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Computer programme for prediction steel parameters after heat treatment

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Analysis and modelling

ABSTRACT

Purpose: The purpose of this paper is presentation of the computer program for calculating the Continuous Cooling Transformation diagrams for constructional and engineering steels.
Design/methodology/approach: The computer program uses the artificial neural networks for prediction steel properties after heat treatment. Input data are chemical composition and austenitizing temperature. Results of calculation consist of temperature of the beginning and the end of transformation in the cooling rate function, the volume fraction of structural components and hardness of steel cooled from austenitizing temperature with a fixed rate.
Findings: The algorithm can be use in designing new chemical compositions of steels with assumed hardness after heat treatment.
Research limitations/implications: The created method for designing chemical compositions is limited by ranges of mass concentrations of elements. The methodology demonstrated in the paper makes possibility to add new steels to the system.
Practical implications: The method may be used in computer steel selection systems for machines parts manufactured from constructional or engineering steels subjected to heat treatment.
Originality/value: The presented computer program can be used for selecting steel with required structure after heat treatment.
Keywords: Computational material science; Artificial intelligence methods; Neural networks; CCT diagrams

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. The elaboration of CCT is time consuming and requires applying expensive testing equipment. Additionally, strict relation between chemical composition and austenitizing conditions and form of transformation curves of supercooled austenite causes the difference between CCT diagrams for given steel grade. [1]

Therefore, many attempts of modeling austenite transformations in the steel during cooling are being undertaken. The basis of temperature calculations and time of particular transformations of supercooled austenite and volume fraction of particular structural components, as well as hardness obtained after cooling is finished, are most often mathematical models of processes proceeding in the steel during heat treatment or empirical dependences elaborated according to sufficiently big number of experimental data. The dependences allowing for modeling supercooled austenite transformations in isothermal cooling conditions, are based most often on Jonson-Mehl and Avramy equations. The results of calculations obtained using mentioned equations, in many cases differ from experimental data. New relationships are published in the literature, describing various quantities connected to kinetics of supercooled austenite transformations, just for the steel with wide range of alloying elements concentration or advised for specific steel grades. Mass concentrations of elements and austenitising temperature were

used as input data, obtaining the temperature values of the particular transformations depending on cooling rate at the output. In all cases the same neural network was employed, which required using a large number of neurons in the output layer, and consequently a big training set. The amount of data mentioned by the authors for solving the problem seems to be far too small. Presented results indicate to the correct representation by the network of some transformation temperature change trends versus cooling time; however, differ significantly from the experimental results. One should note the attempts of neural networks applications for describing those relationships [2-4], what is consistent with main trends connected to application of artificial intelligence methods in material engineering.[4-9]

In papers [10-15] the authors' method of CCT diagrams calculation has been described. It was assumed that decomposition of general problem, which solution requires application of a few neural networks with less complex structure, allows to calculate anisothermic diagram of the supercooled austenite with considerably smaller error. In the present work a computer program has been presented, allowing to make calculations and graphic presentations of the supercooled austenite transformations, steel hardness and volume fraction of structural components.

2. Structure of the program and presentation of results

Computer program for calculating the anisothermic diagrams of supercooled austenite is based on numerical model, developed using the artificial neural networks. In order to design neural networks, the Statistica Neural Network, version 4.0F, program was used. Designing of neural networks required preparing a proper set of learning data. Representative set of data was created from the 400 of CCT diagrams, published in the literature. The range of mass concentration of elements shown in Table 1 also describes the scope of program usage.

Table 1.
Ranges of mass fractions of elements

	Mass fractions of elements, %							
	C	Mn	Si	Cr	Ni	Mo	V	Cu
Min.	0.08	0.13	0.12	0	0	0	0	0
Max.	0.77	2.04	1.90	2.08	3.65	1.24	0.36	0.3
%Mn+%Cr+%Ni+%Mo≤5								

The program was developed in the Borland C++ Builder 6 compiler. The input data for the program were mass concentration of elements and austenitizing temperature, which can be input by the user or calculated by program as temperature Ac3+50°C. The program consists of dozens of source data files, containing implementation of classes, functions and program structure data. In the program, 21 files with neural networks have been implemented. Because of such approach, it is possible to update the program and expand its range of usage or decrease the error values for specific neural networks models. The only condition is completing the learning set with new cases and elaborating proper models of neural networks again.

The program has a modular structure. The block diagram is shown in Fig.1. Module of classification is a module basing on the four models of neural networks and its role is to identify the structure components present in the steel after finishing the continuous cooling with predetermined cooling rate. It allows for determining the range of cooling rates for specific transformations of supercooled austenite and is a essential information for predicting the steel hardness and participation of ferrite, pearlite, bainite and martensite in the microstructure of steel. In the program, 140 mean cooling rates have been investigated. For each of them, the kind of structural component is recognized, which allows for preparing input data for proper network from calculations unit, starting the network and saving the calculations results in the global table.

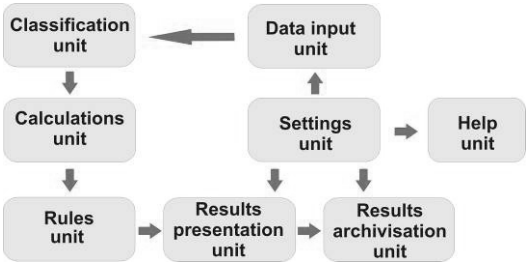

Fig. 1. Block diagram for CCT diagram calculations

Calculations module is used for determining of the temperature values of start and finish of particular transformations of the supercooled austenite, time of transformation start, hardness and volume fraction of structural components for established cooling rate; in this part of a program 16 neural networks have been used. Main information about neural networks used in classification module and in calculations unit are presented in papers [10-15].

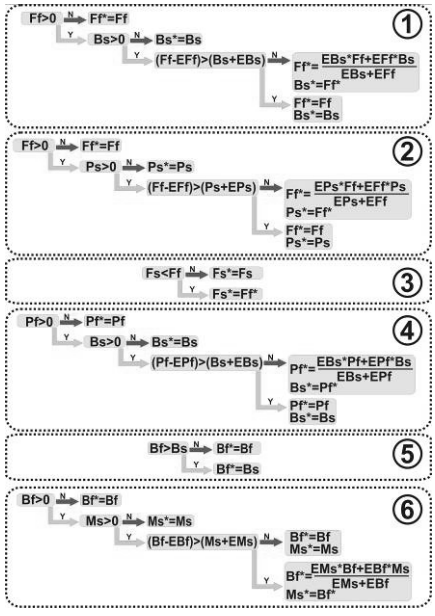

Fig. 2. Algorithm for determining the temperatures of start and finish of the transformations

Rules module verifies the data obtained from calculation unit operation. The application of seven neural networks for calculating

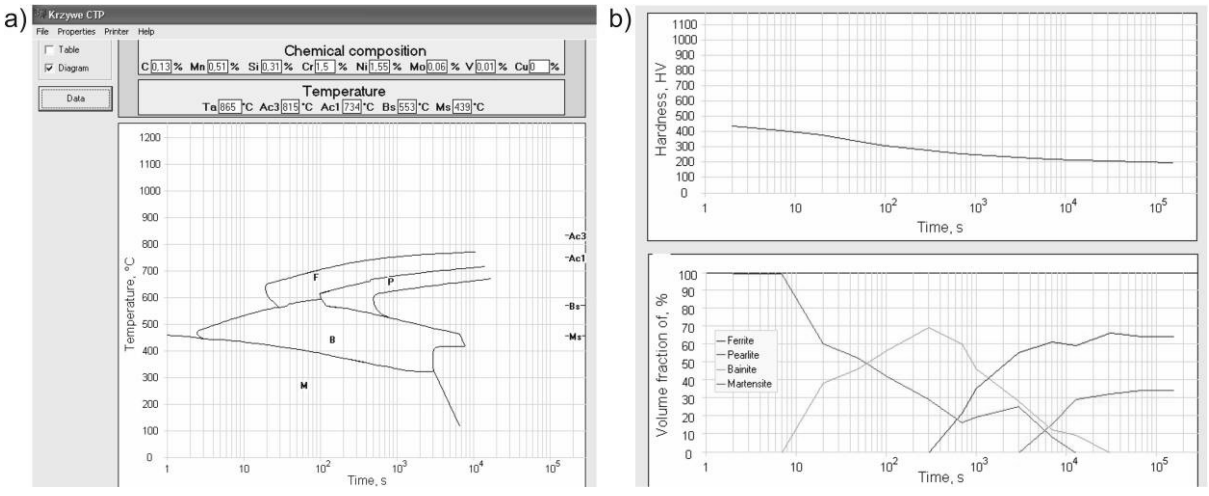

Fig. 3. The program window for steel with following chemical composition: 0.13%C, 0.51% Mn, 0.31%Si, 1.5% Cr, 1.55% Ni, 0.06% Mo, 0.01% Mo; a) CCT diagram view; b) hardness and volume fractions of phases diagrams

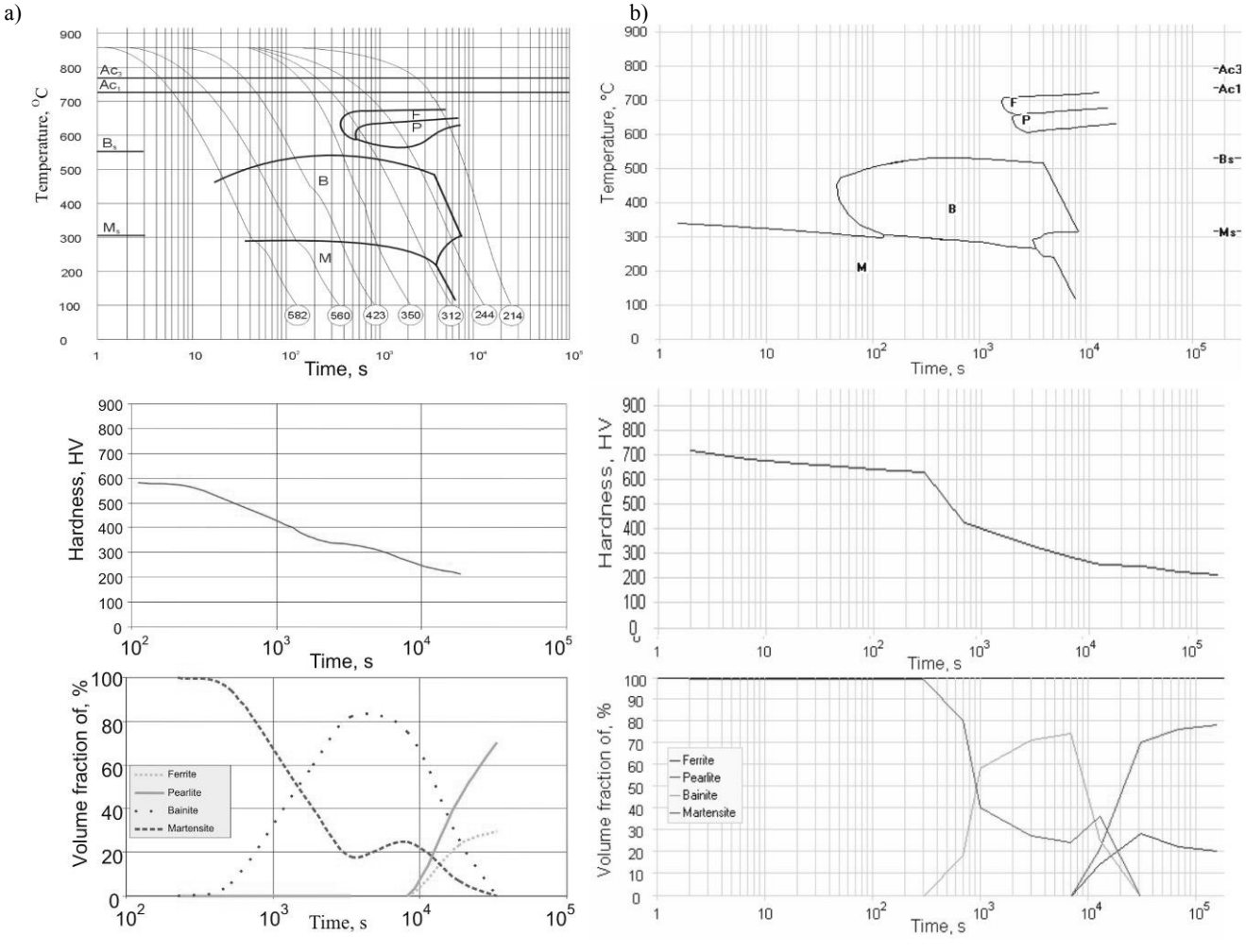

Fig. 4. CCT, hardness and phases volume fractions diagrams of steel with following chemical composition:0.43% C, 0.66% Mn, 0.33% Si, 0.74%Cr, 1,.% Ni, 0.2% Mo, austenitized in 860ºC; a) experimental; b) estimated by program

the temperature of starting and finishing particular transformations of supercooled austenite in the function of cooling rate, with assuming calculations errors, requires carrying out additional analysis of the obtained results. In this analysis the conditions for austenite transformation sequence during decrease of temperature has to be taken into account.

The procedure of final start and finish temperature evaluation is shown in fig. 2. The problem has been described in detail in works [15]. In fig. 2 F_s, F_f, P_s, P_f, B_s, B_f, M_s are the temperature values calculated with using the neural network model, symbols F_s^*, F_f^*, P_s^*, P_f^*, B_s^*, B_f^*, M_s^* describe values of temperature defining, with the cooling rate, the points presented in the temperature-time coordinate system, being the basis for graphic presentation of CCT diagrams.

Module of results presentation generates corresponding diagrams and tables according to calculated values. Temperatures corrected by system of rules are saved in next global tables. After calculating the temperature, in order to present graphically CCT diagram, the time of beginning and finishing of transformation is calculated for calculated temperature and assumed cooling ratio. The time is calculated by especially designed for that reason neural network and saved in the next table. The temperature values of particular phase transformations in the function of cooling time can be presented in the form of diagram or table, where for assumed fourteen cooling rates, the transformation temperature and time passed from the moment of cooling start from the austenitizing temperature has passed.

Figure 3a presents program window with the calculated CCT diagram. Additionally, two diagrams are presented; the first illustrated changes in steel hardness in the function of cooling time, second, volume fraction of ferrite, pearlite, bainite and martensite, depending on cooling time (Fig. 3b).

The results archivization module allows saving calculated results as text files or in graphic format. Help module facilitates working with program by description of the all program functions. Settings module influences the user's interface and program appearance. The user interface allow to change the language (English, Polish), diagram display options, size of input data set, and ways of results archivization (file, print).

Predicted values of steel hardness and calculated volumes fractions of phases give very well results. Shapes of the CCT diagrams generated by program are very similar to experimental diagrams. Most of the received values of parameters had Pearson coefficient close to 0.95. Comparison of calculated and experimental diagrams for example steel is shown on fig. 4.

3. Summary

One of the assumptions during program design phase was possibility of making changes in case of neural network model development, which would allow for calculations of temperature of any transformation, hardness or finally the volume fraction of particular structural components with higher precision. Therefore, the source code for each network is saved in a different file, and data entered by the user as well as calculations results, are stored in tables of global variables.

It allows not only for fast modification of the program, but also its adapting for other groups of steel, provided that sufficient number of experimental data will be accumulated. All functions have been saved according to object language standards, what allows, after making necessary modifications, to elaborate the version available on internet site, for example in PHP language.The investigations on computer system helping the steel selection with assumed course of the CTT diagrams are carried out. The possibility of using the hybrid method connecting artificial neural networks and genetic algorithms is considered.

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