POLISH ACADEMY OF SCIENCES - MATERIALS SCIENCE COMMITTEE
SILESIAN UNIVERSITY OF TECHNOLOGY OF GLIWICE
INSTITUTE OF ENGINEERING MATERIALS AND BIOMATERIALS
ASSOCIATION OF ALUMNI OF SILESIAN UNIVERSITY OF TECHNOLOGY

Conference Proceedings

11th INTERNATIONAL SCIENTIFIC CONFERENCE
ACHIEVEMENTS IN MECHANICAL & MATERIALS ENGINEERING

Application of neural networks to forecasting the CCT curves for constructional steels*

L.A. Dobrzański#, J. Trzaska#

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

The original CCT curve evaluation method for the constructional steels, employing the neural networks is presented in the paper. The data needed to develop the model were collected basing on the CCT curves published in the literature.

1. INTORODUCTION

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. Attempts to develop a model making it possible to evaluate the CCT curves basing on the chemical composition and austenitizing temperature for some selected steel groups had been made, among others, in [3-7]. A single neural network was used in all these cases. Mass fractions of elements and austenitizing temperature were used as input data, yielding temperatures of the particular transformations at the output, depending on the cooling rate. The results presented show the correct mapping by the network of some trends of transformation temperatures as functions of cooling time, however they differ significantly from the experimental results.

2. MATERIAL AND EXPERIMENTAL METHODOLOGY

Literature data were used for developing a method for evaluation of the anisothermic transformation curves of the supercooled austenite, including chemical composition, autenitizing temperature, and the CCT curves of the constructional steels. The obtained curves were analysed, assuming mass fractions of the alloying elements as the criterion. The ranges of the assumed mass fractions of elements and austenitizing temperature are included in Table 1. 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%.

---

* Authors participate in the CEEPUS No PL-013/02-03 project headed by Prof. L.A. Dobrzański.
# Investigations were financed within the framework of the Polish State Committee for Scientific Research No 4 T08A 009 23 grant headed by Prof. L.A. Dobrzański.

Table 1
Ranges of mass fractions of elements and austenitizing temperatures for the analysed constructional steels

Range	Mass fractions of elements, %								Austenitizing temperature, °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

It was found out, basing on analysis of works [3-7], in which neural networks were employed for determining the supercooled austenite transformation curves at the continuous cooling, that development of a model making it possible to calculate the complete CCT diagrams based on a simple mapping: chemical composition and austenitizing temperature → CCT diagram, must be subject to a significant forecast error. Calculating curves of the beginning and end of the transformations using a single neural network forces using a big number of neurons in the output layer, which – at the limited number of the available training curves and relatively big changes of the input values' ranges – does not allow do work out a representative training set. A satisfactory increase of the training set size is difficult because of the lack of literature data, whereas a significant limiting of the number of neurons in the output layer must result in a loss of the important information pertaining the flow of the supercooled austenite transformation. In case of a complex task, there is a possibility of splitting it into some less complicated ones and using separate networks for solving each of these problems. Therefore, while developing the algorithm for evaluating the CCT curves using the neural networks, the tasks were isolated, that could be solved with networks having less complicated structure, and organisation of the training set makes it possible to increase the number of examples with the number of the CCT curves remaining unchanged. Figure 1 shows the block diagram of the developed method for determining the complete transformation curves of the supercooled austenite during its continuous cooling.

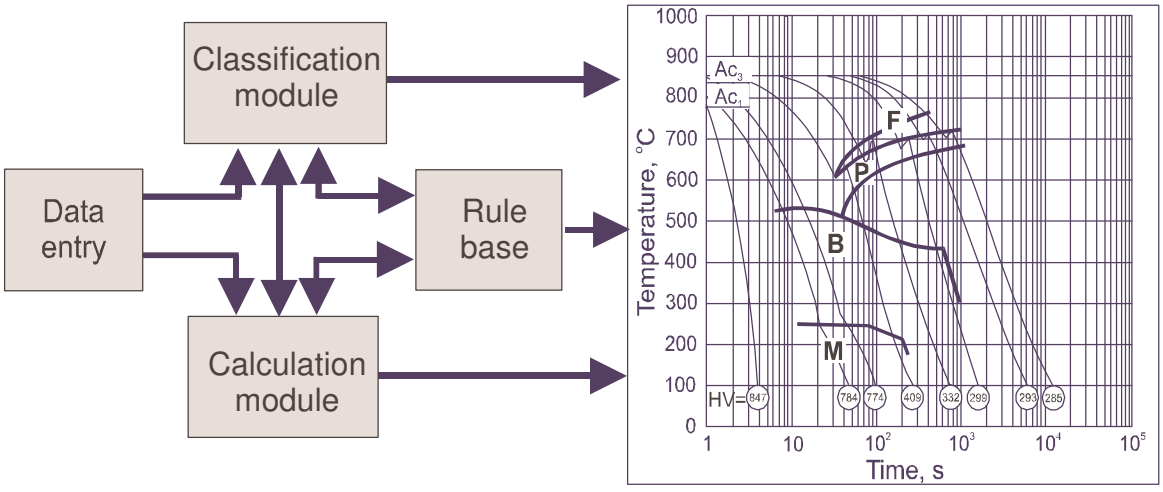

Figure 1. Block diagram of the method for calculation of the CCT curves

The algorithm has been based on four modules. The task of the data entry module is receiving information like chemical composition and austenitizing temperature and linking them with the cooling rates. The classification module composed of classifiers based on the neural networks carries out the task of identification of the structural elements occurring in the steel after completing its continuous cooling at a pre-determined rate. The calculation module employs neural networks for determining the critical values of the time and temperature of transformations, temperatures of beginning and end of transformations, hardness, as well as fractions of the structural elements. Some information from the classification and calculation modules is processed using rules included in the fourth module, safe-guarding from errors that may occur because of splitting the general task. The outputs from the particular modules feature the data that unequivocally defines the form of the CCT diagram and are the basis for its graphical representation.

The data set used to develop the model employing the neural network was split into four subsets: training, validating, testing, and verifying one. Allocation of data to the particular subsets was done randomly. The optimum type and structure of the neural network, error function form, normalisation method for the input data, as well as training method and parameters were assumed after analysing their influence on the quality assessment coefficients of the developed models. The following quality assessment coefficients were assumed for classification problems: coefficient expressing in [%] the number of correct classifications and the area under the ROC curve. The ROC curve expresses the network sensibility (second class classified correctly) as a function of the incorrectly classified first class. In case of random classifications the area under the ROC curve assumes value of 0.5. In case of the „ideal" classifier, the area under the ROC curve assumes value of 1. For the regression issues the following were analysed: the average network forecast error (E_j), ratio of standard deviations of errors and data, which for the ideal forecasts assumes value of 0, as well as the Pearson's correlation coefficient R.

Determining the temperatures of the beginning and end of the supercooled austenite transformations as a function of chemical composition, austenitising temperature, and cooling rate was split into three tasks. The first one yielded the structural constituents of the steel cooled at a particular rate from the austenitising temperature, the second one calculated the temperatures of the beginning and end of the particular transformations occurring during cooling at a particular rate, the third one checked if, between the areas limited by curves of the beginning and end of the consecutive transformations, there is an area of austenite stability, or else, if the transformations occur immediately one after another. After the initial evaluation of temperatures of the beginning and end of transformations, the final values of these temperatures were determined using the conditional and calculation instructions worked out. Four models were worked out to solve the first task, making it possible to check if along the analysed cooling rate the areas of ferrite, pearlite, and bainite occur, and if the martensitic transformation occurs. Having classified the results, the cooling time range was determined – characteristic for the particular transformations and also types of the structural constituents were determined occurring in the steel after completing the cooling. For all transformations the feedforward networks (MLP) were used with one hidden layer and the learning method based on the conjugate gradients algorithm. The structures of the particular networks, input data, training parameters, and sizes of the particular data sets are given in Table 2. In the second task seven models were worked out employing neural networks (MLP) for calculating, depending on the cooling rate, of the values of the temperatures of beginning and end of the areas of occurring of: ferrite (F_s, F_k), pearlite (P_s, P_k), bainite (B_s, B_k), as well as of the

beginning of the martensitic transformation (M_s). Only in case of the B_k temperature, the network was used realising the generalised regression (GRNN). The structures of the particular networks, method and training parameters, as well as sizes of the particular data sets are presented in Table 3.

Table 2
Specifications of the developed classifiers based on neural networks

Transformation area	Input parameters	Network structure	Number of training epochs	Number of cases in data sets:
Ferritic	C, Mn, Si, Cr, Ni, Mo, V, Cu, v_{ch}, T_a	10-7-1	85	Training - 1692
Pearlitic		10-15-1	456	Validating - 846
Bainitic		10-20-14-1	506	Testing - 846
Martensitic		10-12-1	1008	Verifying - 610

Table 3
Specifications of the neural networks used for calculating the temperatures of the beginning and end of the supercooled austenite transformations

Tempe-rature	Number of cases in data sets				Input parameters	Network structure	Training method	No of epochs
	training	validating	testing	verifying				
F_s	918	459	459	327	C, Mn, Si,Cr, Ni, Mo, V, Cu, v_{ch}, T_a	10-11-1	quasi-Newton	627
F_k						10-7-1	quasi-Newton	1248
P_s	755	377	377	273		10-5-1	conjugate gradients	258
P_k						10-15-1	quasi-Newton	2124
M_s	854	427	427	319		10-11-1	conjugate gradients	84
B_s	830	415	415	284	C, Mn, Si, Cr, Ni, Mo, V, Cu, v_{ch}, T_a, B_{smax}	11-7-1	Lavenberg-Marquardt	430
B_k	1250	200	200	284	C, Cr, M_s, v_{ch}, B_{smax}	5-1250-2-1	k-averages	-

3. CALCULATION RESULTS FOR TRANSFORMATION TEMPERATURES

In Table 4 the quality assessment coefficients of the neural networks are presented, used as classifiers yielding information on the successive transformations occurring along the analysed cooling curves. The error values, ratio of standard deviations, and the Pearson's correlation coefficient R for neural networks are given in Table 5, making it possible to determine the temperatures of beginning and end of the particular transformations as functions of cooling rate. Examples of the CCT diagrams, worked out basing on the calculations carried out, along with the experimental plots, are presented in Figures 3 and 4.

Table 4
Quality assessment coefficients for neural networks, used as classifiers for determining the types of occurring transformations

Transformation areas	Testing set		Verifying set
	Coefficient of correct classifications, %	ROC	Coefficient of correct classifications, %
Ferritic	90	0.959	91
Pearlitic	92	0.975	92
Bainitic	88	0.945	89
Martensitic	92	0.973	94

Table 5
Error values and correlation coefficients for the temperatures of beginning and end of transformations calculated for data from the testing / verifying data sets

Tempe -rature	Error E_j, ºC	Error E_j, %	Standard deviation of the error, ºC	Ratio of standard deviations	Pearson's correlation coefficient R
F_s	18.2 / 21.6	2.6 / 3.0	18.1 / 20.3	0.52 / 0.54	0.87 / 0.85
F_k	19.4 / 20.5	3.1 / 3.2	19.2 / 17.7	0.49 / 0.50	0.87 / 0.86
P_s	15.5 / 17.1	2.4 / 2.6	14.5 / 14.8	0.54 / 0.54	0.85 / 0.84
P_k	22.8 / 21.6	3.8 / 3.6	21.3 / 18.9	0.57 / 0.55	0.80 / 0.85
B_s	25.8 / 28.4	5.3 / 5.9	27.2 / 28.0	0.58 / 0.62	0.80 / 0.79
B_k	24.1 / 26.6	7.2 / 8.0	30.9 / 32.3	0.62 / 0.64	0.78 / 0.77
M_s	21.2 / 22.4	7.1 / 8.0	19.9 / 22.2	0.53 / 0.51	0.83 / 0.86

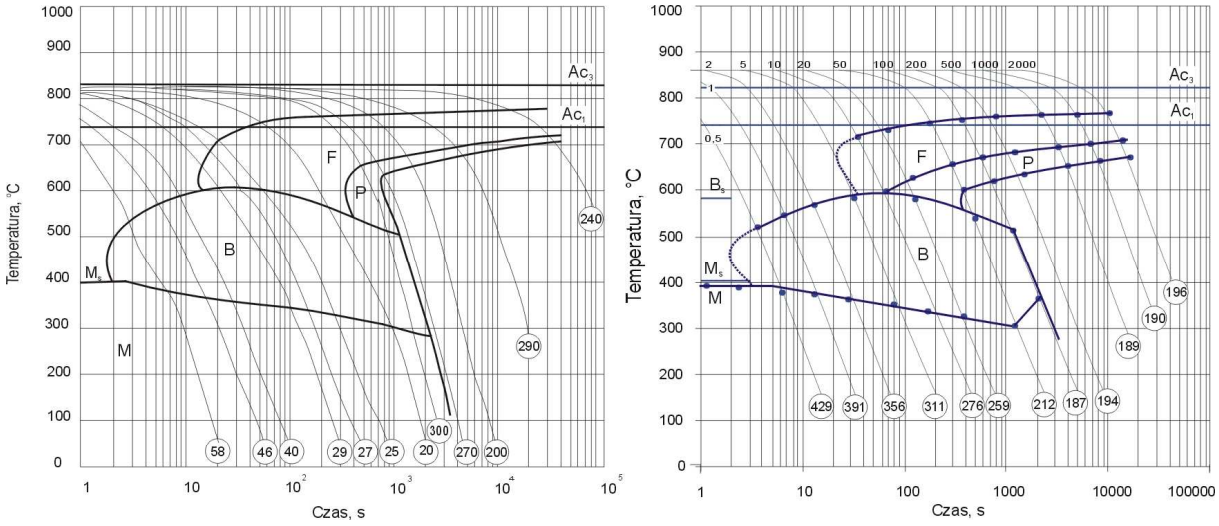

Figure 2. CCT diagram for steel with concentrations: 0.22% C, 0.64% Mn, 0.25% Si, 0.97%Cr, 0.33% Ni, 0.23% Mo, 0.01% V, 0.16% Cu, austenitised at a temperature of 875ºC; a) experimental, b) calculated

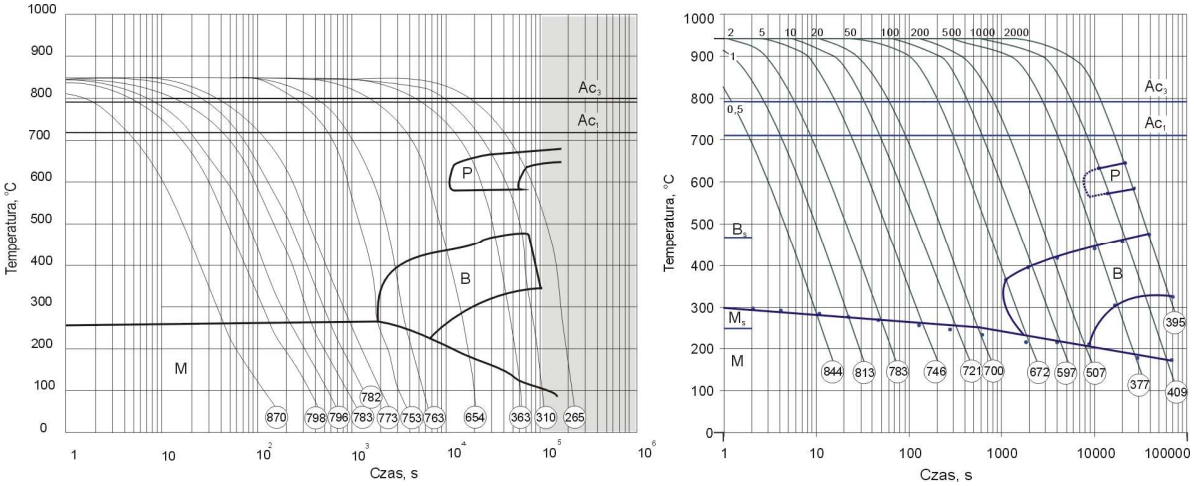

Figure 3. CCT diagram for steel with concentrations: 0.52% C, 0.7% Mn, 0.29% Si, 1.09%Cr, 1.72% Ni, 0.43% Mo, 0.14% V, austenitised at a temperature of 950ºC; a) experimental, b) calculated

4. SUMMARY

The paper presents the methodology of modelling using the neural networks of the relationship between the chemical composition and austenitising temperature, and the supercooled austenite transformation kinetics during the continuous cooling. The model worked out makes it possible to calculate a complete CCT diagram for the steel with a known chemical composition and analysis of the influence of particular elements on the characteristic points and transformation curves of the supercooled austenite, and also the hardness resulting from cooling. It makes also possible forecasting of the structure developed in steel as a result of cooling at a particular rate, by the quantitative description of the percentages of ferrite, pearlite, bainite, and martensite with the retained austenite [1, 2].

REFERENCES

1. J. Trzaska: Methodology of the computer modelling of the supercooled austenite transformations of the constructional steels, PhD thesis - unpublished, Main Library of the Silesian University of Technology, Gliwice 2002 (in Polish).
2. L.A. Dobrzański, J. Trzaska and R. Maniara: Proc. 10th Int. Sc. Conf. "Achievements in Mechanical and Materials Engineering AMME'2001", (2001) 175.
3. H.K.D.H. Bhadeshia: ISIJ International, Vol. 39, 10 (1999), 966.
4. http://huizen.dds.nl/~pwolk/MK/postersnn.html
5. P.J. van der Wolk, W.G. Vermeulen and S. van der Zwaag: 2nd Int. Conf. on Modelling of Metal Rolling Processes, London (1996) 378.
6. W.G. Vermulen, S. van der Zwaag, P. Morris and T. de Weijer: Steel Research, 68 (1997) 72.
7. J. Wang, P.J. van der Wolk and S. van der Zwaag: ISIJ International, Vol. 39, 10 (1999) 1038.