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EMPIRICAL FORMULAE FOR THE CALCULATION OF AUSTENITE SUPERCOOLED TRANSFORMATION TEMPERATURES

ZALEŻNOŚCI EMPIRYCZNE DO OBLICZANIA TEMPERATURY PRZEMIAN AUSTENITU PRZECHŁODZONEGO

The paper presents empirical formulae for the calculation of austenite supercooled transformation temperatures, basing on the chemical composition, austenitising temperature and cooling rate. The multiple regression method was used. Four equations were established allowing to calculate temperature of the start area of ferrite, perlite, bainite and martensite at the given cooling rate. The calculation results obtained do not allow to determine the cooling rate range of ferritic, pearlitic, bainitic and martensite transformations. Classifiers based on logistic regression or neural network were established to solve this problem.

Keywords: CCT diagram, modeling, heat treatment, steel

W pracy przedstawiono zależności empiryczne do obliczania temperatury przemian austenitu przechłodzonego na podstawie składu chemicznego, temperatury austenityzowania i szybkości chłodzenia. Zastosowano metodę regresji wielorakiej. Opracowano cztery równania, które umożliwiają obliczenie temperatury początku przemiany ferrytycznej, perlitycznej, bainitycznej i martenzytycznej. Wyniki obliczeń nie pozwalają na wyznaczenie zakresu szybkości chłodzenia, dla których występują przemiany ferrytyczna, perlityczna, bainityczna i martenzytyczna. Do rozwiązania problemu opracowano klasyfikatory stosując regresję logistyczną lub sztuczne sieci neuronowe.

1. Introduction

Computer modelling make improvement of engineering materials properties possible, as well as prediction of their properties, with the significant reduction of expenditures and time necessary for their investigation. Calculation methods provide an alternative to experimental measurement in providing the material data required for heat treatment process simulation [1-10].

The continuous cooling transformation (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, fully annealed or normalized steels. 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. 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 grain size, austenite homogenisation degree, temperature and austenitisation time. Fluctuations of the chemical composition of steel, allowable even within the same steel grade, and also changes of the austenitising conditions cause that published in catalogues CCT diagrams cannot provide reliable information on austenite transformations during continuous cooling. The dilatometric method supplemented with metallographic investigations for different samples and their hardness measurements are usually used for establishing a CCT diagrams. The measurements are time consuming and require expensive research apparatuses [11, 12].

The attempts to employ computer techniques for solving this problem are connected with calculation of the characteristic transformation points or curves of the diagram, based on a mathematical model, empirical formulae or using the artificial intelligence methods.

A method of modelling the supercooled austenite transformations with the use of neural networks has been described in detail in the publications [13-16].The elaborated calculation models were used in the custom software for the graphical presentation of a CCT diagram [17]. Another example of hybrid method application for CCT diagrams calculation is a model presented in [18] that employs artificial neural networks and multiple regression.

The paper presents the methodology of modelling using the regression method of the relationship between the chemical composition and the supercooled austenite transformations temperatures of the steel cooling from the austenitising temperature.

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2. Material and method

The preparation of a representative set of empirical data has had a important significance for preparing a method of calculating supercooled austenite transformations start temperatures. The data set was developed on the basis of on literature data, including chemical compositions, austenitising temperature and the CCT diagrams for structural and engineering steels. The obtained curves were worked out, assuming mass fractions of the alloying elements as the criterion. A range of the accepted mass concentrations of the elements has been presented in Table 1. The data set consisted of 500 CCT diagrams. The number of cases for particular data sets has been presented in Table 2.

TABLE 1

Ranges of mass concentrations of elements

Range	Mass fractions of elements, %							
	C	Mn	Si	Cr	Ni	Mo	V	Cu
min	0.21	0.28	0.13	0	0	0	0	0
max	0.68	2.0	1.9	2.5	3.85	1.05	0.38	0.38

TABLE 2

Number of cases in data sets

	Data set			
	Fs	Ps	Bs	Ms
Regression	1827	1460	1930	1688
Classification	2925			

Based on the analysis of different forms, general formulae embracing the influence of the chemical composition and optionally the austenitising temperature as well as the cooling rate on the temperature transformations value, including the interrelations accounted for synergy of alloy elements' interactions, the general forms of equation have been accepted:

$$Ts(^{\circ}C) = a_0 + a_1 \cdot C + a_2 \cdot Mn + a_3 \cdot Si + a_4 \cdot Cr + a_5 \cdot Ni + a_6 \cdot Mo + a_7 \cdot V + a_8 \cdot Cu + a_9 \cdot T_A + a_{10} \cdot v_R \quad (1)$$

where:

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

a_0, a_1.., a_{12} – coefficients calculated with the regression analysis;

T_A – austenitising temperature, °C;

V_R – cooling rate, °C/min.

Created, with the help of multiple regression, formulae do not allow for determining the range of the cooling rate for which ferritic, pearlitic, bainitic and martensite transformations occur. That is why, the values of the cooling rate, for which ferritic, pearlitic, bainitic and martensite transformations take place, have been determined with the help of the classifiers, worked out using the logistic regression method. A classifier had to be developed, to obtain this information, using as input data the chemical composition, cooling rate and austenitising temperature. The problem amounts to the calculation of the highest cooling rate value for which a ferrite, pearlite and bainite occur and the lowest cooling rate value for which bainite and martensite occur in the structure of the steel. The range of cooling rate for particular transformations and the type of structural components existing in steel after continuous cooling with the set cooling rate are determined as a result of the classification made.

The general forms of formulae used for forecasting occurrences of the particular structural constituents in steel for assumed cooling rate are presented in equations (2)-(3).

$$P_X = \exp(K_X)/\{1 + \exp(K_X)\} \quad (2)$$

$$K_X = b_{0X} + b_{1X} \cdot C + b_{2X} \cdot Mn + b_{4X} \cdot Si + b_{4X} \cdot Cr + b_{5X} \cdot Ni + b_{6X} \cdot Mo + b_{7X} \cdot V + b_{8X} \cdot Cu + b_{9X} \cdot T_A + b_{10X} \cdot v_R \quad (3)$$

where:

C, Mn, Si, Cr, Ni, Mo, V, Cu – mass fractions of the alloying elements;

T_A – austenitising temperature, °C;

v_R – cooling rate, °C/min;

b_{0X}, b_{1X}.., b_{12} – coefficients calculated with the logistic regression analysis;

X=F (ferrite), P (pearlite), B (bainite), M (martensite).

Occurrence of transformations have been predicted based on the value of the variable Px. The transformation occurs if the calculated Px value is higher or equal to 0.5.

3. Calculation result

Evaluation of the worked out empirical formulae has been made on the basis of the analysis of the mean absolute error value, the standard deviation of the error, 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. The formulae describing the influence of the chemical composition on the temperature of the beginning of transformations in the function of the cooling rate, worked out using the multiple regression, are presented in equations (4)-(7). The assessment of the significance of the regression coefficients are presented in Tables 3-6. 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 particular transformations temperatures are given in Table 8.

$$Fs = 857 - 257 \cdot C - 69 \cdot Mn + 23 \cdot Si - 20 \cdot Cr - 38 \cdot Ni - 20 \cdot Mo + 34 \cdot V + 26 \cdot Cu + 0.07 \cdot T_A - 17 \cdot v_R^{0.25} \quad (4)$$

$$Ps = 780 - 30 \cdot C - 65 \cdot Mn + 24 \cdot Si - 29 \cdot Ni - 26 \cdot Mo - 21 \cdot Cu - 17 \cdot v_R^{0.25} \quad (5)$$

$$Bs = 675 - 212 \cdot C - 57 \cdot Mn - 17 \cdot Si - 49 \cdot Cr - 29 \cdot Ni - 60 \cdot Mo - 94 \cdot V + 0.056 \cdot T_A - 1.6 \cdot v_R^{0.25} \quad (6)$$

$$Ms = 411 - 328 \cdot C - 13 \cdot Mn - 3 \cdot Cr - 9 \cdot Ni - 16 \cdot Mo + 34 \cdot Cu + 6.7 \cdot v_R^{0.25} \quad (7)$$

Classifiers used for forecasting occurrences of the particular structural constituents in steel are presented in equations

(8)-(13). The values of the coefficient of the correct classifications for the particular transformations temperatures are presented in Table 8.

TABLE 3
The assessment of significance of regression coefficients for the ferritic transformation temperature

	Coefficients	Standard Error	t Stat	p-value
Intercept	857.1805	12.69909	67.49935	0
C	-257.512	6.062584	-42.4757	2.4E-274
Mn	-68.5837	2.196809	-31.2197	1.2E-171
Si	22.78437	2.158293	10.55666	2.52E-25
Cr	-19.8011	1.35543	-14.6087	8.79E-46
Ni	-37.8265	0.820115	-46.1234	4.3E-308
Mo	-20.271	3.790368	-5.34803	1E-07
V	33.7432	11.15142	3.02591	0.002514
Cu	26.47218	7.864241	3.366146	0.000778
T_A	0.074651	0.01348	5.537811	3.51E-08
$V_R^{0.25}$	-17.1635	0.352848	-48.6426	0

TABLE 4
The assessment of significance of regression coefficients for the pearlitic transformation temperature

	Coefficients	Standard Error	t Stat	p-value
Intercept	779.7969	3.675802	212.1433	0
C	-29.7173	5.402673	-5.50049	4.47E-08
Mn	-65.1811	2.214819	-29.4295	1.1E-149
Si	23.78078	1.954424	12.16766	1.66E-32
Ni	-29.2803	0.936806	-31.2554	2E-164
Mo	-25.9124	4.296364	-6.03124	2.06E-09
Cu	-21.1773	8.495378	-2.4928	0.012785
$V_R^{0.25}$	-17.4238	0.48057	-36.2566	1.7E-205

The logistic regression appeared to be a very useless method for calculating the range of cooling rate for bainitic transformations. The accepted for the assessment of the worked out formulae coefficient of correct classification indicated the considerable difference between the calculated and empirical values (Table 8). The neural networks, applied for the calculation of these range, ensure greater correctness of these calculations. The details were presented in papers [18].

$$P_F = \exp(K_F)/\{1 + \exp(K_F)\} \quad (8)$$

$$K_F = 20 - 17 \cdot C - 2.1 \cdot Mn + 1.03 \cdot Si - 2.4 \cdot Cr - 1.6 \cdot Ni - 5.6 \cdot Mo + 1.6 \cdot V + 4.2 \cdot Cu - 0.005 \cdot T_A - 1.17 \cdot v_R^{0.25} \quad (9)$$

$$P_P = \exp(K_P)/\{1 + \exp(K_P)\} \quad (10)$$

$$K_P = 14 - 1.93 \cdot C - 2.7 \cdot Mn + 0.3 \cdot Si - 2.2 \cdot Cr - 1.5 \cdot Ni - 7.2 \cdot Mo + 2.7 \cdot V + 1.1 \cdot Cu - 0.004 \cdot T_A - 1.33 \cdot v_R^{0.25} \quad (11)$$

$$P_M = \exp(K_M)/\{1 + \exp(K_M)\} \quad (12)$$

$$K_M = -17 + 3.9 \cdot C + 2.2 \cdot Mn + 0.4 \cdot Si + 2.4 \cdot Cr + 1.2 \cdot Ni + 0.9 \cdot Mo - 0.04 \cdot V + 3 \cdot Cu + 0.009 \cdot TA + v_R^{0.25} \quad (13)$$

TABLE 5
The assessment of significance of regression coefficients for the bainitic transformation temperature

	Coefficients	Standard Error	t Stat	p-value
Intercept	675.0608	16.49892	40.91547	1.1E-263
C	-212.146	7.945826	-26.6991	8E-134
Mn	-56.827	3.486541	-16.299	4.86E-56
Si	-17.1918	3.611832	-4.75987	2.08E-06
Cr	-48.7544	1.929019	-25.2742	6.6E-122
Ni	-28.8722	1.139604	-25.3353	2.1E-122
Mo	-60.5141	4.727671	-12.8	4.67E-36
V	-93.9168	14.52657	-6.46518	1.28E-10
T_A	0.056393	0.016837	3.349301	0.000826
$V_R^{0.25}$	-1.65855	0.409525	-4.04993	5.33E-05

TABLE 6
The assessment of significance of regression coefficients for the martensitic transformation temperature

	Coefficients	Standard Error	t Stat	p-value
Intercept	410.6985	4.495101	91.3658	0
C	-327.886	5.241376	-62.5572	0
Mn	-12.7126	2.549301	-4.9867	6.78E-07
Cr	-2.51486	1.414075	-1.77845	0.075511
Ni	-8.56036	0.716145	-11.9534	1.15E-31
Mo	-16.3256	3.179085	-5.13533	3.14E-07
Cu	34.45196	8.215225	4.193673	2.89E-05
$V_R^{0.25}$	6.692919	0.223038	30.00796	8.9E-159

TABLE 7
Error values and correlation coefficients for the temperatures of the beginning of transformations

Temperature	Error E_j, °C	Standard deviation of the error, °C	Ratio of standard deviations	Pearson's correlation coefficient
F_s	19.5	17.4	0.33	0.86
P_s	19.4	16.3	0.38	0.80
B_s	30.6	23.0	0.41	0.72
M_s	20.5	17.2	0.30	0.88

The comparative plots for the experimental and calculated temperature values of the particular transformations are presented in Fig. 1. To verify the model worked out, the experimental CCT diagrams were compared with curves calculated using equations (4)-(13). Examples of the calculated values of

the transformations' temperature along with the experimental CCT diagrams are presented in Figs. 2-3.

TABLE 8
Quality assessment coefficients for models, used as classifiers for determining the types of occurring transformations for assumed cooling rate

Transformation areas	Coefficient of correct classifications, %
Ferritic	87
Pearlitic	87
Bainitic	60
Martensitic	84

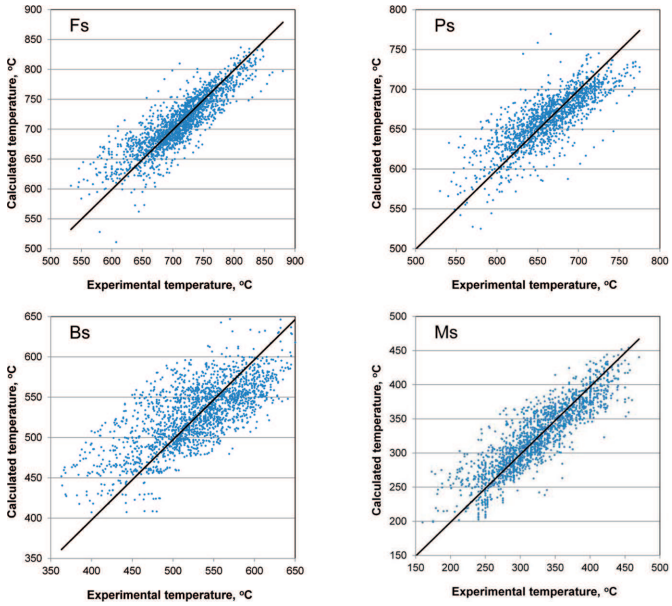

Fig. 1. Comparison of the experimental temperatures with values calculated using the regression model

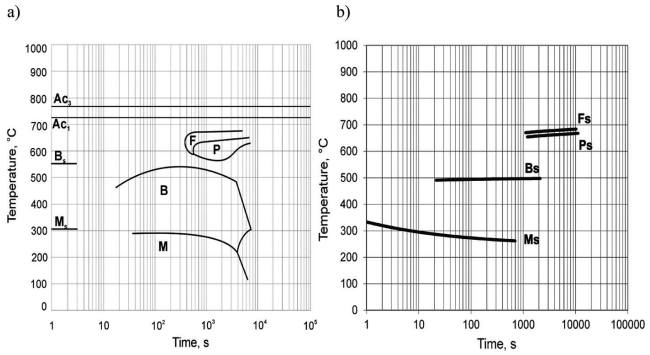

Fig. 2. CCT diagram for steel with concentrations: 0.43% C, 0.66% Mn, 0.33% Si, 0.74%Cr, 1.4% Ni, 0.2% Mo, austenitised at temperature of 860°C: a) experimental, b) calculated

4. Summary

The model worked out makes it possible to calculate austenite supercooled transformation start temperatures for the steel with a known chemical composition. The applied numerical verification of the worked out formulae allows to state that in the range of the assumed mass concentrations of the alloy elements, the proposed method makes also possible to make some parts of CCT diagrams for the newly worked out types of steel grades. The presented model facilitates the analysis of the interaction of the chemical composition on the start transformations temperature of the steel cooled from the austenitising temperature. The austenite grain size and the time of austenitising, 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.

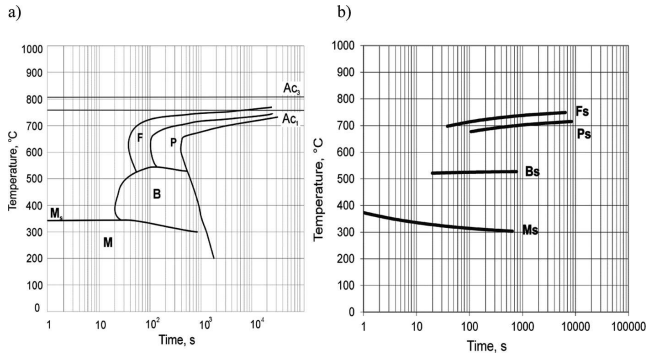

Fig. 3. CCT diagram for steel with concentrations: 0.36% C, 0.49% Mn, 0.25% Si, 1.54%Cr, 0.21% Ni, 0.03% Mo, 0.16% Cu, austenitised at temperature of 860°C: a) experimental, b) calculated

A model describing supercooled austenite star transformations in the function of alloying elements of steel enables to solve an inverse task consisting of calculating the chemical compositions of steel with the required form of a CCT diagrams.

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