Journal of Achievements in Materials and Manufacturing Engineering
VOLUME 17
ISSUE 1-2
July-August
2006

An artificial intelligence approach in designing new materials

W. Sitek*, J. Trzaska, L.A. Dobrzański
[a] 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: wojciech.sitek@polsl.pl

Received 15.03.2006; accepted in revised form 30.04.2006

Analysis and modelling

ABSTRACT

Purpose: The paper presents the computer aided method of chemical composition designing the metallic materials with a required property.
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: Obtained results show that AI tools used are effective and very useful in designing new metallic materials.
Research limitations/implications: The presented models may be used in the ranges of mass concentrations of alloying elements presented in the paper. The methodology presented in the paper makes it possible to add new grades of steel to the models.
Practical implications: The worked out models may be used in computer systems of steel selection and designing for the heat-treated machine parts.
Originality/value: The use of the artificial intelligence method, particularly the neural networks as a tool for designing the chemical composition of steels with the required properties.
Keywords: Design; Computational material science; Artificial intelligence methods

1. Introduction

Since many years the investigations in the area of materials science have been carrying out to develop new materials, among them tool ones with higher working properties and fulfilling economical and ecological requirements. The main aim of this activity is the development of materials for suitable application having a few of the following required features: hardness, heat resistance, high-temperature creep resistance, wear resistance, corrosion resistance, impact strength, elasticity, strength, life, ecological manufacturing technology, recycling, low cost and other. Fulfilling this demand is extorted by the changes still speeded up in global free-market economy where the role of inexpensive series/mass production grows up significantly. The evolution of science at the end of the 20th century take effect in the development of new research, manufacturing and forming method of engineering materials. One can observe gradual leaving the empirical way of mastering/learning of the reality for the advantage of new, mainly computerised, methods using mathematical model of the object of investigations.

The paper presents the computer aided methods of chemical composition designing the metallic materials with a required property.

2. Designing the chemical composition of steel with required hardenability

The new method is dedicated for the conventional carburising and heat-treatable steels. Carbon, silicon, manganese, chromium, nickel and molybdenum are the main alloying elements used in

the carburising and heat-treatable groups of conventional alloy constructional steels considered. The chemical composition calculations were assumed to be made basing on the given hardenability curve shape, presented as the successive hardness values at 15 fixed distances from the Jominy specimen face. Initial classification of steels was done to obtain a high conformity of the computational results with the experimental data. The basis of the classification is the value of the alloy factor (AF) describing digitally the fraction of alloying elements in steel according to standard ASTM A255. The problem is discussed in detail in [1]. Basing on the investigations carried out, it was found out that classification of steels into three classes within the framework of each group of carburising and heat-treatable steels is sufficient to obtain a good conformity of the calculations with the experimental data of the chemical composition.

For designing of the chemical composition of the steel with the required hardenability, unidirectional multilayer neural networks were employed with the learning method based on the error backpropagation algorithm. Fifteen input nodes and 6 output ones assumed in the network structure are the consequence of the assumption that the hardenability of the steels' analysed is affected mainly by the concentration of six basic alloying elements. And additionally, hardenability curve is plotted by the values of hardness measured at fifteen successive points in fixed distances from Jominy specimen face. Finally, after preliminary tests, the 15-30-6 network model was assumed for the calculations, with the learning coefficient η=0.15 and momentum parameter α=0.3. Networks with such structures were trained individually for each steel class, using a data set prepared basing on the results of the experiments carried out. The neural networks developed were experimentally verified, which consisted in the evaluation of the conformity of the computational results (obtained by using the network models) with the experimental data. As a criterion of the evaluation a coefficient of assessment of the computation method adequacy *s* was employed. The coefficient defines the difference between the required hardenability and the one obtained for an actual heat. As a result of the investigations performed, the limiting value 2.5 HRC of the coefficient *s* was assumed [2].

Verification procedure for such a model consists in calculating the chemical composition of the steel with the required Jominy curve shape and in making the heat of the steel with the chemical composition calculated. Then, the relevant hardenability investigation is carried out and the actual experimental hardenability curve of the heat is compared to the required Jominy curve shape. For experimental verification hardenability curves with the assumed and distinctly different shapes were selected. Calculations of the chemical composition for the curves with the required shape were made within the framework of a particular steel grade only when the required hardenability curve was within the experimental hardenability band for the class considered. Then, investigations of hardenability of the heats with the actual chemical compositions the nearest to the calculated ones were made. Hardenability curves' shapes, the required and the actual ones, were compared afterwards. As an example of the calculations made, the results for two of the required shapes of hardenability curves are presented (curve I for carburising steel, curve II for heat-treatable steel). The chemical compositions calculated within the framework of each steel class for which the required hardenability curve is within the experimental hardenability band and the relevant chemical compositions of the actual heats are included in Table 1. Figure 1 presents the graphical comparison of the required hardenability curve and the experimental ones for the steel heats with the designed chemical composition. Basing on such calculations made for about 550 testing industrial heats it was found out that the neural network model developed secures the satisfactory adequacy with experimental data since in each case the calculated coefficient of adequacy assessment s is smaller than its critical value 2.5 HRC.

Table 1
Comparison of the calculated and the relevant chemical compositions of the actual heats

Required curve	Alloying element	Mass concentration, %		
		calculated 1	calculated 2	calculated 3
		actual 1	actual 2	actual 3
I	C	0.20	0.24	0.22
		0.18	0.23	0.26
	Mn	0.91	0.80	0.59
		0.95	0.78	0.60
	Si	0.29	0.26	0.23
		0.28	0.29	0.20
	Cr	0.93	0.59	1.01
		0.95	0.53	1.06
	Ni	0.12	0.53	0.18
		0.12	0.45	0.16
	Mo	0.25	0.32	0.22
		0.23	0.32	0.21
II	C	0.41	0.40	0.42
		0.41	0.40	0.41
	Mn	0.60	0.77	0.79
		0.68	0.72	0.69
	Si	0.25	0.29	0.26
		0.28	0.31	0.36
	Cr	0.75	1.01	1.02
		0.74	1.03	1.06
	Ni	1.29	1.29	0.23
		1.35	1.35	0.26
	Mo	0.16	0.18	0.07
		0.16	0.17	0.07

3. Designing the chemical composition of steel with the assumed hardness after cooling from the austenitising temperature

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.

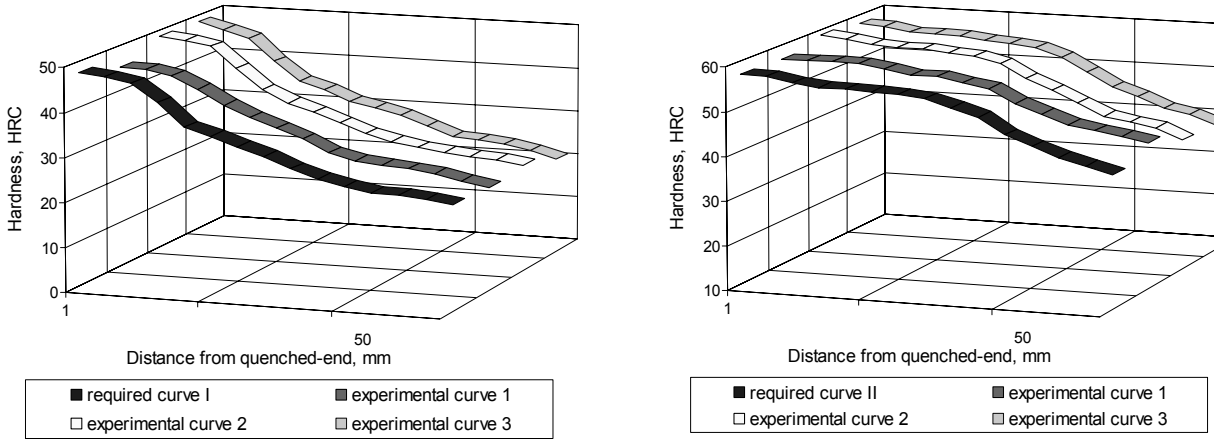

Fig. 1. Comparison of the required hardenability curves and the experimental ones of the steels' with designed chemical composition

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 Ac3+50°C) using the neural network model described in [3],
- calculating hardness of steel cooled continuously from the austenitising temperature for various cooling rates using the model developed employing the neural networks,
- selecting the chemical composition of steel meeting the assumed criterion.

The data set was developed basing on literature data, including chemical compo-sitions, austenitising temperature (TA) 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 2.

To develop the relationship between the chemical composition, austenitising temperature, and cooling rate, and hardness of the constructional steel the feedforward neural network (MLP) was used. The data was divided into four sets: training, validating, test, and verifying 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 verifying set was used for verifying the model when the network training was completed. Allocation of data to the particular subsets was done randomly. The number of vectors was determined in the particular sets: 1582, 791, 790, and 369. The activation level of the successive fourteen network input nodes depended on: mass concentration of elements (C, Mn, Si, Cr, Ni, Mo, V, Cu), austenitising temperature, cooling rate, and structure type. The type of structure developed after cooling the steel at a particular rate was specified using four binary nominal variables.

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, and also method and training parameters were specified analyzing the effect of these quantities on the network performance coefficient values for the test set. The number of training epochs was determined by observing the network forecast error for the training and validating sets. The model developed was subjected to the numerical verification using the data that were not used in its development. The network with two hidden layers and numbers of neurons in these layers as twenty and two was assumed to be optimal. Table 3 presents error values and correlation coefficients for calculated hardness. Training method was used based on the conjugate gradient algorithm. The detailed problem description was presented in [4,5].

To prepare the database containing the information about the randomly selected chemical compositions of steel, taking into account limitations presented in Table 2, 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,
- maximum sum of the selected elements' concentrations,
- additional parameter (cooling time from the austenitising temperature to the ambient temperature).

Austenitising temperature was determined as the Ac3+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.

Table 2.
Ranges of mass concentrations of elements and austenitising temperature for the analysed steels

Range	Mass concentrations 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

Table 3.
Error values and correlation coefficients for hardness calculated for data from the training/validating/testing /verifying data sets

Data set	Error E_{HV}, HV	Standard deviation of the error, HV	Quotient of standard deviations	Pearson correlation coefficient
Training	28.7	27.2	0.24	0.97
Validating	34.8	35.1	0.29	0.96
Testing	36.1	37.3	0.31	0.95
Verifying	38.4	38.5	0.32	0.95

Table 4.
Chemical composition of steel calculated for the assumed versus cooling time from the austenitising temperature

Cooling time, s	3	20	50	100	250	500	1000	5000	$2 \cdot 10^3$	$\cdot 10^5$
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
Ferrit	No	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Pearlit	No	No	No	No	No	No	No	Yes	Yes	Yes
Bainit	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	No	No
Martensit	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	No	No

Predicted mass concentration of alloying 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

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.

Figure 2 present comparison of the required curve of hardness changes versus cooling time with the curve calculated for the assumptions presented in Table 4.

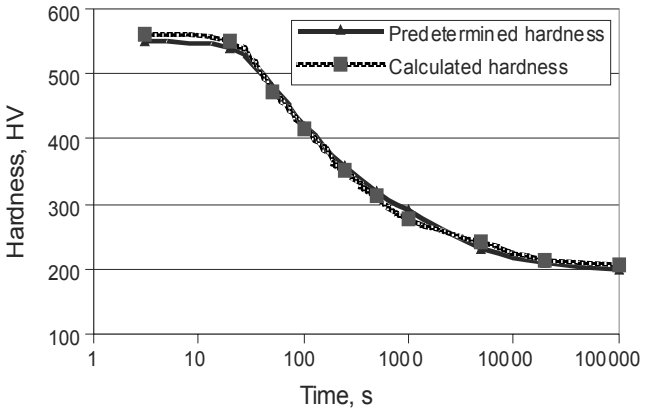

Fig. 2. Comparison of the assumed and calculated curves

4. Final remarks

The paper presents some examples of application of artificial intelligence tools, i.e. neural networks and genetic algorithms in designing of new materials with required properties. Results of numerical simulation show that AI tools used are effective and very useful in designing new metallic materials.

References

[1] L.A. Dobrzański, W. Sitek: "Application of neural network in modelling of hardenability of constructional steels", Journal of Materials Processing Technology, 78 (1998) 59-66.

[2] L.A. Dobrzański, W. Sitek: "The modelling of hardenability using neural networks", Journal of Materials Processing Technology, 92-93 (1999) 8-14.

[3] L.A. Dobrzański, J. Trzaska: "Application of neural networks for prediction of critical values of temperatures and time of the supercooled austenite transformations", Journal of Materials Processing Technology, 155-156 (2004) 1950.

[4] J. Trzaska PhD Thesis, Silesian University of Technology, Poland, 2002.

[5] L.A. Dobrzański, J. Trzaska: "Application of neural networks for prediction of hardness and volume fractions of structural components in constructional steels cooled from the austenitizing temperature", Material Science Forum, 437–438 (2003) 359-362.