Journal of Achievements in Materials and Manufacturing Engineering

VOLUME 27
ISSUE 2
April
2008

Project of neural network for steel grade selection with the assumed CCT diagram

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Received 30.01.2008; published in revised form 01.04.2008

Analysis and modelling

ABSTRACT

Purpose: The aim of this paper was developing a project of neural network for selection of steel grade with the specified CCT diagram – structure and of harness after heat treatment.

Design/methodology/approach: The goal has been achieved in the following stages: at the first stage characteristic points of CCT diagram have been determined. At the second stage neural network has been developed and optimized.

Findings: The neural network was developed in this paper, that allowed selection of steel grade with the assumed CCT diagram.

Research limitations/implications: Created method for designing chemical compositions is limited by the established ranges of mass concentrations of elements. The methodology demonstrated in the paper makes it possible to add new steel grades to the system.

Practical implications: The method worked out may be used in computer steel selection systems for the machine parts put to heat treatment.

Originality/value: Presented computer aided method makes use of neural networks, and may be used for selecting the steel with the required structure after heat treatment.

Keywords: Computational Material Science; Artificial Intelligence Methods; CCT diagram

1. Introduction

Despite advance in development of materials with special properties, for instance ceramics, composites or polymers, steel is still the most commonly used resource in today's engineering. The advantage of steel over other engineering materials lies in connection of high mechanical properties with large number of manufacturing processes, forming processes and heat treatment processes.

Steel properties depend first of all on chemical composition and structure. These steel properties may be formed in heat treatment process – quenching and tempering. Structure composition and hardness of steel after hardening, tempering or full annealing may be determined using continuous cooling transformation (CCT) diagrams [1-3].

At present an artificial intelligence (neural networks) is engaged for CCT diagram calculation. This move allows to reduce the necessary time and costs of obtaining the CCT diagrams [4,15].

Artificial neural networks imitate functioning of human brain, which is able to learn by experiment, associate, predict, or make rational decisions. These properties feature the advantages of neural networks. The networks are built by many artificial neurons, which are connected by a net. Each neuron calculates the weighted sum of input signals and compares it to the threshold. Weights are determined by the process itself [5,6]. Neural networks are widely used in medicine, economy, engineering, and materials engineering [7-15]. Currently, a reverse process to predict the course of the supercooled austenite transformations is being developed using neural networks. The purpose is to investigate the steel grade with the assumed CCT diagram and properties.

2. Material and methodology

Steels for hardening and tempering were used to develop an neural network for selection of steel grades with the assumed CCT diagrams. Marks of steel grade and ranges of mass concentrations of elements are shown in Table 1. The steel grades were chosen from the point of view of unrepeatability of ranges of elements mass concentration.

At first, 3000 random chemical composition were generated, 300 cases for every of steel grade. For all generated compositions, CCT diagrams were computed [15].

CCT diagram was determined to develop neural network for steel grade selection with the specified CCT diagram.

An effort was made to create system, which can determine diagram in a clear-cut matter. Characteristic data was assumed and read from diagrams. The characteristic data are points, which are presented in Fig. 1.:

- for martensitic transformation:
  - temperature of start-transformation (point 1),
  - maximum time during which transformation occurs (point 1);
- for bainitic transformation:
  - temperature of the shortest supercooled austenite life point (point 2),
  - time of the shortest supercooled austenite life point (point 2),
  - temperature of start-transformation at maximum time during which transformation occurs (point 3),
  - maximum time during which transformation occurs (point 3);
- for pearlitic transformation:
  - temperature of start-transformation at minimum time during which transformation occurs (point 4),
  - minimum time during which transformation occurs (point 4);
- for ferritic transformation:
  - temperature of start-transformation at minimum time during which transformation occurs (point 5),
  - minimum time during which transformation occurs (point 5).

All of temperature data are given in ºC, and time data are stated in seconds. Additionally, structural participation of martensite and bainite and hardness of steel (HV) after five different cooling rates were read from CCT diagrams for every of chemical composition. The cooling rates were determined as: 160 ºC/s, 40 ºC/s, 8 ºC/s, 2 ºC/s, 0.15 ºC/s.

Data set was divided into three subsets: training (1500 data), validating (750 data) and testing (750 data). 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 subset was done randomly.

Task of designing a classifier consist in selection of the steel grade with the assumed CCT diagram and required structure and hardness after heat treatment.

Neural networks were designed using "Statistica Neural Networks 4.0 F" application.

Qualitative evaluation of neural networks was realized on the basis of coefficient of correct classifications.

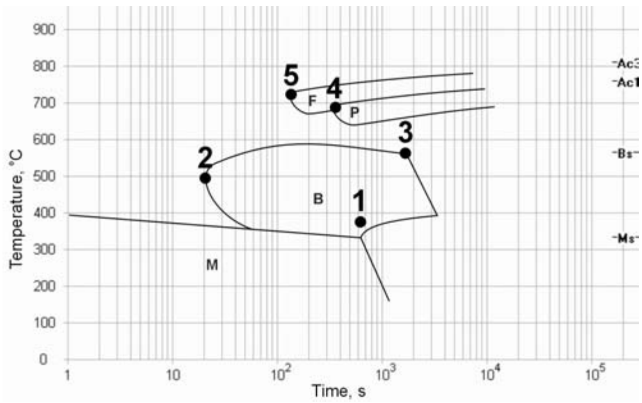

Fig. 1. CCT diagram with characteristic points marked

Table 1.
Grades of steel and chemical compositions [16]

Steel grade mark	Elements' mass concentrations[1)], %					
	C	Mn	Si	Cr	Ni	Mo
C22E	0.17–0.24 –	0.40–0.70		≤0.40	≤0.40	≤0.10
C35E	0.32–0.39	0.50–0.80		≤0.40	≤0.40	≤0.10
C45E	0.42–0.50	0.50–0.80		≤0.40	≤0.40	≤0.10
C60E	0.57–0.65	0.60–0.90		≤0.40	≤0.40	≤0.10
28Mn6	0.25–0.32	1.30–1.65	≤0.40	≤0.40	≤0.40	≤0.10
38Cr2	0.35–0.42	0.50–0.80		0.40–0.60	-	-
41Cr4	0.38–0.45	0.60–0.90		0.90–1.20	-	-
25CrMo4	0.22–0.29	0.60–0.90		0.90–1.20	-	0.15–0.30
42CrMo4	0.38–0.45	0.60–0.90		0.90–1.20	-	0.15–0.30
36CrNiMo4	0.32–0.40	0.50–0.80		0.90–1.20	0.90–1.20	0.15–0.30

[1)] Cr+Mo+Ni≤0.63, P≤0.035, S≤0.035

3. Description of results

The feedforward neural networks have been applied for calculations – Multi Layer Perceptron (MLP). The number of nodes in input layer was defined as 25 – ten of them correspond to five points (Fig. 1), ten correspond to structural participation of martensite and bainite for five different cooling rates and five nodes correspond to hardness of steel after five different cooling rates. Number of nodes in output layer was defined as 10, which is depended on number of steel grades.

Mutual entropy has been applied as error function. This type of error function, designed especially for classification problems, is used with softmax as type of output layer activation function. Union of these parameters allow to interpret the neuron's activation level of the output layer as the estimated probability of certain class affiliation.

In this neural network, one-of-N conversion type has been applied. This conversion type using neurons number answers one nominal variable is equal number of values achieves by this variable. In order to represent selected variable, appropriate neuron is activated and the rest of them staying inactive.

The number of hidden layers, number of nodes in these layers and the number of training epochs were determined by observing the neural forecast error for the training and validating sets. Neural networks training was carried with errors back-propagation method and conjugate gradient algorithm.

The neural network with one hidden layer and numbers of neurons in this layer as 25 was assumed to be optimal.

The minimal number of unqualified or mistakenly qualified cases was achieved for MLP neural network, that was trained by error back propagation method in 50 epochs and conjugate gradient algorithm in 264 epochs.

The values of the coefficient of the correct classifications for the training, validating and testing data set have been presented in Table 2. The number and type of network false classifications have been presented in Table 3.

A large majority of steel grades were classified correctly. Steel grade 36CrNiMo4 (as 42CrMo4), 38Cr2 (as C35E) and 42CrMo4 (as 41Cr4) were false classified once by developed neural network. C35E steel was false classified five times – as 38Cr2 steel 3 times and as C22E steel 2 times. In all 19 false classified cases, 11 of them concerned C45E steel (see Table 3).

C45E steel was classified as C60E steel five times. The reason is most probably similarity of CCT diagrams and structure participation of martensite and bainite and hardness of steel after hardening with five different cooling rates of these cases. The two similar CCT diagrams of C45E and C60E steel have been presented in Fig. 2. Similarity of these two CCT diagrams is a effect influence of alloyed elements (chromium, molybdenum and nickel), which concentrations are situated in the top ranges. Transformations are shifted to the right – to lower cooling rates. High concentrations of alloyed elements increase also the structure participation of martensite and bainite and hardness of steel.

C45E steel was also classified wrong, three times, as 41Cr4 steel. The reason of these false responses is probably the same like previous case (C45E steel classified as C60E). Additionally, errors are possible, because ranges of elements mass concentrations partially overlapped. The two similar CCT diagrams of C45E and C60E steel have been presented in Fig. 3. Locations of supercooled austenite transformations curves on CCT diagram is depended on chemical composition of steel.

Table 2.
The value of the coefficient of the correct classifications

Data sets		
training	validating	testing
99.9%	99.3%	98.4%

Table 3.
The number of network false responses

Neural network response	Learning pattern	Data sets		
		training	validating	testing
28Mn6	C45E	1	-	1
38Cr2	C35E	-	1	2
38Cr2	C45E	-	1	-
41Cr4	42CrMo4	-	-	1
41Cr4	C45E	-	-	3
42CrMo4	36CrNiMo	-	1	-
C22E	C35E	-	-	2
C35E	38Cr2	-	1	-
C60E	C45E	1	1	3

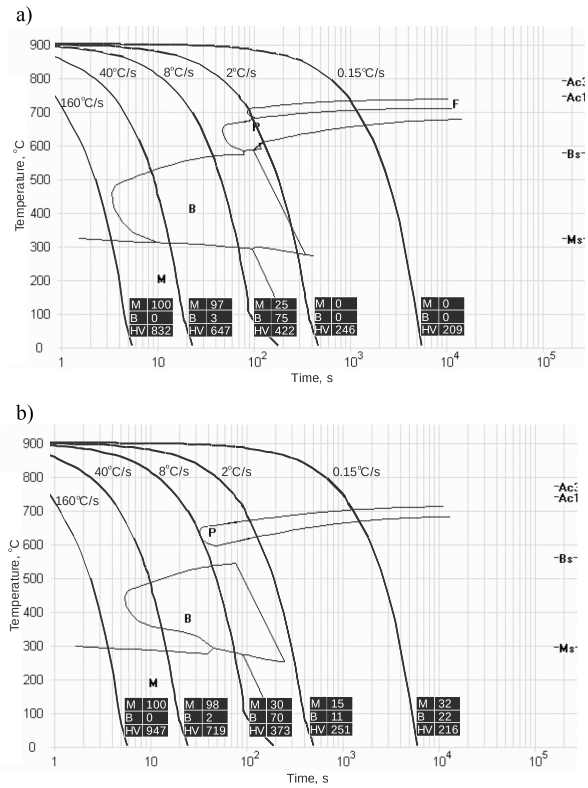

Fig. 2. Comparison of the CCT diagram with marked structural participation of martensite (M) and bainite (B) and hardness of steel (HV) for five different cooling rates: a) accepted as a model (C45E), b) suggested by the neural network (C60E)

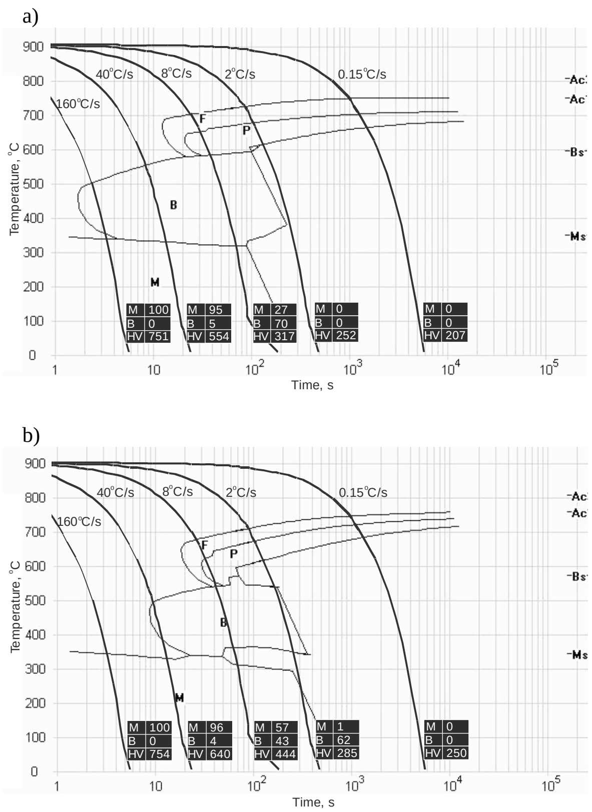

Fig. 3. Comparison of the CCT diagram with marked structural participation of martensite (M) and bainite (B) and hardness of steel (HV) for five different cooling rates: a) accepted as a model (C45E), b) suggested by the neural network (41Cr4)

4. Conclusions

Good quality neural network was developed as a result of calculations. This network classified correctly over 99.3% steel grades from 3000 cases. Classifier selected the steel grade based on 25 variables: coordinates of five points were described CCT diagram, martensite participation in the structure (for five different cooling rates), bainite participation in the structure (for five different cooling rates) and steel hardness after cooling at five different cooling rates.

Presented calculations were limited to only ten grades of steel for quenching and tempering. Presented system could be extended by widening ranges of steel grades.

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