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Selection method of steel grade with required hardenability

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Analysis and modelling

ABSTRACT

Purpose: The purpose of this paper is to work out the computer aided method for selecting grades of steel with a required hardenability.

Design/methodology/approach: The purpose has been achieved in two stages. In the first stage a neural network model for calculating the Jominy curve on the basis of the chemical composition has been worked out. This model made possible to prepare, in the second stage, a representative set of data and to work out the neural classifier that would aid the selection of steel grade with the required hardenability.

Findings: The calculations made in the paper have confirmed the purposefulness of applying artificial neural networks for aiding the selection of steel with the required hardenability.

Research limitations/implications: The presented system may be used in the range of the accepted in the paper mass concentrations of elements. The methodology demonstrated in the paper makes it possible to add new grades of steel to the system.

Practical implications: The worked out model may be used in computer systems of steel selection for the parts of machines exposed to the heat treatment.

Originality/value: The use of the artificial neural networks as an aiding tool for selecting the steel with the required hardenability.

Keywords: Computational material science; Metallic alloys; Artificial intelligence methods; Hardenability

1. Introduction

New requirements are established for designers of systems and machines due to development of contemporary software tools, especially of computer aided design systems, as well as methods of artificial intelligence. Contemporary designing of machines and their parts consists in making concurrent and proper selection of design features, of manufacturing process and of the most suitable material. Therefore, extending of CAD/CAM systems by adding CAMS system (Computer Aided Material Selection) is justified. Employment of such computer systems will undoubtedly eliminate subjective factors, or even errors in the materials selection [1-6]. As far as CACSS (Computer Aided Constructional Steel Selection) systems for machines parts are concerned, it is necessary to have a calculation model for hardenability forecasting adequate to the experimental results [7,8]. 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.

The purpose of this paper 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.

2. Material and method

The aim of this paper 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.

A representative data set has been prepared on the basis of the information concerning the chemical composition and the hardness measured for the consecutive distances from the quenched end for 500 constructional and engineering steel alloys.

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.

3. Calculation of Jominy curve

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 data was divided into three sets: training, validating and testing one. The training set was used for development of the neural network model, the validating set was used for checking the model during establishing the values of weights, and the testing set was used for verifying the model when the network training was completed. Allocation of data to the particular subsets was done randomly. Additionally, a verifying set has been separated, which consisted of 30 casts and served as the numerical verification of the worked out neural network models.

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 structure, method, training parameters and the mean error values of the neural networks for which the most beneficial values of the coefficient factors in both considered response coding variants have been obtained are presented in Table 2. 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 input layer. The approximate values of the mentioned coefficients for particular data sets indicate the ability of the network to generalize the knowledge acquired in the training process. The mean error value, ratio of standard deviations and the correlation coefficient for the selected distances from the quenched end have been compared in Table 3.

Table 2.
The structure, training parameters and the mean error values for networks designed for calculating the hardenability curve.

Network structure	Training method / No of epochs	Average error, HRC			
		training	validating	testing	verifying
7-10-1	CG/3600	1.45	1.48	1.46	1.45
6-13-13	CG/263	1.65	1.81	1.82	1.70

CG - conjugate gradients

Table 3.
The neural network quality coefficients with one neuron in the output layer in the selected distances from the quenched end.

	Data set	Distance from quenched end, mm					
		1.5	3	11	25	30	50
Average error, HRC	training	0.9	0.9	1.4	1.6	1.6	1.9
	validating	1.1	1.0	1.7	1.4	1.5	2.1
	testing	1.0	1.0	1.5	1.6	1.5	1.8
	verifying	1.1	1.1	1.3	1.6	1.6	1.9
Ratio of standard deviations	training	0.20	0.19	0.20	0.25	0.28	0.35
	validating	0.23	0.25	0.22	0.26	0.27	0.24
	testing	0.22	0.25	0.23	0.25	0.25	0.33
	verifying	0.22	0.25	0.18	0.23	0.24	0.30
Correlation coefficient	training	0.98	0.98	0.98	0.97	0.96	0.94
	validating	0.97	0.97	0.97	0.96	0.96	0.94
	testing	0.98	0.97	0.97	0.97	0.97	0.95
	verifying	0.98	0.97	0.98	0.97	0.97	0.97

In Figures 1 and 2 the Jominy curve has been compared, that has been calculated with the help of the neural network and determined experimentally.

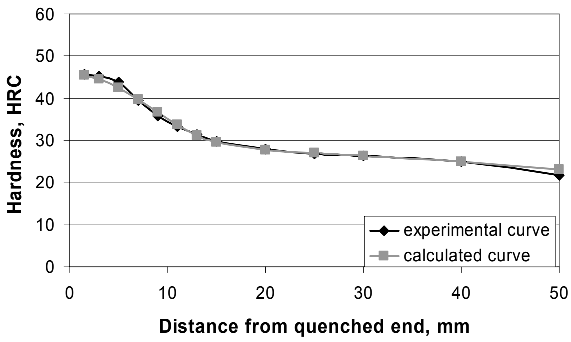

Fig. 1. The comparison of the experimental and calculated curves for the steels with a mass concentration of elements: 0.19%C, 0.94%Mn, 0.28%Si, 0.94%Cr, 0.17%Ni, 0.23%Mo

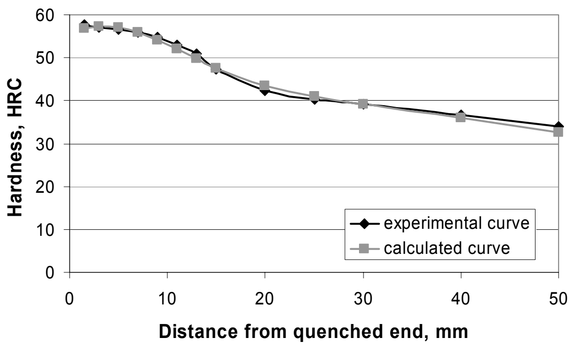

Fig. 2. The comparison of the experimental and calculated curves for the steels with a mass concentration of elements 0.4%C, 0.54%Mn, 0.24%Si, 0.69%Cr, 1.39%Ni, 0.2%Mo

4. Selection of steel grade

For calculations the feed-forward 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. 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.

4.1. Selection of steel grade by means of one output variable

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-z-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.

The numbers of neurons in the hidden layer, as well as the method and training parameters, were assumed by analyzing the effect of these quantities on the network quality evaluation parameters. Training method was used based on the conjugate gradient algorithm. The number of training epochs was determined by observing the network forecast error for the training and validating sets. The network with one hidden layer and numbers of neurons in these layer as 31 was assumed to be optimal.

On the basis of network response analysis it has been stated that the network provides most often false responses for the same steel grades. It has been observed that for a certain steel grade the network usually indicates the same equivalent. It is true of the steel grades whose ranges of element concentration mass partially overlap, but ranges of steel hardness change in function of distance from quenched end have common values. It has been acknowledged that such cases can be regarded as correct network responses because the assumed hardness curve is included in the hardness range of both steel grades.

Figure 3 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.

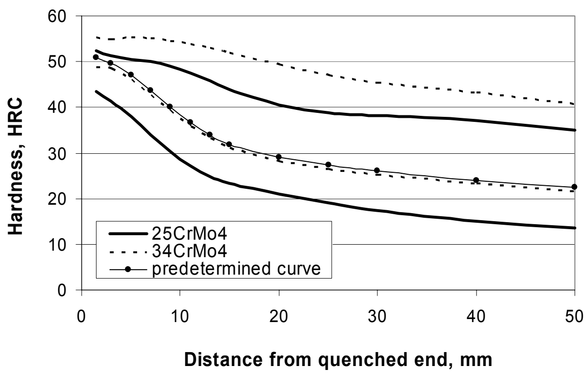

Fig. 3. Comparison of the predetermined Jominy curve and range of hardness change accepted as a model (34CrMo4) and suggested by the neural network (25CrMo4)

4.2. Selection of steel grade by means of many output variables

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.

The presented method of the neuron network response coding makes it possible for unclassified cases to arise, that is the ones whose value of activation of the output neuron is between the acceptance and rejection levels. The change of values of the acceptance and rejection levels allows to eliminate unclassified cases; however, in the investigated case such action seems pointless. The application of the error function in the form of mutual entropy and the output layer activation function of the softmax type allows to interpret the value of the signal as probability of class affiliation. Similar values of signals for several output neurons should be regarded as possibility of several steel grades selection. In this case, the result of the artificial neuron network calculations is a set of possible outcomes but the final decision is to be made by the user.

As a result of optimization of neuron network parameters a network of a hidden layer with 31 neurons has been accepted. The training method based on the conjugate gradient algorithm has been applied. The training set of 597 training epochs has been applied to the neural network. All the unclassified cases have been analysed by means of Jominy curve graphs in function of distance from quenched end against the background of steel hardness ranges suggested as possible outcomes. Figures 4 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.

5. Summary

In the paper a project of the system of selecting a steel grade with the required hardenability is presented. For working out the system the artificial neural networks have been used. There have been presented two solution variants. The use of the error function in the form of the reciprocal entropy and the softmax input activation layer has made it possible to interpret the output neuron activation values as the probability of the class affiliation and creating a set of possible solutions.

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.

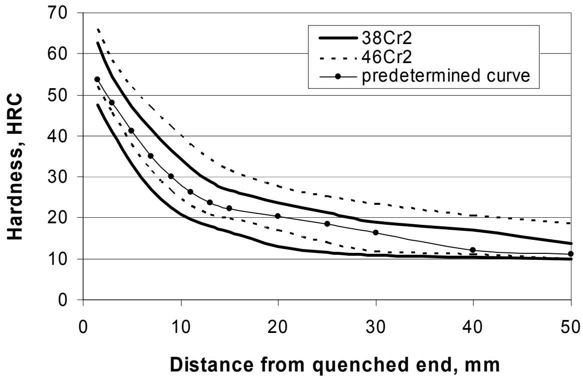

Fig. 4. Comparison of the predetermined Jominy curve and hardness ranges for steel grades suggested by the neural network: variant 1-38Cr2; variant 2 – 46Cr2

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