



Calculation of the steel hardness after continuous cooling

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ABSTRACT

Purpose: The paper presents method in predicting hardness of steel cooled continuously from the austenitizing temperature, basing on the chemical composition, austenitizing temperature and cooling rate.

Design/methodology/approach: In the paper it has been applied a hybrid approach that combined application of various mathematical tools including logistic regression and multiple regression to solve selected tasks from the area of materials science.

Findings: Modelling make improvement of engineering materials properties possible, as well as prediction of their properties, even before the materials are fabricated, with the significant reduction of expenditures and time necessary for their investigation and application.

Practical implications: The worked out relationships may be used in computer systems of steels' designing for the heat-treated machine parts.

Originality/value: The paper presents the method for calculating hardness of the structural steels, depending on their chemical composition, austenitizing temperature and cooling rate.

Keywords: Computational material science; Steels; Statistic methods; CCT diagrams

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METHODOLOGY OF RESEARCH, ANALYSIS AND MODELLING

1. Introduction

Computer-aided modeling is becoming increasingly present in research and in industrial practice. Computer modelling make improvement of engineering materials properties possible, as well as prediction of their properties, even before the materials are fabricated, with the significant reduction of expenditures and time necessary for their investigation and application. Research in the area of mathematical modelling, computational intelligence, and artificial intelligence indicate to the big potential connected with using this methods [1-7].

The knowledge of kinetics of supercooled austenite transformations occurring during steel cooling continuously from

the austenitisation temperature, as shown in CCT diagrams, is underlying the selection of parameters of many steel heat treatment operations. CCT diagrams are applied for determining the structure and hardness of hardened, normalised steel or steel subjected to full annealing. The position and shape of curves of supercooled austenite transformations applied onto CCT diagrams depend most of all on the chemical composition of steel, austenite homogenisation degree, austenite grain size. Fluctuations of the chemical composition of steel, allowable even within the same steel grade, and also changes of the austenitizing conditions cause that published in catalogues CCT diagrams cannot provide reliable information on austenite transformations during cooling. The dilatometric method supplemented with metallographic investigations with different velocities of samples and their

hardness measurements are usually used for establishing a CCT diagrams. The investigations are time consuming and require costly research apparatuses [8-9].

The paper presents the methodology of modelling using the regression method of the relationship between the chemical composition and the hardness of the steel cooling from the austenitizing temperature.

2. Examples of the hardness calculating methods

The method proposed in the paper [10] employs two applications of the neural networks: classification and regression. To develop the relationship between the chemical composition, austenitising temperature, cooling rate, and hardness of the structural steel the feedforward neural network (MLP) was used. The activation level of the successive fourteen network input nodes depended on: mass concentration of elements (C, Mn, Si, Cr, Ni, Mo, V, Cu), austenitizing 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, whose values were determined basing on the model presented in [11-13]. The values of the network quality evaluation coefficients for the training, validation and test set, were: for the average absolute error 37HV, a quotient of standard deviations 0.32, a correlation coefficient 0.95.

Research workers at the Creusot Laboratory have been studying the effect of chemical composition and austenitisation conditions on the continuous cooling transformation diagrams for carbon and low alloy steels [14-17]. They have derived the following Equations:

$$\log v_M = 9.81 - (4.62 \cdot C + 1.05 \cdot Mn + 0.5 \cdot Cr + 0.66 \cdot Mo + 0.54 \cdot Ni + 0.00183 \cdot P_A) \quad (1)$$

$$\log v_{M90} = 8.76 - (4.04 \cdot C + 0.96 \cdot Mn + 0.58 \cdot Cr + 0.97 \cdot Mo + 0.49 \cdot Ni + 0.001 \cdot P_A) \quad (2)$$

$$\log v_{M50} = 8.50 - (4.13 \cdot C + 0.86 \cdot Mn + 0.41 \cdot Cr + 0.94 \cdot Mo + 0.57 \cdot Ni + 0.0012 \cdot P_A) \quad (3)$$

$$\log v_B = 10.17 - (3.8 \cdot C + 1.07 \cdot Mn + 0.57 \cdot Cr + 1.58 \cdot Mo + 0.7 \cdot Ni + 0.0032 \cdot P_A) \quad (4)$$

$$\log v_{B90} = 10.55 - (3.65 \cdot C + 1.08 \cdot Mn + 0.61 \cdot Cr + 1.49 \cdot Mo + 0.77 \cdot Ni + 0.0032 \cdot P_A) \quad (5)$$

$$\log v_{B50} = 8.74 - (2.23 \cdot C + 0.86 \cdot Mn + 0.59 \cdot Cr + 1.60 \cdot Mo + 0.56 \cdot Ni + 0.0032 \cdot P_A) \quad (6)$$

$$\log v_{FP} = 6.36 - (0.43C + 0.49 \cdot Mn + 0.26 \cdot Cr + 0.38 \cdot Mo + 2 \cdot Mo^{0.5} + 0.78 \cdot Ni + 0.0019 \cdot P_A) \quad (7)$$

$$\log v_{FP90} = 7.51 - (1.38 \cdot C + 0.35 \cdot Mn + 0.11 \cdot Cr + 2.31 \cdot Mo + 0.93 \cdot Ni + 0.0033 \cdot P_A) \quad (8)$$

where:

C, Mn, Cr, Ni, Mo, - mass concentration of the alloying elements; v_i [°C/h] - critical cooling rates at 700°C are referred to as:

v_M -for martensite; v_{M90} - denotes 90% of martensite with 10% of other constituents; v_{M50} - denotes 50% of martensite with 50% of other constituents; v_B -for bainite; v_{B90} - denotes 90% of bainite with 10% of other constituents; v_{B50} - denotes 50% of bainite with 50% of other constituents; v_{FP} -for ferrite-pearlite; v_{FP90} -denotes 90% of ferrite-pearlite with 10% of bainite;

P_A is an austenitising parameter whose value in °C/h is given by:

$$P_A = \left[\frac{1}{T} - \frac{nR}{\Delta H} \log \frac{t}{t_0} \right]^{-1} \quad (9)$$

where:

T-temperature, K,

t - time,

t_0 - unit of time,

R - gas constant 8.314 J/K·mol,

n - $\log_e 10$,

ΔH - the activation energy of the phenomenon which for grain growth in most low alloy steels has a value of 460.55 kJ/mol.

The hardness of the microstructures produced are given by the Equations (10-12).

$$HV_M = 127 + 949 \cdot C + 27 \cdot Si + 11 \cdot Mn + 16 \cdot Cr + 8 \cdot Ni + 21 \cdot \log v_R \quad (10)$$

$$HV_B = -323 + 185 \cdot C + 330 \cdot Si + 153 \cdot Mn + 144 \cdot Cr + 191 \cdot Mo + 65 \cdot Ni + (\log v_R) \cdot (89 + 53 \cdot C - 55 \cdot Si - 22 \cdot Mn - 20 \cdot Cr - 33 \cdot Mo - 10 \cdot Ni) \quad (11)$$

$$HV_{FP} = 42 + 223 \cdot C + 53 \cdot Si + 30 \cdot Mn + 7 \cdot Cr + 19 \cdot Mo + 12.6 \cdot Ni + (\log v_R) \cdot (10 - 19 \cdot Si + 8 \cdot Cr + 4 \cdot Ni + 130 \cdot V) \quad (12)$$

where: v_R is the cooling rate.

Maynier and coworkers have developed a useful method to predict steel hardness. Their equations were derived from 107 tests on 40 industrial grades. The total hardness of steel is calculate dependent on the volume fractions of the constituents of the microstructure.

$$HV = (\%FP \cdot HV_{FP} + \%B \cdot HV_B + \%M \cdot HV_M) / 100 \quad (13)$$

A disadvantage of the Creusot-Loire method is that knowledge is required of the amount of the starting constituents of the microstructure. This can be estimated by the Equations (1-8).

3. Materials and method

The preparation of a representative set of empirical data has had a fundamental significance for preparing a method of hardness calculating. The data set, made on the basis of available publications, included the chemical composition, austenitizing temperature and CCT diagrams for structural and engineering steels. The obtained diagrams have been subjected to a selection, taking the mass concentration of alloy elements as a criterion. A range of the accepted mass concentrations of the elements has been presented in Table 1. The data set consisted of 1200 cases.

On the basis of the analysis of different forms, general formulae embracing the influence of the chemical composition and optionally, the austenitizing temperature as well as the cooling rate on the hardness, including the interrelations accounted for synergy of alloy elements' interactions, the general forms of Equations have been accepted:

$$HV = a_0 + a_1 \cdot C + a_2 \cdot Mn + a_3 \cdot Cr + a_4 \cdot Ni + a_5 \cdot Mo + a_6 \cdot V + a_7 \cdot T_A + a_8 \cdot v_R + a_9 \cdot F + a_{10} \cdot P + a_{11} \cdot B + a_{12} \cdot M \quad (14)$$

where:

C, Mn, Cr, Ni, Mo, V - mass fractions of the alloying elements;

a_0, a_1, \dots, a_{12} - coefficients calculated with the regression analysis;
 T_A - austenitizing temperature, °C;
 V_R - cooling rate, °C/min;
 F, P, B, M - binary nominal variables, whose values (0 or 1) were determined basing on the logistic regression model.

Table 1.
 Ranges of mass concentrations of elements

Range	Mass fractions of elements, %					
	C	Mn	Cr	Ni	Mo	V
min	0.22	0.40	0	0	0	0
max	0.55	1.15	2.10	2.15	0.55	0.25
average	0.37	0.71	0.78	0.52	0.17	0.02
standard deviation	0.09	0.14	0.49	0.67	0.16	0.05

The type of structure developed after cooling the steel was specified using four binary nominal variables, whose values were determined basing on the logistic regression model. A classifier had to be developed, to obtain this information, using as input data the mass concentrations of the alloying elements, austenitizing temperature, and cooling rate.

$$P_X = \exp(K_X) / \{1 + \exp(K_X)\} \quad (15)$$

where:

$X = F, P, B, M,$

$$K_X = b_{0X} + b_{1X} \cdot C + b_{2X} \cdot Mn + b_{3X} \cdot Cr + b_{4X} \cdot Ni + b_{5X} \cdot Mo + b_{6X} \cdot V + b_{7X} \cdot V_R \quad (16)$$

4. Calculation results

Evaluation of the worked out empirical formulae has been made on the basis of the analysis of the mean error value, the deviation of the average absolute error and Pearson's correlation coefficient. The formulae describing the influence of the chemical composition and cooling rate on the hardness worked out using the multiple regression, are presented in Equation 17. Classifiers used for forecasting occurrences of the particular structural constituents in steel are presented in Equations 18-25.

$$HV = -86 + 492 \cdot C + 92 \cdot Mn + 69 \cdot Cr + 25 \cdot Ni + 102 \cdot Mo + 267 \cdot V + 0.064 \cdot T_A + 27.7 \cdot V_R^{0.25} - 38 \cdot F - 70 \cdot P - 32 \cdot B + 72 \cdot M \quad (17)$$

where:

$F = 1$ for $P_F \geq 0.5$ or $F = 0$ for $P_F < 0.5$

$P = 1$ for $P_P \geq 0.5$ or $P = 0$ for $P_P < 0.5$

$B = 1$ for $P_B \geq 0.5$ or $P = 0$ for $P_B < 0.5$

$M = 1$ for $P_M \geq 0.5$ or $P = 0$ for $P_M < 0.5$

$$P_F = \exp(K_F) / \{1 + \exp(K_F)\} \quad (18)$$

$$K_F = 17 - 20.9 \cdot C - 0.01 \cdot Mn - 2.3 \cdot Cr - 1.2 \cdot Ni - 7.4 \cdot Mo - 6.5 \cdot V - 1.5 \cdot V_R^{0.25} \quad (19)$$

$$P_P = \exp(K_P) / \{1 + \exp(K_P)\} \quad (20)$$

$$K_P = 16 - 3.5 \cdot C - 4 \cdot Mn - 3.5 \cdot Cr - 1.5 \cdot Ni - 11.8 \cdot Mo - 1.7 \cdot V - 1.9 \cdot V_R^{0.25} \quad (21)$$

$$P_B = \exp(K_B) / \{1 + \exp(K_B)\} \quad (22)$$

$$K_B = 0.0015 - 2.54 \cdot C - 0.74 \cdot Mn - 0.3 \cdot Cr - 0.2 \cdot Ni - 2.3 \cdot Mo - 1.85 \cdot V - 0.018 \cdot V_R^{0.25} \quad (23)$$

$$P_M = \exp(K_M) / \{1 + \exp(K_M)\} \quad (24)$$

$$K_M = -10.9 - 1.7 \cdot C - 2.9 \cdot Mn - 3.7 \cdot Cr - 0.9 \cdot Ni - 3.7 \cdot Mo - 2.5 \cdot V - 1 \cdot V_R^{0.25} \quad (25)$$

The assessment of the significance of the regression coefficients are presented in Table 2. Significance level was specified of 0.05. The input variable is statistically significant if the p-value is less than 0.05. The mean error values, the standard deviation of the error and the correlation coefficient for the hardness model are given in Table 3. In Table 4 the quality assessment coefficients of the classifier are presented, used as classifiers yielding information on the successive transformations occurring along the analysed cooling curves.

Table 2.
 The assessment of significance of regression coefficients

	Coefficients	Standard Error	t Stat	P-value
Intercept	-86.3305	35.70162	-2.41811	0.015753
C	491.6927	24.263	20.26512	1.68E-78
Mn	92.34665	14.82571	6.228819	6.54E-10
Cr	69.01353	4.360176	15.82815	2.81E-51
Ni	24.92482	3.172811	7.855754	8.95E-15
Mo	101.742	13.58629	7.488582	1.37E-13
V	267.2312	40.81646	6.547145	8.76E-11
T_A	0.063932	0.03227	1.981182	0.047805
$V_R^{0.25}$	21.70305	0.950688	22.82877	1.06E-95
F	-37.6321	5.582585	-6.74098	2.46E-11
P	-70.5438	6.369514	-11.0752	3.52E-27
B	-31.6706	4.233635	-7.48071	1.45E-13
M	72.08688	5.671254	12.71092	9.11E-35

Table 3.
 Error values and correlation coefficients for hardness model

Error E_{HV} , HV	Standard deviation of the error, HV	Quotient of standard deviations	Pearson correlation coefficient
46.9	35.6	0.23	0.92

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

Transformation areas	Coefficient of correct classifications, %
Ferritic	88
Pearlitic	88
Bainitic	63
Martensitic	83

To verify the model worked out, the experimental hardness change curves were made as functions of cooling time were compared with curves calculated using hardness model. Examples of the curves worked out are shown in Figures 1-6. The comparative plots for the experimental and calculated hardness are presented in Figure 7. The distribution of the residuals calculated for pearlitic and martensitic transformation are presented in Figures 8-9.

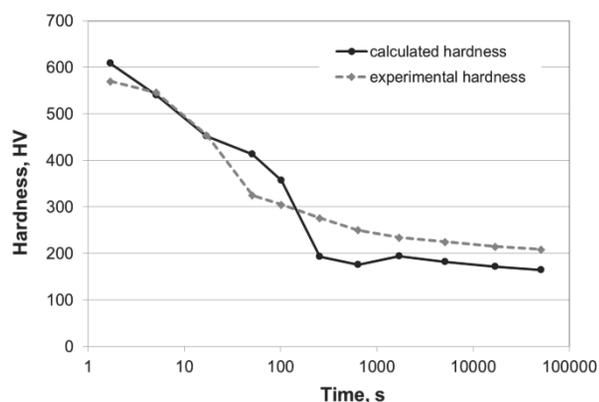


Fig. 1. The comparison of the experimental and calculated curves for the steels with a mass concentration of elements: 0.3% C, 0.5% Mn, 1.0% Cr, 0.2% Mo austenitised at temperature of 850°C

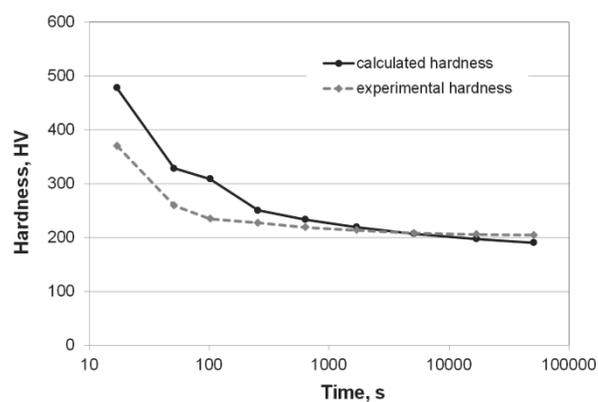


Fig. 4. The comparison of the experimental and calculated curves for the steels with a mass concentration of elements: 0.44% C, 0.8% Mn, 0.14% Cr, 0.2% Ni, austenitised at temperature of 850°C

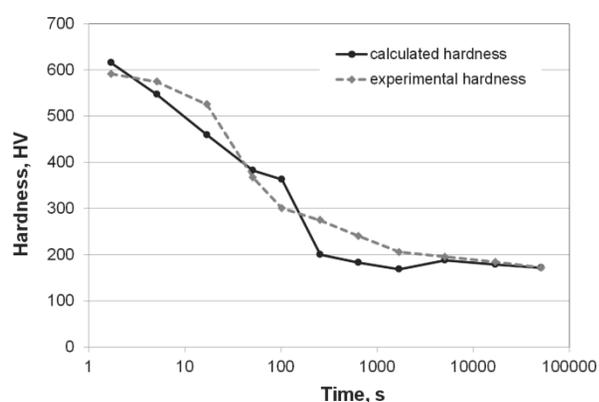


Fig. 2. The comparison of the experimental and calculated curves for the steels with a mass concentration of elements: 0.3% C, 0.8% Mn, 0.5% Cr, 0.55% Ni, 0.2% Mo austenitised at temperature of 850°C

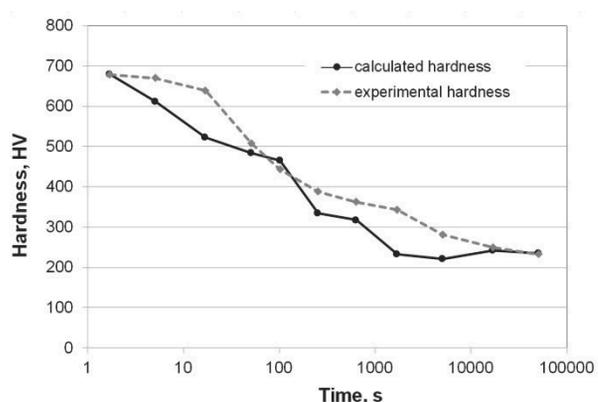


Fig. 5. The comparison of the experimental and calculated curves for the steels with a mass concentration of elements: 0.41% C, 0.85% Mn, 0.5% Cr, 0.55% Ni, 0.25% Mo austenitised at temperature of 850°C

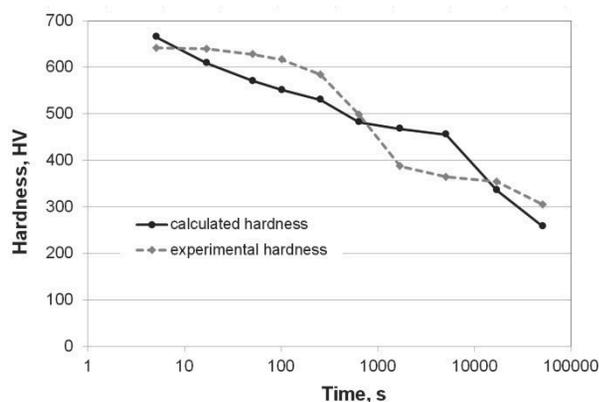


Fig. 3. The comparison of the experimental and calculated curves for the steels with a mass concentration of elements: 0.36% C, 0.7% Mn, 1.5% Cr, 1.5% Ni, 0.25% Mo austenitised at temperature of 850°C

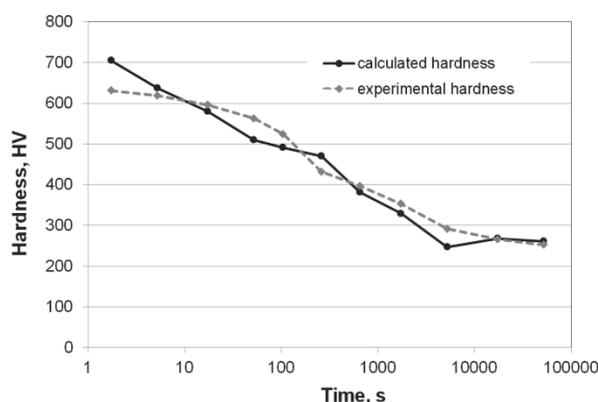


Fig. 6. The comparison of the experimental and calculated curves for the steels with a mass concentration of elements: 0.4% C, 0.85% Mn, 1.05% Cr, 0.3% Mo, austenitised at temperature of 870°C

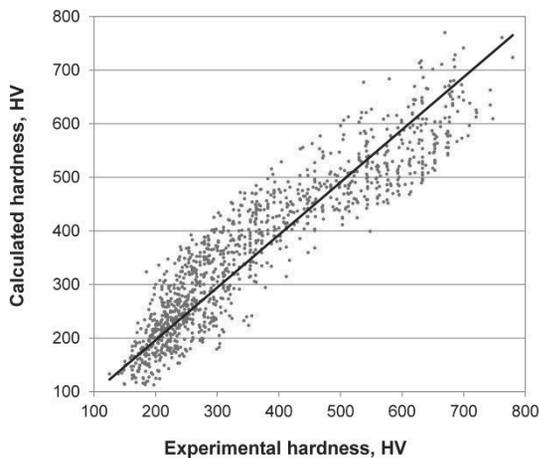


Fig. 7. Comparison of the experimental HV hardness with values calculated using the regression model

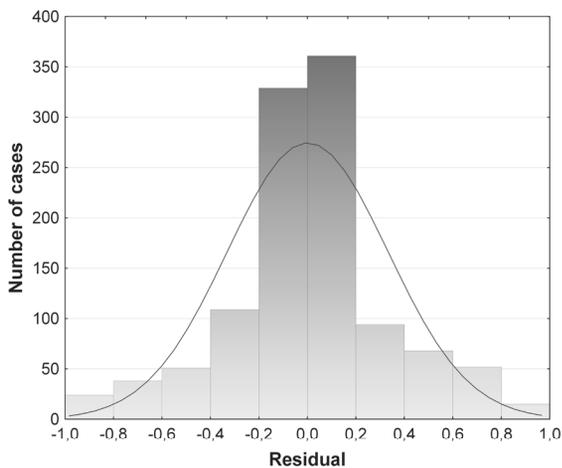


Fig. 8. Distribution of residuals for classifier-martensitic transformation

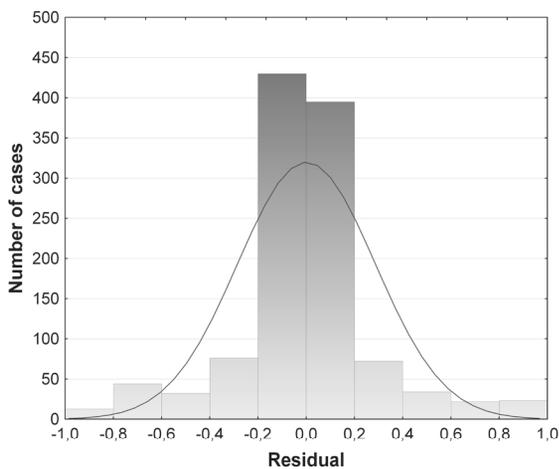


Fig. 9. Distribution of residuals for classifier-pearlitic transformation

5. Summary

The model worked out makes it possible to calculate hardness for the steel with a known chemical composition. Determining the curve of hardness changes versus cooling time, 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 cooling rate.

The presented model facilitates the analysis of the interaction of the chemical composition on the hardness curves of the steel cooled from the austenitizing temperature. This model delivers crucial information for the reasonable choice of steel for those parts of the machines that are subjected to the heat treatment. The presented interrelations may also be of use when selecting the chemical composition and determining the austenitizing temperature for steels with a complex course of the supercooled austenite transformations.

In the paper, the size of the austenite grain and the time of austenitizing, have not been taken into account because of the lack of the information in the majority of CCT diagrams used for preparing the data set. Moreover, simplifications concerning the chemical composition of the examined steels are often used and there are only mass concentrations of the basic elements of a given type of steel demonstrated.

Calculation methods provide an alternative to experimental measurement in providing the material data required for heat treatment process simulation.

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