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Neural networks model for prediction of the hardness of steels cooled from the austenitizing temperature

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ABSTRACT

Purpose: The paper presents the new neural networks model making it possible to estimate the hardness of continuously-cooled steel from the austenitizing temperature.

Design/methodology/approach: The method proposed in the paper employs two applications of the neural networks of: classification and regression. Classification and consists in determining the value of dichotomous variables describing the occurrence of: ferrite, pearlite, bainite and martensite in the microstructure of a steel. The values of dichotomous variables have been used for calculating steel hardness. The other task is regression, which aims at calculating the steel hardness.

Findings: The presented neural networks model can be used only in the range of concentrations of alloying elements shown in this paper.

Practical implications: The model worked out makes it possible to calculate hardness for the steel with a known chemical composition. This model deliver important information for the rational selection of steel for those parts of the machines that are subjected to the heat treatment. The presented model make it possible the analysis of the interaction of the chemical composition on the hardness curves of the steel cooled from the austenitizing temperature.

Originality/value: The paper presents the method for calculating hardness of the structural and engineering steels, depending on their chemical composition, austenitizing temperature and cooling rate.

Keywords: Computational Material Science; Steel; Neural Networks; CCT diagram

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METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

1. Introduction

The recent years have seen a considerable progress as regards the methods and tools allowing for modelling and simulation of the technological processes of manufacturing, processing and shaping the operating properties and structure of materials. Computer aided modelling is present both in research and in industrial

practice. It is a relatively cheap and effective method of optimising, among others, the chemical composition and conditions of technological processes, making it easier to obtain desired characteristics of materials. Modelling of heat treatment requires an analysis of many inter-related factors that influence the process and concentrates on comprehensive solutions and selected issues. The most popular numeric methods in modelling technological processes are characterised by a high level of flexibility, allow for an analysis of the issue in complex geometry objects and taking into account changes of thermo-physical parameters [1]. Aside from mathematical modelling and the numerical methods related to it, bio-inspired methods are used increasingly frequently.

The increasing popularity of artificial intelligence and computational intelligence methods in many fields of science and engineering is also reflected by the area of materials engineering [2-7]. Use of hybrid methods is a visible trend related to modelling in materials engineering [8,9].

Selection of steel for construction elements and machines parts requires analysis of working conditions and assuring appropriate values, taking into account their changes in profile. In case of structural and engineering steels the required values are obtained due to correctly adjusted chemical composition of steel and correct microstructure shaping resulting from thermal, thermal-plastic or thermal-chemical processing. Time-Temperature-Transformation diagram provides material information on the opportunity of obtaining the required steel microstructure and hardness depending on the course of its cooling from the austenitizing temperature. Knowledge of austenite transformation kinetics occurring during continuous cooling of steel from the austenitizing temperature presented at CCT diagrams helps determine the conditions of operations such as hardening, normalising or full annealing. The position and shape of austenite transformation curves marked on CCT diagrams depend primarily on the chemical composition of steel, the initial condition of material and the conditions of austenitizing [10].

Attempts to modelling austenite transformation were and still are taken, in parallel to experimental studies [11]. A popular method of modelling in this area is multiple regression [12,13]. Although first equations describing temperatures of phase transformations were described by Payson and Savage [14] and Carapella [15] more than fifty years ago, new models are still proposed and might be used for various groups of steels. Many of the empirical formulae available in literature was collected in the work [16]. Aside from the multiple regression method, artificial neural networks are used as well. Results of the first works presenting neural models of temperatures of austenite transformations were published at the end of 20th century [17,18] and, similarly to the case of multiple regression, new solutions are still being presented.

A popular model taken advantage for the purpose of the calculations of microstructural constituents and the hardness of a continuously-cooled steel from the austenitizing temperature is the Maynier model [19]. The Maynier model was developed upon the basis of the data acquired from approximately 300 CCT diagrams. The Maynier equations make it possible to calculate the typical cooling rates at the temperature of 700°C, for which in the microstructure of steels the following quantities are formed: 100%, 90% and 50% of martensite, 90% and 50% of bainite, and also 90% and 100% of ferrite and pearlite respectively. In the literature, there are as well examples of the calculations of the hardness of a continuously-cooled steel upon the basis of the Jominy hardenability curve [20].

The first results of own research connected with modelling the hardness of steel cooled from the austenitizing temperature were presented in the papers [21,22]. For the purpose of developing the hardness model, the method of artificial neural network was applied.

Complementing and extending the collection of empirical data made it possible to develop equations connecting the chemical composition of a steel, the cooling rate and the austenitizing temperature with the hardness of a steel. The collection of empirical data was prepared upon the basis of more than 500 CCT diagrams. In paper [2323], the equations applied for the purpose of the calculations of the hardness of continuously cooled structural steels upon the basis of the chemical composition as well as austenitizing temperature. In the hardness models developed with the application of multiple regression method [23], the significant variables were constituted by dichotomous variables describing the occurrence of: ferrite, pearlite, bainite and martensite in the microstructure of a steel. For the purpose of the calculation of those variables, the classifier developed with the application of the logistic regression method was applied.

In the paper, the new neural networks model was presented making it possible to estimate the hardness of continuously-cooled steel from the austenitizing temperature.

2. Data for calculation

Modelling hardness with the application of the neural networks method required preparing a representative empirical data set. New results of research conducted for

commercial steel, experimental steel and model alloys as well as easier access to information offer significant opportunities in this regard. The data set was developed upon the basis of available publications containing experimentally-determined CCT diagrams for structural and engineering steels.

A set of empirical data has been compiled by digitalising CCT diagrams. More than 500 structural and engineering steel have been analysed. The selection of variables is the result of the knowledge of the modelling process. However, the availability of data often requires the adoption of necessary simplifications. Vectors that contain examples used in modelling should include the values of all variables. The information connected with the austenite grain size and the austenitizing time was not provided on the majority of the CCT diagrams. For that very reason, it was necessary to adopt simplifications connected with the number of independent variables describing the model. It was presumed that the independent variables of the model would be the mass concentrations of the following elements: C, Mn, Si, Cr, Ni, Mo, V and Cu, the cooling rate, and also the austenitizing temperature.

The data set applied for the purpose of developing the model contained 2845 cases. In addition to that, a verification data set was separated, and that data set was taken advantage of for the purpose of the numerical verification of the model. The verification data set contained 300 cases. Upon the basis of one CCT diagram, several vectors containing the values of independent variables and the respective value of hardness were developed.

An analysis of the range of values of independent variables, in which the developed models can be used, was carried out. An analysis of data involving, among others: descriptive statistics, an analysis of outlying data, distribution of values for independent variables and an assessment of collinearity of independent variables allowed to define the scope of using the model. The maximum and minimum values of the mass fractions of elements were presented in Table 1. The additional conditions, relevant to the sums of the mass fractions of selected elements, were presented in Table 2.

The data set used to develop the model by the neural networks was divide into four subsets such as: training, validating, testing, and verifying. Allocation of data to the particular subsets was done randomly. The data from a training set were used for determining the values of weights in the training process. The validating set was used for checking the model during establishing the values of weights, the testing and verifying sets was used for verifying the model when the network training was completed. For hardness HV model the numbers of cases in the sets: training, validating, testing and verifying one were respectively: 1405, 550, 550, 300.

Table 1.
Ranges of mass concentrations of elements

Range	Mass fractions of elements, %							
	C	Mn	Si	Cr	Ni	Mo	V	Cu
min	0.10	0.25	0.13	0	0	0	0	0
max	0.68	1.82	1.68	2.3	3.69	1.05	0.38	0.38
average	0.32	0.79	0.33	0.72	0.75	0.17	0.02	0.04
SD	0.13	0.34	0.27	0.56	1.01	0.21	0.06	0.08

SD – standard deviation

Table 2.
Additional conditions for limiting the scope of model application

	Mass fractions of elements, %			
	Mn+Cr	Mn+Cr+Ni	Cr+Ni	Mn+Ni
max	3.6	5.6	5.3	4.5

3. Method and results

In the hardness models developed with the application of the artificial neural networks method [21] as well as the multiple regression and logistic regression method [23], the significant variables were constituted by dichotomous variables describing the occurrence of: ferrite, pearlite, bainite and martensite in the microstructure of a steel. The values of dichotomous variables obtained that way, identifying the transformations occurring during cooling with assumed speed have been used for calculating steel hardness. Therefore, the hardness model is based on the assumption that it is necessary to solve two types of tasks for their correct calculation. One task is classification and consists in determining the scope of cooling rate for individual phase transformations. The other is regression, which aims at calculating the steel hardness. The classification task defined that way might be equated with an answer to the question whether austenite-ferrite, austenite-perlite, austenite-bainite and austenite-martensite

transformations occur during cooling rate with known speed. The classifiers have been drawn up using the artificial neural networks method. The dichotomous dependent variable Wx describing the occurrence in the microstructure of the steels of the following: ferrite (W_f), pearlite (W_p), bainite (W_b) and martensite (W_m). The four classifiers based on neural networks were developed. Independent variables in the models were constituted by the mass concentrations of elements, the austenitizing temperature (T_A) and the cooling rate (v_c).

To develop the relationship between the chemical composition, austenitizing temperature, cooling rate, and hardness of the steels the feedforward neural networks (MLP - Multi-Layer Perceptron) were used. An MLP is the most universal type of neural network intended for solving tasks related to classification as well as regression [6]. Neural networks design consists of determining the parameters characterizing the network and then training as well as testing the network. In the case of MLP-type network basic parameters include the number of hidden layers and number of neurons in the particular layers, a variable scaling method, error functions, activation functions, and postsynaptic potential functions, method and parameters of training. The number of hidden layers and number of neurons in these layers, and also method and training parameters were specified analyzing the effect of these quantities on the neural network quality assessment coefficient values for the training and validating data sets as well as test set. The number of training epochs was determined by observing the network forecast error for the training and validating data sets. Methodology for the design of artificial neural networks was presented in work [6].

Information on neural network models used for determining the types of structural constituents occurring in the steel after the completed cooling process at a particular rate were compiled in Table 3.

The correctness of the classifiers was assessed upon the basis of the coefficient of correct classifications as well as the area under the ROC (Receiver Operating Characteristic) curve. The coefficient of correct classifications which was being determined as the quotient of correctly classified cases and all the examples in the data sets. The ROC curve expresses the neural network sensibility (second class classified correctly) as a function of the incorrectly classified first class. In case of the „ideal" classifier, the area under the ROC curve assumes value of 1. In case of random classifications, the area under the ROC curve assumes value of 0.5. The statistics of the classifiers were presented in Table 4.

Table 3.
Specifications of the developed classifiers based on neural networks

Output variable	Input variables	Neural network type	Neural network structure	Training method/No of epochs
W_f	C, Mn, Si, Cr, Ni, Mo, V, Cu, T_A, v_c	MLP	10-8-1	BP/50,CG/330
W_p			10-8-1	BP/50,CG/119
W_b			10-10-1	BP/50,CG/188
W_m			10-6-1	CG/100

BP – back propagation method; CG – conjugate gradients method

Table 4.
Quality assessment coefficients for models, used as classifiers for determining the types of occurring transformations

	Data sets	Transformation areas, output variable			
		Ferritic	Pearlitic	Bainitic	Martensitic
		W_f	W_p	W_b	W_m
Coefficient of correct classifications, %	training	0.92	0.92	0.86	0.89
	validating	0.91	0.92	0.86	0.86
	testing	0.89	0.91	0.84	0.86
ROC	training	0.97	0.97	0.93	0.95
	validating	0.97	0.97	0.92	0.94
	testing	0.96	0.97	0.92	0.93

Moreover, the hardness of steel was described in addition to that with the application of two neural networks which may be applied for a martensitic structure (HV_m) and also for the ferritic - pearlitic one (HV_{f-p}). The hardness models for a martensitic structure, and for the ferritic-pearlitic one, may be applied after obtaining the appropriate results of classifications. In the case of uncertain results of classifications, it is a better solution to apply the general model. Information on neural network models used for calculating the hardness occurring in the steel after the completed cooling process at a particular rate were presented in Table 5.

The hardness models were being assessed upon the basis of: the mean absolute error, the standard deviation of error, correlation coefficient and also the standard deviation quotient of the calculation error, as well as the standard deviation of the dependent variable value. The statistics of the hardness models were presented in Table 6.

Table 5.
Specifications of the neural networks used for calculating the steel hardness

Output variable	Input variables	Neural network type	Neural network structure	Training method/No of epochs
HV	C, Mn, Si, Cr, Ni, Mo, V, Cu, T_A, v_c, W_f, W_p, W_b, W_m	MLP	14-10-1	BP/50, CG/489
HV_m	C, Mn, Cr, Ni, V, Cu, v_c,		7-10-1	BP/50, CG/184
HV_{f-p}	C, Mn, Si, Cr, Ni, Mo, V, T_A, v_c		9-9-1	CG/189

Table 6.
Values of statistics used to evaluate the quality of the developed models

	Data sets	Mean absolute error, HV	Standard deviation of the error, HV	Ratio of standard deviations	Pearson's correlation coefficient
HV	training	31.5	45.4	0.28	0.96
	validating	33.8	47.5	0.29	0.96
	testing	33.1	48.9	0.30	0.95
HV_m	training	28.8	36.8	0.37	0.93
	validating	28.7	36.9	0.34	0.94
	testing	24.9	31.1	0.28	0.96
HV_{f-p}	training	17.1	21.0	0.46	0.89
	validating	17.5	22.0	0.43	0.90
	testing	18.2	22.3	0.44	0.90

The hardness model was numerically verified by means of comparison between the hardness curves determined experimentally and the calculated ones. The calculations were performed for data which were not taken advantage of for the purpose of developing the neural network models. The verification data set was composed of 25 chemical compositions of structural steel. The examples of the results were presented in Figures 1-3. The comparative plots for the experimental and calculated hardness were presented in Figures 4-6. Scatter plots of the experimental vs calculated values of the steel hardness were calculated using the HV, HV_m as well as HV_{f-p} models.

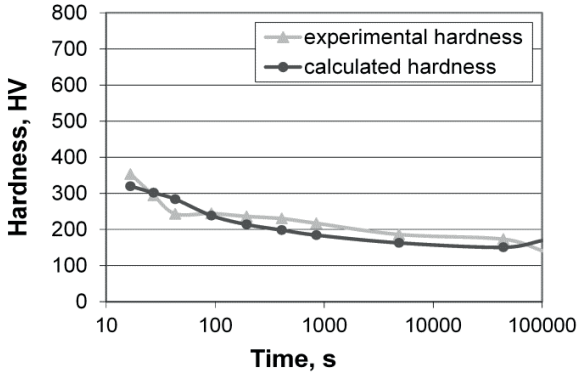

Fig. 1. The comparison of the experimental and calculated hardness curves for the steels with a mass concentration of elements: 0.14%C, 1.2%Mn, 0.1%Si, 0.15%Cr, 0.48%Ni, 0.15%V, 0.15%Cu austenitised at temperature of 900°C

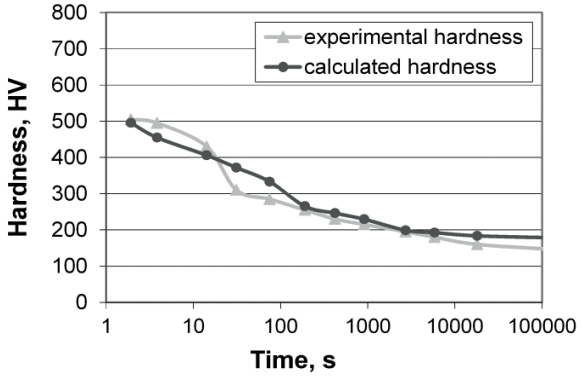

Fig. 2. The comparison of the experimental and calculated hardness curves for the steels with a mass concentration of elements: 0.22%C, 0.66%Mn, 0.3%Si, 0.56%Cr, 0.15%Ni, 0.44%Mo, 0.18%Cu austenitised at temperature of 890°C

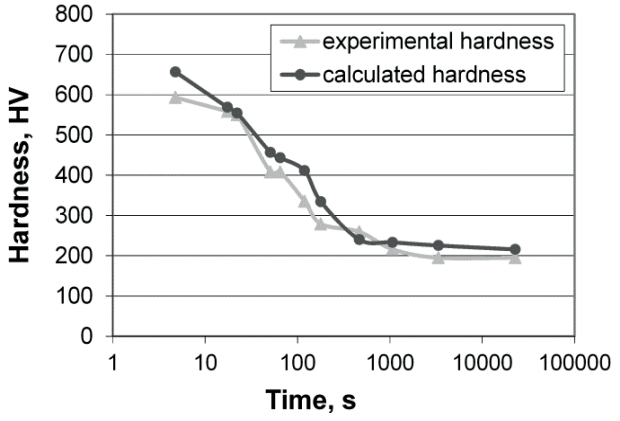

Fig. 3. The comparison of the experimental and calculated hardness curves for the steels with a mass concentration of elements: 0.38%C, 0.76%Mn, 0.26%Si, 0.9%Cr, 0.26%Ni, 0.17%Cu austenitised at temperature of 880°C

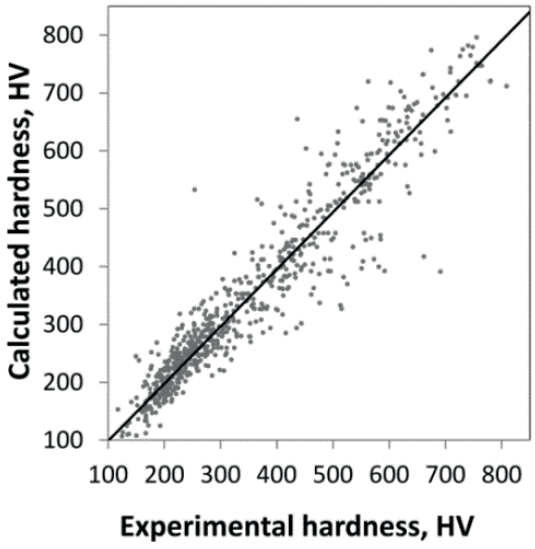

Fig. 4. Comparison of the experimental hardness with values out of the testing set calculated using the HV model

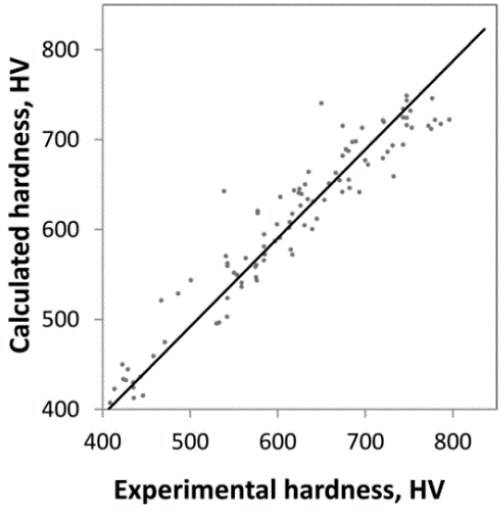

Fig. 5. Comparison of the experimental hardness with values out of the testing set calculated using the HV_m model

The results of the calculation of the steel hardness are burdened with some errors. Those results both from simplifications applied in the course of modelling, as well as from the specific character of empirical data. The data set was prepared based on the published CCT diagrams. Every vector of data taken advantage of in the course of the training of the neural network has to contain the values of all variables. Information relevant to the austenitizing time, and also to the austenite grain size, was not being provided on the majority of the CCT diagrams, and, for that very reason, it was not taken under consideration in the model. A significant problem is constituted as well by the graphic form of data and errors connected with making CCT diagrams and printing them, and also errors resulting from the digitalization of data. Moreover, simplifications concerning the chemical composition of the steels are often used. In this case, only mass concentrations of the basic elements are presented.

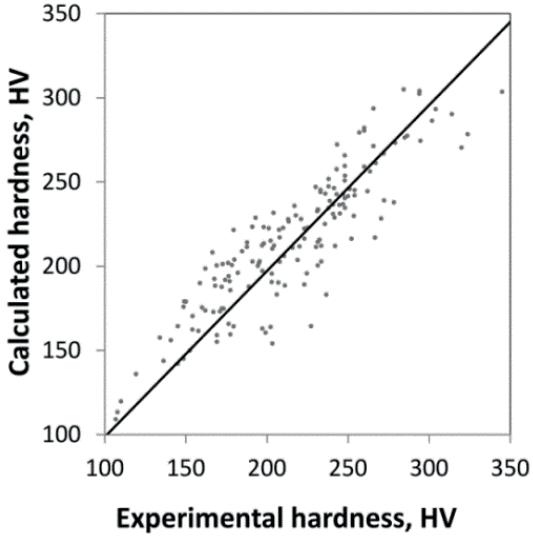

Fig. 6. Comparison of the experimental hardness with values out of the testing set calculated using the $HV_{f\text{-}p}$ model

4. Conclusions

The model worked out makes it possible to calculate hardness for the steel with a known chemical composition. The presented neural networks model can be used only in the range of concentrations of alloying elements shown in the Table 1. Simultaneously, the conditions set out in the Table 2 should be complied with. The hardness model for structural and engineering steels, continuously cooled from the austenitizing temperature, was developed as well with the application of the multiple regression and logistic regression method [23].

The presented model make it possible the analysis of the interaction of the chemical composition on the hardness curves of the steel cooled from the austenitizing temperature. This model deliver important information for

the rational selection of steel for those parts of the machines that are subjected to the heat treatment.

New models describing the hardness of steels have been applied for the purpose of modification of a computer program [24] for predictions of CCT diagrams for structural and engineering steels. Because of the limited publication volume, only the most important information characterising the developed model was presented. The detailed problem description was presented in [25]. Presented method might be used for other alloys and similar calculating tools might be developed for these alloys when having the required experimental data.

Computer aided modelling is a relatively cheap and effective method of optimising, among others, the chemical composition and conditions of technological processes, making it easier to obtain desired characteristics of materials. Computer aided calculations help reduce costs – also due to decreasing the number of necessary experiments.

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