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Application of neural networks for designing the chemical composition 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

Abstract: The method presented in the paper makes it possible to determine the mass concentrations of the alloying elements for steels with the required curve of hardness changes versus cooling rate. Search for the optimum chemical composition is carried out in two stages. The first stage consists in preparing the data file consisting of chemical compositions of steels and calculated curves of hardness change versus cooling rate. Hardness of steel cooled from the austenitising temperature is calculated with the model using the artificial neural networks. At the second stage the chemical composition of steel is searched for - the closest to the assumed criterion.

Keywords: Neural network; CCT diagrams; Hardness, Modelling

1. INTRODUCTION

The CCT diagrams containing the quantitative data pertaining to the dependence of steel structure and hardness on temperature and time of the supercooled austenite transformations are used for determination of the structure and hardness of the quenched, normalised, or fully annealed steels. Locations and shapes of the supercooled austenite transformations' curves, plotted on the CCT diagrams, depends mostly on the chemical composition of the steel, extent of austenite homogenising, austenite grain size, as well as on austenitising temperature and time. Fluctuations of the chemical composition of steel, allowable even within the same steel grade, and also changes of the austenitising conditions make that using the CCT diagrams published as catalogues does not provide reliable information on austenite transformations during cooling [1]. In [2-4] the modelling methodology was worked out for relationships between the chemical composition and austenitising temperature, and kinetics of the supercooled austenite transformations during continuous cooling, using neural networks as the computer science tool.

Neural networks have become, since several years, the tool being used more and more in the area of Materials Engineering, which is confirmed by many publications presenting research results obtained in many scientific centres in the world. Multi-network structures are used more and more often in designing the classifiers employing the artificial neural networks. This solution, called most often modular neural network, consists in employing

many neural networks independently developed and in determining the response of the entire system using the supervisor module. In many complex issues a network mapping its specific fragment only of the modelled problem fulfils its task much better. Using the modular networks of less complex structure prevents many a time from the excessive matching the network to the data from the training set, which leads to losing by the network its capability to generalise the acquired knowledge. Neural networks linked in parallel may be also used to develop the classifier, where the response of the entire system is determined using the accordingly designed decision block. However, employment of the collective decision of the modular neural network gives hope that it will be subjected to a smaller error than the response of a single network. [5]

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 constructional and engineering steels. The obtained curves were worked out, assuming mass fractions of the alloying elements as the criterion. Basing on the collected data it was assumed in addition that total of the mass fractions of manganese, chromium, nickel, and molybdenum does not exceed 5%. The ranges of the assumed mass fractions of elements and austenitising temperature are included in Table 1.

Table 1
Ranges of mass concentrations of elements and austenitising temperature for the analysed steels

Range	Mass fractions of elements, %								Austenitising temperature T_A, °C
	C	Mn	Si	Cr	Ni	Mo	V	Cu	
min	0.08	0.13	0.12	0	0	0	0	0	770
max	0.77	2.04	1.90	2.08	3.65	1.24	0.36	0.3	1070

The method presented in the paper makes it possible to determine the mass concentrations of the alloying elements for steels with the required curve of hardness changes versus cooling rate obtained during the continuous cooling from the austenitising temperature. Designing the optimum chemical composition is carried out in three stages:

- preparing the database containing information on mass concentrations of the elements,
- calculating the austenitising temperature (temperature A_{c3}+50°C) using the neural network model described in [4],
- calculating hardness of steel cooled continuously from the austenitising temperature for various cooling rates using the model developed employing the neural networks [6],
- selecting the chemical composition of steel meeting the assumed criterion.

3. CALCULATION OF STEEL HARDNESS

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 cooking rate. The following assumptions of the neural network based classifier were analysed:

- neural network analyses occurrences of four structural constituents (four neurons in the output layer),
- neural network recognizes only one structural constituent of the supercooled austenite transformations in the entire range of cooling rate,
- neural network recognizes only one structural constituent of the supercooled austenite transformations in the limited range of cooling rate.

In each case possibility of employing the modular neural networks was analysed. To select the optimum method of choosing the classifier's final response the following were checked:

- method based on the absolute majority of votes of neural networks included in the module
- method of the vote priority of the network providing a more reliable response, where the response reliability was determined basing on the activation values of the output layer neurons,
- method consisting in assigning weight values to responses of the particular networks, depending on the number of errors made.

Data required for model development were prepared basing on the CCT diagrams. Mass concentrations of the particular alloying elements, cooling rate, and austenitising temperature were used as input data. Influence of copper was omitted in case of the network with nine neurons in the input layer. The ranges of mass concentrations of the particular alloying elements are presented in Table 1. The numbers of cases in the sets: training, validating and the test one were respectively: 2580, 1290, 1290. The biggest number of the correct responses was obtained using the modular neural networks forecasting a single transformation in the full range of cooling rate. The particular classifiers were developed using the unidirectional neural networks of the MLP type (multilayer perceptron) with one or two hidden layers. The voting method based on the absolute majority of votes was chosen. Specifications of the particular classifiers used for forecasting occurrences of the particular structural constituents in steel are presented in Tables 2-5 . Figure 1 presents the comparison of the experimentally determined and calculated ranges of occurrences of the particular transformations depending on the average cooling rate for the steel from the verifying set.

Table 2.
Specification of the classifier forecasting occurrence of ferrite in the structure of steel cooled from the austenitising temperature

		1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Network structure		9-18-17-1	9-12-1	9-14-1	10-27-19-1	10-20-14-1	10-8-5-1	9-16-12-1	9-18-1	9-13-1	9-20-17-1
Training method/ No of epochs		CG 245	CG 258	CG 297	BP 250	CG 360	BP 272	BP 148	CG 187	CG 235	CG 331
Cc, %	Training set	99.1									
	Validating set	97.4									
	Testing set	97.7									

Cc - Coefficient of the correct classifications for the modular neural networks, BP – back propagation method; CG - conjugate gradients method

Table 3.
Specification of the classifier forecasting occurrence of pearlite in the structure of steel cooled from the austenitising temperature

		1	2	3	4	5	6	7	8	9
Network structure		10-20-11-1	10-5-2-1	10-25-1	10-31-1	10-17-5-1	10-17-10-1	10-19-16-1	10-8-5-1	10-25-10-1
Training method/ No of epochs		BP 131	CG 127	CG 149	CG 91	BP/111; QN5	BP 232	CG 77	BP/174; CG23	BP/60; QN11
Cc, %	Training set	98.0								
	Validating set	97.1								
	Testing set	97.0								
QN - quasi-Newton method										

Table 4.
Specification of the classifier forecasting occurrence of bainite in the structure of steel cooled from the austenitising temperature

		1	2	3	4	5	6	7	8	9
Network structure		10-32-6-1	10-26-10-1	10-31-25-1	10-47-37-1	10-20-14-1	9-23-19-1	10-31-29-1	9-20-18-1	9-45-32-1
Training method/ No of epochs		CG/176	CG/198	CG/218	CG/165	CG/166; BP/96	BP/268	CG/157; BP/77	CG/257; BP/173	BP/312
Cc, %	Training set	97.8								
	Validating set	95.5								
	Testing set	96.3								

Table 5.
Specification of the classifier forecasting occurrence of martensite in the structure of steel cooled from the austenitising temperature

		1	2	3	4	5	6	7	8	9
Network structure		10-20-13-1	10-10-1	10-17-1	10-20-14-1	10-20-18-1	10-18-1	10-24-17-1	10-19-6-1	10-13-12-1
Training method/ No of epochs		CG/241	CG/103	CG/98	CG/104	CG/112	CG/90	BP/76	BP/150	BP/63; CG/94
Cc, %	Training set	98.7								
	Validating set	97.9								
	Testing set	97.9								

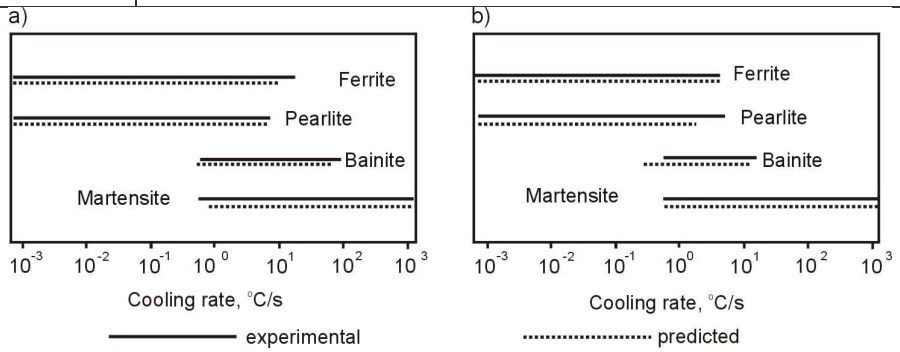

Figure 1. Comparison of the experimentally determined and calculated ranges of occurrences of the particular structural constituents depending on cooling rate for steels with the following compositions: a) 0.38% C, 0.74% Mn, 0.26% Si, 0.26% Ni, 0.90% Cr, 0.04% Mo, 0.17% Cu, austenitised at temperature of 880°C; b) 0.38% C, 0.41% Mn, 0.21% Si, 0.03% Ni, 1.29% Cr, 0.05% Cu, 0.12% V, austenitised at temperature of 925°C

4. CALCULATION OF STEEL CHEMICAL COMPOSITION

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,
- cooling time from the austenitising temperature to the ambient temperature.

Austenitising temperature was determined as the A_{c3}+50°C temperature for the prepared set of 6500 various chemical compositions of steel and next hardness was calculated for ten assumed average cooling rates. Three numerical procedures were developed making it possible selection of the optimum chemical composition in respect to one of the three search criteria:

- required hardness for the assumed cooling rate,
- required hardness in the assumed range of cooling rate changes,
- required curve of hardness change in the entire range of cooling rate changes.

In the first method, the chemical composition of steel is searched, for which the module value of difference between the calculated and expected hardness (for the assumed cooling rate) is the smallest. In the second method, the chemical compositions of steels are searched, for which hardness is within the range defined by specifying the minimum and maximum values at the assumed cooling rate range. In the third method, calls for specifying the expected hardness for the successive ten values of cooling time from the austenitising temperature to 100°C. The chemical composition of steel is searched, for which the sum of the absolute differences between the calculated and expected hardness, for the successive cooling time values, is the smallest. The values of the assumed hardness values, calculated hardness values, types of structural constituents occurring in the steel after cooling from the austenitising temperature and calculated chemical compositions of the steels are presented in Table 6.

Table 6.
Chemical composition of steel calculated for the assumed hardness versus cooling time from the austenitising temperature

Cooling time, s	3	20	50	100	250	500	1000	5000	20000	10^5
Predetermined hardness, HV	550	540	480	420	360	320	290	230	210	200
Calculated hardness, HV	560	552	473	417	353	312	277	240	215	207
Error, HV	9.8	12.0	7.4	2.9	7.2	8.2	12.6	10.2	5.1	7.1

Predicted mass fractions of elements, %								
C	**Mn**	**Si**	**Cr**	**Ni**	**Mo**	**V**	**Cu**	**T_A**
0.2	0.63	0.43	0.53	0.21	0.24	0.29	0.03	912

Figure 2 present comparison of the required curves of hardness changes versus cooling time with the curves calculated for the assumptions presented in tables 7 respectively.

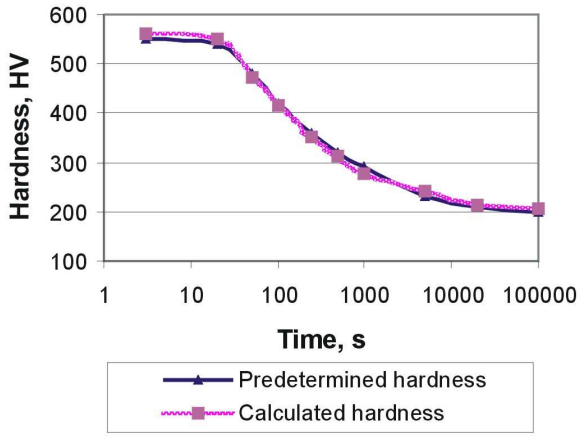

Figure 2. Comparison of the assumed and calculated curves of hardness change versus cooling time

5. CONCLUSIONS

The appropriate selection or design of a material meeting the assumed requirements features an essential stage in the contemporary design process of machines and their elements. The extensive set of the available materials and the need for the multi-criteria optimization of their selection causes employment of the computer aided material selection becoming a necessity, especially in the presence of the growing demands that the contemporary products have to satisfy. The computer aided materials selection system (CAMS) should have the auxiliary tools making possible, for instance such tasks as computer simulation of the chemical composition effect on the required properties or optimization of the feasible solutions basing on the assumed criteria - all these tasks are not supported by the engineering materials databases. Meeting the requirements mentioned above calls for the appropriate numerical model.

The model presented in the paper of the relationship between the chemical composition and austenitising temperature – and hardness of the machinery steels - and procedure making it possible to determine the chemical composition of the steel with the required hardness across the transverse section of the quenched or normalised element may become a part of the computer based steel selection system for elements of machinery and structures.

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