Journal of Achievements in Materials and Manufacturing Engineering
VOLUME 16
ISSUE 1-2
May-June
2006

Application of neural networks for selection of steel with the assumed hardness after cooling from the austenitising temperature

J. Trzaska, L.A. Dobrzański*
Division of Materials Processing Technology and Computer Techniques in Materials Science, Institute of Engineering Materials and Biomaterials, Silesian University of Technology, ul. Konarskiego 18a, 44-100 Gliwice, Poland
* Corresponding author: E-mail address: leszek.dobrzanski@polsl.pl

Received 15.11.2005; accepted in revised form 15.04.2006

Analysis and modelling

ABSTRACT

Purpose: The aim of the study is to establish a system that supports the choice of steel grade for quenching and tempering at a required hardness curve as function of cooling rate from the austenitising temperature.

Design/methodology/approach: It has been assumed that the steel will meet the criterion provided that the hardness curve, defined by the user, is included within the range of hardness change that is characteristic of a certain steel grade. In order to determine the steel hardness ranges it has been necessary to work out a suitable calculation model. Therefore, a neural network has been designed and verified numerically to calculate the steel hardness on the basis of chemical content for the predetermined cooling rate. To develop the relationship between the chemical composition, austenitising temperature, cooling rate and hardness of the steels for quenching and tempering the artificial neural network was used. The obtained results were used for determination of neural classifier. The classifiers based on the neural networks carries out the task of selection of the steel grade.

Findings: Artificial neural networks can be applied for selection of steel with the assumed hardness after cooling from the austenitising temperature.

Practical implications: The system presented can be applied to selection of steel grade intended for machine parts of predetermined hardness in the section of a hardened or normalized element.

Originality/value: The research presented in this paper offers a new strategy useful in selection of steel grade.

Keywords: Metallic alloys; Artificial intelligence methods; Heat treatment; CCT Diagram; Hardness

1. Introduction

The appropriate selection of the material for the particular application, based on the multi-criterion optimisation taking into account its chemical composition, manufacturing conditions, operating conditions, and the material waste disposal method in its after-service phase, as well as the price-dependant issues connected with obtaining the material, its transforming into a product, the product itself, and also costs of disposal of the industrial waste and scrap, as well as modelling of all processes and properties connected with materials, feature the fundamentals of the dynamically developing computational materials science. Various models are employed in the computational materials science, depending on scale and also possibilities of using the engineering materials modelling, their synthesis, structure, properties, and phenomena. The experimental verification enables to check the computer simulation in various scales and using the artificial intelligence methods, for employing the new materials and their manufacturing processes.

The Computer Aided Materials Selection Systems (CAMS) and the Computer Aided Materials Design ones (CAMD) have found their right position within the framework of the Computer

Aided Design (CAD) and Computer Aided Manufacturing (CAM) systems. Simultaneously, the designer's personal experience and intuition, and even his customary attitude roles' importance are gradually decreasing in the engineering materials selection for the particular applications. The subjective factors, and even mistakes, are being eliminated more and more, and the selected materials have the most advantageous mechanical, functional, and technological properties, with the right density, meet the ecological requirements, and all that at the lowest attainable materials' costs and products made from them. The intensive research dedicated to this topic is to go on in many centres. [1]

The need for making more and more effective and reliable systems of processing information that are able to recognize, forecast, associate and control, has caused the development of artificial neural networks. Artificial neural networks are applied to solve practical tasks in very diverse areas like finance, medicine, physics, geology, military science or engineering. Artificial neural networks have, in recent years, become the tool also used in materials science as many publications in this field prove. [2-6] The essential reason for such a growing popularity of neural networks is the fact that creating relations between the examined quantities does not require mathematical description of the analyzed problem but only a representative analysis of the experimental data sets. In most cases, the analysis of the results received, using neural networks justifies the application of this method. Among the most important properties of neural networks one can enumerate the ability of parallel signal transformation as well as the ability to learn which consists in estimating the weight values describing the connections between particular lattice points on the basis of presented examples. The attribution of a proper semantic interpretation to the signals and artificial neural networks' cells enables to collect knowledge in its structure. Artificial neural networks can be applied as knowledge basis in expert systems. The process of gaining knowledge amounts in this case to preparing a set of learning signals in the form of examples and to determining the type and structure of neural network as well as defining other parameters like error function, activation function, variable scaling method. It also helps to determine the weight values for connections between neurons in the learning process of the neural network according to the established algorithm. [7]

2. Material and experimental methodology

The data set was developed basing on literature data, including chemical compositions, austenitising temperature (T_A) and the CCT diagrams of the steels for quenching and tempering.. The obtained curves were worked out, assuming mass fractions of the alloying elements as the criterion. The ranges of the assumed mass fractions of elements are included in Table 1.

The aim of the study is to establish a system that supports the choice of steel grade for quenching and tempering at a required hardness curve as function of cooling rate from the austenitising temperature. It has been assumed that the steel will meet the criterion provided that the hardness curve, defined by the user, is included within the range of hardness change that is characteristic of a certain steel grade. The hardness range for the certain steel grade has been defined by the highest and lowest hardness calculated for ten predetermined successive time units until the end of steel cooling from the austenitising temperature. The example of the hardness range changes as function of cooling rate for the 38Cr2 steel grade has been presented in Figure 1.

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

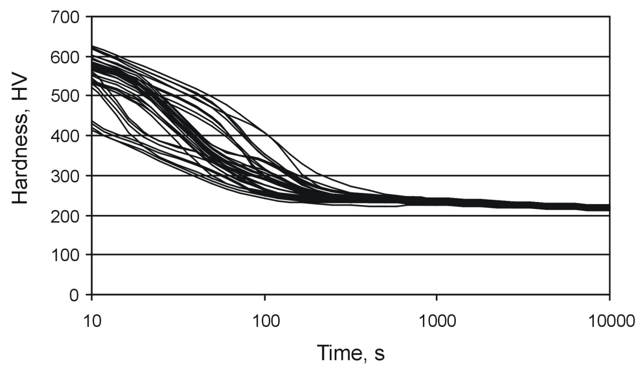

Fig. 1. Hardness range changes as function of cooling rate for the 38Cr2 steel grade

In order to determine the steel hardness ranges it has been necessary to work out a suitable calculation model for the mass concentration range of elements shown in Table 1. Therefore, a neural network has been designed and verified numerically to calculate the steel hardness on the basis of chemical content for the predetermined cooling rate. The training set has been established due to literature data. Then for each steel grade (according to EN-10083-1) 150 chemical contents have been made at random and the hardness for ten predetermined cooling rates has been calculated. As a result, there has been made a training set for another artificial neural network whose task is to suggest the steel grade after the hardness for 10 average cooling rates have been defined by the user.

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.

The following quantities determined for the testing set were used as the basic coefficients for evaluation of the neural network model performance: average network prediction error, standard deviation of the network prediction error, quotient of the standard deviations of the prediction errors and of the standard deviation of the resulting variable, Pearson correlation coefficient and for classification problems: coefficient expressing in [%] the number of correct classifications.

3. Calculation of steel hardness

To develop the relationship between the chemical composition, austenitising temperature, cooling rate, and hardness of the steel the feedforward neural network (MLP) was used. The activation level of the successive 13 network input nodes depended on: mass concentration of elements (C, Mn, Si, Cr, Ni, Mo, V), austenitising temperature, cooling rate, and structure type. The average cooling rate has been calculated on the basis of the time until the end of steel cooling from the austenitising temperature. As the cooling rate in the CCT graphs is within the range of 1 second and 10^5 seconds, the obtained value of average cooling rate has been normalized by calculation of the fourth root of the value. The number of vectors was determined in the particular sets: 1000, 368, 368. The type of structure developed after cooling the steel at a particular rate was specified using four binary nominal variables.

Determining the curve of hardness changes versus cooling rate, according to the method proposed in the paper, calls for determining the types of the structural constituents that occur in the steel after cooling from the austenitising temperature. The types of the structural constituents were determined using four bivalued nominal variables containing the information if the following constituents are present in the structure: ferrite, pearlite, bainite, martensite. A classifier had to be developed, to obtain this information, using as input data the mass concentrations of the particular alloying elements, austenitising temperature, and cooling rate. The detailed problem description was presented in [8-12].

Hardness was determined basing on the activation level of a single neuron in the network output layer. The number of hidden layers and number of nodes in these layers, were specified analyzing the effect of these quantities on the network performance coefficient values. 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 13 was assumed to be optimal. Training method was used based on the conjugate gradient algorithm. Values of errors as well as quotients of standard deviations and the Pearson correlation coefficient r obtained for the steel hardness calculations, depending on the cooling rate for the developed neural network model are presented in Table 2. The comparative plots for the experimental and calculated hardness values are presented in Figure 2.

Table 2
Error values and correlation coefficients for hardness calculated for data from the training / validating / testing data sets

Data set	Error E_{HV}, HV	Quotient of standard deviations	Pearson correlation coefficient
Training	31.2	0.24	0.97
Validating	36.3	0.29	0.96
Testing	33.5	0.28	0.96

4. Selection of steel grande

It has been required to prepare a representative training database in order to design a neural network as a classifier that on the basis of the hardness curve defined by the user is able to select the optimal steel grade.

To prepare the database containing the information about the randomly selected chemical compositions of steel, taking into account limitations presented in Table 1, the computer program was developed generating random chemical compositions of steel basing on user specified parameters:

- range of mass concentrations for each element,
- number of cases.

Austenitising temperature was determined as the A_{c3}+50°C temperature for the prepared set of 150 various chemical compositions for each steel grade and next hardness was calculated for ten assumed average cooling rates. To calculate the A_{c3} temperature on the basis of element mass concentrations, the artificial neural network presented in the paper [13] has been applied .

It has been assumed that average cooling rates will be calculated for the time until the end of steel cooling from the austenitising temperature. The following values of cooling rates have been accepted: 5, 10, 20, 50, 100, 200, 500, 1000, 5000 and 100000 seconds.

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. For calculations the feedforward 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.

4.1. Selection of steel grade 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 10 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 26 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 five 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 cooling rate from the austenitising temperature 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. On that basis an amended coefficient of the correct classifications has been calculated. The values of the coefficient of the correct classifications have been calculated and the amended coefficient of the correct classifications for the training, validating and testing sets have been presented in Table 3. The number of network false responses for the successive data sets have been presented in Table 4. Figures 3-4 show the examples of hardness curve in function of time necessary for sample cooling from the austenitising temperature against a background of the range of hardness change for steel grades accepted as a model and suggested by the network.

Table 3
The values of the coefficient of the correct classifications

	Data sets		
	training	validating	testing
Coefficient of the correct classifications, %	91.0	92.0	93.0
Amended coefficient of the correct classifications, %	99.6	98.9	98.1

Table 4
The number of network false responses

Neural network response	Learning pattern	Data sets		
		training	validating	testing
37Cr4	34Cr4	39	15	14
37Cr4	41Cr4	34	12	12
38Cr2	46Cr2	8	5	6
48Si7	56Si7	5	4	3
42CrMo4	50CrMo4	2	2	1

3.1. 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 12 neurons has been accepted. The training method based on the conjugate gradient algorithm has been applied. The training set of 311 training epochs has been applied to the neural network. Table 5 presents coefficients of correct classifications and amended coefficients calculated on the assumption that ambiguous responses (unclassified cases) can be interpreted as different variants of the network correct responses. The number of unclassified cases for each data sets have been presented in Table 6. All the unclassified cases have been analysed by means of hardness curve graphs in function of cooling rate against the background of steel hardness ranges suggested as possible outcomes. Figures 5-7 show the example of predetermined hardness curve in function of time necessary for cooling the sample from the austenitising temperature against the background of hardness ranges for steel grades: the one assumed as a model and the one suggested by the neural network.

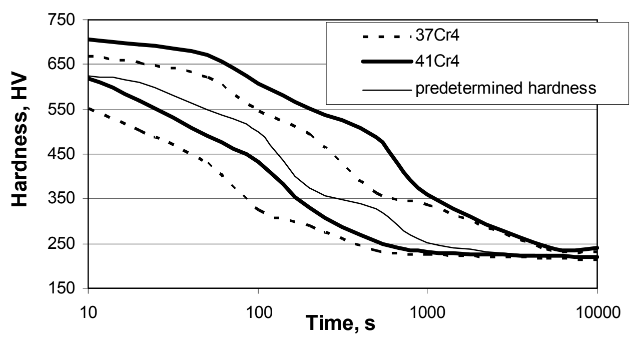

Fig. 3 Comparison of the predetermined hardness curve and range of hardness change accepted as a model (37Cr4) and suggested by the neural network (41Cr4)

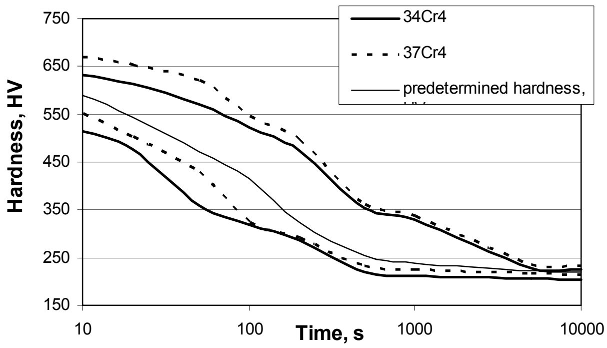

Fig. 4 Comparison of the predetermined hardness curve and range of hardness change accepted as a model (34Cr4) and suggested by the neural network (37Cr4)

Table 5
The values of the coefficient of the correct classifications

	Data sets		
	training	validating	testing
Coefficient of the correct classifications, %	71.6	71.6	69.2
Amended coefficient of the correct classifications, %	99.5	98.7	98.5

Table 6
The number of unclassified cases

Variant 1	Variant 2	Data sets		
		training	validating	testing
37Cr4	34Cr4	36	13	14
37Cr4	41Cr4	82	40	51
38Cr2	46Cr2	97	50	65
48Si7	56Si7	8	3	5
42CrMo4	50CrMo4	4	7	2

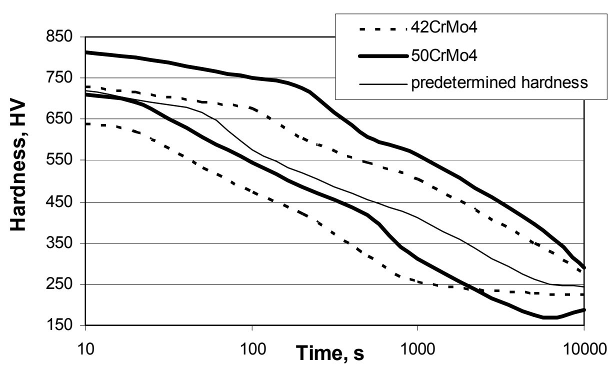

Fig. 5. Comparison of the predetermined hardness curve and hardness ranges for steel grades suggested by the neural network: variant 1-42CrMo4; variant 2 – 50CrMo4

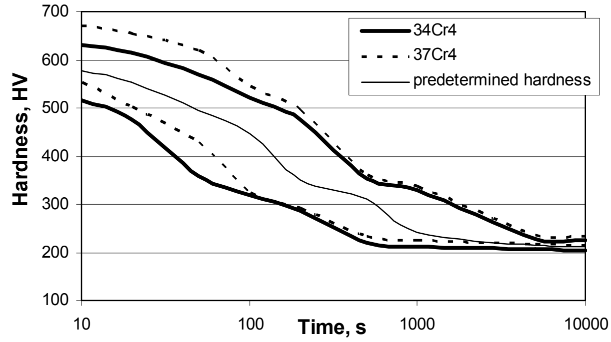

Fig. 6. Comparison of the predetermined hardness curve and hardness ranges for steel grades suggested by the neural network: variant 1-34Cr4; variant 2 – 37Cr4

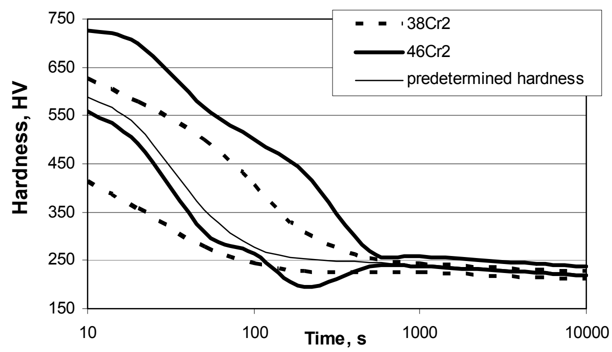

Fig. 7. Comparison of the predetermined hardness curve and hardness ranges for steel grades suggested by the neural network: variant 1-38Cr2; variant 2 – 46Cr2

5. Summary

The study presents a design of the advisory system whose task is to support the selection of steel grade of predetermined hardness in function of cooling rate from the austenitising temperature. The artificial neural networks have been applied to develop the project. Two options of neural network response coding have been used. The first one, by means of one variable whose value is equal to the number of classes of possible outcomes, and the other, by means of the number of output variables that is equal to the number of classes, where each variable can have two nominal values: confirming and rejecting value of class affiliation. The application of 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 output neuron activation as probability of class affiliation. There may appear such cases in which the function of the artificial neural network can be limited to development of a set of possible outcomes and the final decision should be made by the user.

The system presented can be applied to selection of steel grade intended for machine parts of predetermined hardness in the section of a hardened or normalized element. Differences of chemical content acceptable within the same steel grade and also altering of austenitising conditions are the reason that it is difficult to evaluate possible hardness in the section of the element only on the basis of steel grade and it must produce great error. It has been confirmed by ranges of hardness change in function of cooling rate calculated for different steel grades for quenching and tempering. As it has been shown in the study, the model of relationship between chemical content, the austenitising temperature, cooling rate and steel hardness can be applied to determine a difference between the predetermined hardness and the hardness feasible in the casting of certain chemical content. The project of advisory system presented in the study can be supplemented with other steel grades. At present research is done to work out system supporting selection of steel of predetermined content, in the section of a hardened or normalized part, of volume fractions of structure elements, such as ferrite, pearlite, bainite and martensite. Promising results of preliminary calculations have also been obtained for a project of system supporting selection of steel of predetermined course in the CCT diagrams.

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