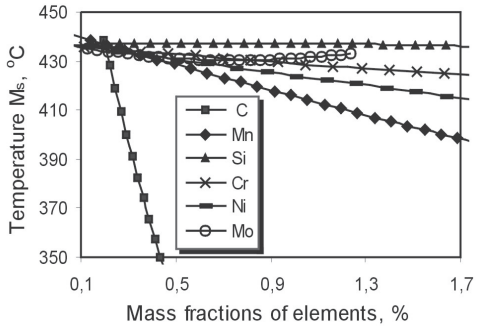

Fig. 4. Effect of the alloying elements on the M_s temperature of the steel of the remaining elements: 0.2%C, 0.2%Mn, 0.15%Si, 0.05%Cr, 0.05%Ni, 0.05%Mo

4. Summary

The paper presented application of method of hardenability modelling for evaluation of the effect of the alloying elements on steels' hardenability, using neural networks. Vast potential use of the computer tools developed was pointed out, and their practical usefulness was illustrated by examples. The developed neural network model can also be employed for simulations of the relationship between hardness at a given distance from the Jominy specimen face and the chemical composition of steel. This can be done in the entire range of concentrations of the main alloying elements occurring in constructional alloy steels. Application of the presented method, using the computer program developed, enables a scientist to make free analyses of the effect of the alloying elements occurring in heat-treatable alloy constructional steels using only computer simulation, without having to carry out additional and expensive experimental investigations

The synergetic effect of the alloying elements on austenite transformations during the continuous cooling is the reason for which analysing the influence of single elements does not reveal fully their real effect. The influence of the alloying elements should be analyzed for the particular elements at the fixed concentration of the remaining constituents in the analysed steel. The artificial intelligence tools, including the neural networks, make it possible to substitute partially the costly and time consuming experimental investigations with the computer simulation and using the obtained results as data for further analyses. Thanks to the method developed in the project, analyses can be made referring to the effect of the selected elements on any temperature or time describing the austenite transformation and also hardness and volume fractions of the structural constituents which originate due to cooling the steel from the austenitising temperature. One should also stress the big potential of employment of the developed model in the didactic process.

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