APPLICATION OF THE CONTROL THEORY FOR MODELLING AUSTENITE-FERRITE PHASE TRANSFORMATION IN STEELS

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Abstract

Problem of the phase transformation kinetics is investigated in the paper. Experimental observations and results of modelling showed that, when temperature changes are imposed, then the response of the material represented by the kinetics of changes of volume fraction of the new phase, is similar to the response of the second order inertia term in electrical systems. Therefore, possibility of application of the control theory to simulations of austenite-ferrite phase transformation in steels was the main objective of the paper. Equilibrium state was determined as a function of the temperature using ThermoCalc software. Description of the kinetics of phase transformation in transient states by the second order differential equation was proposed. Time constants in this equation were introduced as functions of the temperature. Identification of the model parameters was performed using inverse analysis of the results of dilatometric tests. Model based on the control theory was applied to describe changes of the new phase volume fraction as response to the changes of the temperature. Performed numerical tests confirmed good predictive capabilities of the model.

Key words: Control theory, phase transformation model, identification

1. INTRODUCTION

As far as phase transformations are considered, a number of papers dealing with modelling of these phenomena in steels can be found in the scientific literature. The objective of the present paper is searching for a simple model with reasonable accuracy, which can be applied in optimization of metallurgical processes involving varying temperatures. Johnson-Mehl-Avrami-Kolmogorov equation (Kolmogorov, 1937; Johnson & Mehl, 1939; Avrami, 1939) is commonly used in calculations of kinetics of phase transformations. However, this equation was derived for isothermal conditions and it is the main disadvantage of JMAK model. To enable calculations for varying temperatures JMAK equation is combined with the Scheil (1935) additivity rule, but an accuracy of this approach is limited. Therefore, development of the model, which would allow avoiding application of the additivity rule, was the main objective of the paper. The basis of the control theory was applied to reach this objective.

2. CLASSIFICATION OF PHASE TRANSFORMATION MODELS

The Johnson-Mehl-Avrami-Kolmogorov equation (Kolmogorov, 1937, Johnson & Mehl, 1939; Avrami, 1939) and its numerous modifications (eg. Donnay et al., 1996) have been used to predict kinetics of phase transformations for more than half of the decade. New models with specific features were developed, such as Suehiro et al. (1992) model based on differential equation, phase field models (Simmons et al., 2000; Mecozzi et al., 2008; Militzer, 2011) or Cellular Automata models (Lanet et al., 2004; Halder et al., 2014). Two aspects decide about accuracy, reliability and effectiveness of the phase transformation modelling. These is a selection

of a relevant model for a particular application and correct identification of this model. The former aspect is considered in the present work.

A classification of phase transformation models with respect to predictive capabilities and computing costs is presented in figure 1 (Szeliga, 2012). The first group (bottom left corner in figure 1) contains models commonly used for fast simulations of industrial processes and they are generally limited to the description of the kinetics of transformations and volume fractions of phases. Additivity rule (Scheil, 1935) has to be applied in these models to account for the temperature changes during transformations. In the second group (the centre in figure 1) there are differential equations or phase field technique models, usually applied to technology design and optimization of processes. These models accurately describe transformations in varying temperatures. The third group (further right in figure 1) includes models based on the FE solution of the diffusion equation with moving boundary (Pernach & Pietrzyk, 2008). Beyond the mentioned earlier parameters, these models are capable to predict distribution of carbon concentration in austenite and resulting hardness of bainite and martensite. Difficulties with identification of coefficients in these models are their weak point.
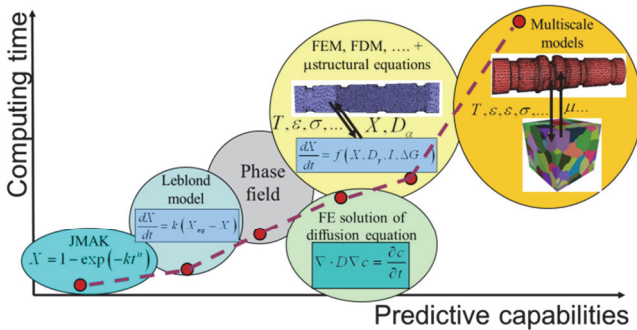

Fig 1. *Classification of selected phase transformation models: computing costs versus predictive capabilities.*

Significant extension of the predictive capabilities is obtained when mentioned earlier models are implemented into the finite difference or finite element codes, which simulate industrial thermomechanical processes (Pietrzyk & Kuziak, 1999). This coupling allows to predict distribution of calculated parameters in the material volume but it involves increase of the computing costs. Finally, the most advanced models (the top right corner in figure 1) connect FE codes with discrete models such as Cellular Automata (CA), Molecular Dynamics (MD) or Monte Carlo (MC). Combining of FE code and CA

model, called CAFE approach, seems to be the most frequently used (eg. Pietrzyk et al., 2010). New quality of information concerning microstructural features during phase transformations is obtained from these models but the increase of the computing costs is significant.

Performed analysis of the phase transformation models and published data (Bhadeshia, 2001) led to the conclusion that various modifications of the JMAK equation are reasonably accurate and efficient enough to be applied in the optimization tasks, when volume fractions of phases are the only optimization parameters. The objective of this paper was searching for a model, which will be as efficient as JMAK equation and will be more flexible to enable realistic description of phase transformation at the varying temperature. The idea of such model was proposed by Leblond and Devaux (1984), who introduced the following evolution equation for phase transformation:

$$\frac{dX}{dt} = \frac{F_{fT} - XF_{f\max}}{\tau(T)} \tag{1}$$

where: X – volume fraction of ferrite with respect to the maximum volume fraction of this phase in steel, F_{fT} - the equilibrium volume fraction of the ferrite at the temperature T, $F_{f\max}$ - the maximum volume fraction of ferrite in steel, τ - the characteristic time of the transformation at constant temperature T.

The proposition of Leblond and Devaux (1984) was extended in this paper by introduction of the second order differential equation. This model was applied to the ferritic transformation only. Pearlitic and bainitic transformation was simulated by the JMAK model and martensitic transformation was simulated by the model proposed by Koistinen and Marburger (1959).

3. MODEL

In the proposed model the equilibrium response (volume fraction) as a function of the temperature was determined using ThermoCalc software. The idea of the model is application of the differential equation, which describes transient state between the two equilibrium states. Introduction of two time constants (second order inertia term) was the main difference comparing to the Leblond and Devaux (1984) model. Following this idea the control theory was used in the present paper to calculate response of the material at varying temperatures.

3.1. Equilibrium

As it has been mentioned, the equilibrium states has been determined using ThermoCalc software. The model is general and can be applied to any carbon steel but main results presented in this paper were obtained for the DP600 steel with the chemical composition given in the first row (A) of table 1. A part of the phase equilibrium diagram for this steel is shown in figure 2. Carbon content at the γ-α boundary ($c_{\gamma\alpha}$) and at the γ-cementite boundary ($c_{\gamma\beta}$) was approximated by the following linear relationships:

$$c_{\gamma\alpha} = c_{\gamma\alpha0} + c_{\gamma\alpha1}T \qquad (2)$$

$$c_{\gamma\beta} = c_{\gamma\beta0} + c_{\gamma\beta1}T \qquad (3)$$

where: T – temperature in °C.

Coefficients in equations (2) and (3), which were determined for the steel A using ThermoCalc software, are given in Table 2. Beyond this, equation describing carbon content in the ferrite (c_α) is also given in this table.

Fig. 2. *Part of the phase equilibrium diagram for the investigated DP steel A.*

Table 1. *Chemical composition of the investigated steels, wt %.*

steel	C	Mn	Si	Cr	Mo	Cu	Al	V	Nb	Ti	N
A	0.071	1.45	0.25	0.55	0.03	0.02	0.022	0.005	0.005	0.002	0.0039
B	0.11	1.45	0.19	0.27	0.03	0.01	0.034	0.005	0.004	0.013	0.0038
C	0.095	1.51	0.23	0.41	0.05	0.02	0.037	0.045	0.005	0.006	0.0039
D	0.08	1.74	0.12	0.23	0.43	-	0.025	-	-	-	0.009

Table 2. *Parameters in equations (2) and (3) describing equilibrium carbon concentrations.*

$c_{\gamma\alpha0}$	$c_{\gamma\alpha1}$	$c_{\gamma\beta0}$	$c_{\gamma\beta1}$
4.8513	-0.005776	-1.46583	0.002887

$c_\alpha = -0.069 + 0.000435T - 9.1658\times10^{-7}T^2 + 6.487\times10^{-10}T^3$	for $T < 637°$ C
$c_\alpha = -0.0487268 + 0.00017839T - 1.50788\times10^{-7}T^2$	for $T > 637°$ C

To evaluate predictive capabilities and performance of the model for different chemical compositions identification of coefficients and validation was also performed for three more DP600 steels. Chemical compositions of these steels are given in rows B, C and D in Table 1.

3.2. Model based on the control theory

Kinetics of ferritic transformation is characterised by three stages. The first stage is some delay due to time needed for nucleation of the new phase grains. The second stage is the maximum rate of the transformation due to growth of a new phase. The third stage is slowing down due to an impingement of the new phase grains. Typical responses 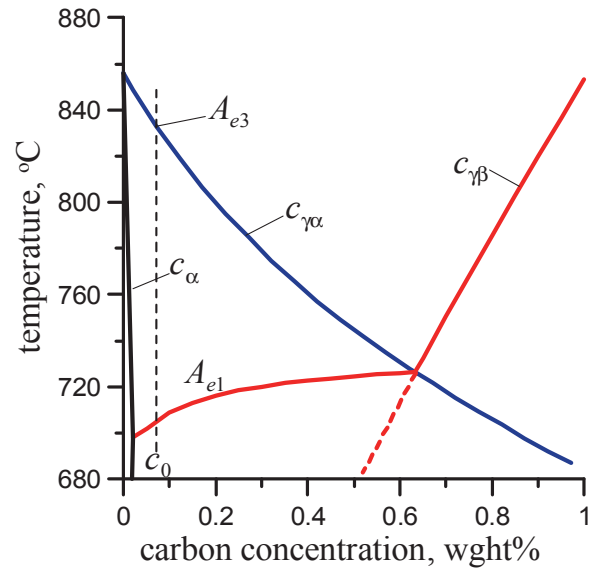of the material during isothermal phase transformations are shown in figure 3. Volume fraction X in this figure is calculated with respect to the maximum volume fraction F in the steel defined as:

$$F_{f\max} = 1 - \frac{(c - c_\alpha)}{(c_{eut} - c_\alpha)} \qquad (4)$$

where: c – carbon content in steel, c_α – carbon content in ferrite, c_{eut} – carbon content at eutectic, which is calculated as crossing point between lines $c_{\gamma\alpha}$ and $c_{\gamma\beta}$ in figure 2.

In all equations below X represents volume fraction of the ferrite with respect to the maximum volume fraction of this phase in steel ($F_{f\max}$) and F represents volume fraction of the ferrite with respect to the whole volume of the material.

Solid line in figure 3 shows the plot when the temperature drops from A_{c3} to A_{c1} (step function) and isothermal transformation takes place at A_{c1}. Dotted

line in figure 3 shows the plot when the temperature drops from A_{c3} to certain temperature T (from the range $A_{c1} < T_1 < A_{c3}$) and isothermal transformation takes place at T_1. In the latter case the volume fraction of ferrite X reaches equilibrium volume fraction calculated as F_{fT}/F_{fmax}, where:

$$F_{fT} = \frac{c_{\gamma\alpha} - c_0}{c_{\gamma\alpha} - c_\alpha} \quad (5)$$

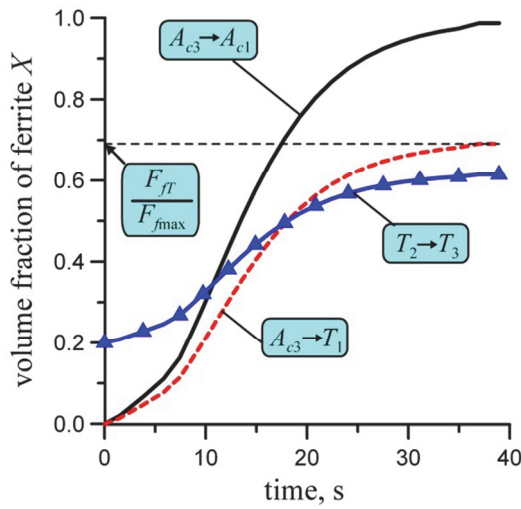is the equilibrium volume fraction of the ferrite at the temperature T_1.

Fig. 3. *Typical responses of the material during isothermal phase transformations.*

When transformed volume fraction at the temperature A_{c1} (solid line in figure 3) achieves 1 it means that the volume fraction of ferrite in the steel reaches F_{fmax}. Step change of the temperature from T_2 to T_3 causes change of the ferrite volume fraction from one equilibrium state $X(T_2)$ to a new equilibrium state $X(T_3)$ and the kinetics of this change is represented by the curve with triangular symbols in figure 3.

Analysis of the plots in figure 3 allows to assume that kinetics of the phase transformation is similar to the response of the second order electrical two-pair terminal network in the control theory. Applicability of this theory to modelling of materials processing, accounting for the microstructure evolution, was confirmed by Svyetlichnyy (2004). This approach was also applied by Pietrzyk and Kuc (2010) to modelling of twinning using internal variable method. Electrical second order two-pair terminal network, which was proposed as representation of the material during phase transformation, is shown in figure 4, where: R – resistance, C – capaci-

ty and L – inductance. Equations, which describe this element, are:

$$U_2 = U_1 - L\frac{di}{dt} - iR \qquad i = \frac{1}{C}\frac{dU_2}{dt} \quad (6)$$
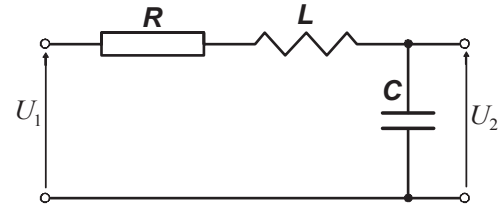
where: i – electrical current.

Fig. 4. *Second order electrical two-pair terminal network.*

After rearrangement of equation (6), the following differential equation was obtained:

$$LC\frac{d^2U_2}{dt^2} + RC\frac{dU_2}{dt} + U_2 = U_1 \quad (7)$$

Thus, Laplace transmittance of this element is:

$$G(s) = \frac{k}{B_1^2 s^2 + B_2 s + 1} \quad (8)$$

where: s – Laplace operator, k – amplifying coefficient, B_1, B_2 – time constants defined as:

$$B_1 = RC \qquad B_2 = \sqrt{LC} \quad (9)$$

In the case of phase transformations the input signal is the temperature drop below A_{e3} ($U_1 \rightarrow \Delta T$) and the output signal is the volume fraction of ferrite ($U_2 \rightarrow X$). In consequence equation (7) has the form:

$$B_1^2 \frac{d^2 X}{dt^2} + B_2 \frac{dX}{dt} + X = f(T) \quad (10)$$

where: B_1, B_2 – time constants.

Right hand side of equation (10) is a function of temperature. This function has to be equal to the equilibrium volume fraction of ferrite at the considered temperature:

$$f(T) = \frac{F_{fT}}{F_{f\max}} \quad (11)$$

where: F_{fT} – equilibrium content of ferrite in steel at the considered temperature defined by (5), $F_{f\max}$ – maximum volume fraction of ferrite in steel defined by equation (4).

3.3. Finite difference solution

Finite difference scheme for equation (10) is given in Table 3. In this table t_{i-1}, t_i and t_{i+1} stand for three subsequent points on the time scale. When response of the material to the step function ΔT is considered, time constant B_1 is responsible for the initial delay of this response. Therefore, this time constant was correlated with the rate of nucleation. Since nucleation rate is directly connected with the undercooling below A_{c3}, the following definition was assumed in the first approach:

$$B_1 = a_4 \exp\left[-a_5\left(A_{e3} - T\right)\right] \qquad (12)$$

where: a_4, a_5 – coefficients.

***Table 3.** Finite difference scheme for equation (10).*

Term	t_{i-1}	t_i	t_{i+1}
$\dfrac{\partial^2 X}{\partial t^2}$	$\dfrac{B_1^2}{h_1^2}$	$\dfrac{-B_1^2\left(h_1 + h_2\right)}{h_1^2 h_2}$	$\dfrac{B_1^2}{h_1 h_2}$
$\dfrac{\partial X}{\partial t}$	$\dfrac{-B_2}{h_1 + h_2}$	0	$\dfrac{B_2}{h_1 + h_2}$
X	0	1	0
scheme	$\dfrac{B_1^2}{h_1^2} - \dfrac{B_2}{h_1 + h_2}$	$1 - \dfrac{B_1^2\left(h_1 + h_2\right)}{h_1^2 h_2}$	$\dfrac{B_1^2}{h_1 h_2} + \dfrac{B_2}{h_1 + h_2}$

Time constant B_2 is responsible for the growth of the ferrite phase. Therefore, this time constant was correlated with the diffusion coefficient and mobility of the interface. It led to the assumption that time constant B_2 is inversely proportional to the modified Gauss function with the nose located at the temperature of the maximum rate of the transformation (a_7 in the model). In consequence the following relation was proposed in the first approach:

$$B_2 = \left\{ a_6 \exp\left[-\left(\frac{a_7 - T}{a_8} \right)^2 \right] \right\}^{-1} \qquad (13)$$

where: a_6, a_7, a_8 - coefficients.

The differential scheme for equation (10) is now:

$$\left(\frac{B_1^2}{h_1^2} - \frac{B_2}{h_1 + h_2} \right) X_{i-1} + \left[1 - \frac{B_1^2\left(h_1 + h_2\right)}{h_1^2 h_2} \right] X_i +$$

$$\left(\frac{B_1^2}{h_1 h_2} + \frac{B_2}{h_1 + h_2} \right) X_{i+1} = \frac{F_{fT}}{F_{f\max}} \qquad (14)$$

where: $h_1 = t_i - t_{i-1}$, $h_2 = t_{i+1} - t_i$ - time steps.

Modelling of phase transformations starts with equation (14) when the temperature drops below A_{e3}. The transformed ferrite volume fraction X is calculated with respect to the maximum volume fraction of this phase in steel $F_{f\max}$. The maximum value of X, which can be obtained, changes when temperature T is changing according to the line $c_{\gamma\alpha}$ in figure 2. This maximum value of X is equal to the right hand side of equation (14). Thus, the current volume fraction of ferrite with respect to the whole volume of the material is $F = X F_{f\max}$.

4. INVERSE ANALYSIS

Identification of coefficients in the proposed model is crucial for its accuracy and reliability. In the present work inverse analysis for the results of dilatometric tests was used to identify coefficients $a_4 - a_8$.

4.1. Basic idea of application of the inverse analysis to phase transformation models

The inverse algorithm dedicated to identification of material models consists of three steps (Szeliga et al, 2006):
- Performing physical experiments and collecting the obtained data.
- Performing simulations of the experiments at selected physical conditions and elaborating the collected data.
- Running optimization procedure to minimize the difference between measured and calculated data with respect to the parameters of the material model.

This algorithm was developed for identification of rheological models of materials (Szeliga et al, 2006) and was applied by Pietrzyk and Kuziak (2012) to identification of ferritic, pearlitic, bainitic and martensitic phase transformation models. In the latter approach the experiment was dilatometric tests performed at various cooling rates. The modified JMAK model described in (Donnay et al, 1996) applied to transformations was identified in (Pietrzyk & Kuziak, 2012) and the same procedure was used in the present work for identification of the coefficients $a_4 - a_8$. Any phase transformation model can be written as the set of equations of the following form:

$$\mathbf{y} = f(\mathbf{x}) \qquad (15)$$

where: **y** – vector of model outputs, **x** = {**p,a**} – vector of model inputs **p** (e.g. cooling rate) and parameters of the model **a**.

The problem of parameters **a** identification, if model outputs **y** and inputs **p** are known, is called an inverse one:

$$\mathbf{a} = f^{-1}(\mathbf{y}, \mathbf{p}) \qquad (16)$$

Inverse function f^1 can be found analytically for some linear problems only. Phase transformations model is nonlinear, therefore, the problem of parameters **x** identification is transformed to the optimization task:

$$\Phi(\mathbf{x}) = \left\| \mathbf{y}^c(\mathbf{x}) - \mathbf{y}^m \right\|^2 \qquad (17)$$

where: $\mathbf{y}^c(\mathbf{x})$ – the model output vector, $\mathbf{y}^m$ – measured vector.

It can be proved (Kirsch, 1996) that minimum of the goal function (17) is the solution of the inverse problem (16). Identification of the phase transformation model parameters $\mathbf{a} = \{a_4, \ldots, a_8\}$ was performed with the goal function defined as (17), which in the particular case of phase transformations is of the form:

$$\Phi(\mathbf{a}, \mathbf{p}) = \sqrt{\frac{1}{Ncr} \sum_{i=1}^{Nt} \left\{ \left[\frac{T_{ij}^c(\mathbf{a}, \mathbf{p}) - T_{ij}^m}{T_{ij}^m} \right]^2 + \left[\frac{F_i^c(\mathbf{a}, \mathbf{p}) - F_i^m}{F_i^m} \right]^2 \right\}} \qquad (18)$$

where: a – vector of the coefficients in equations (12) and (13), T^m, T^c – measured and calculated start temperatures for transformation, F^m, F^c – measured and calculated volume fractions of ferrite, Ncr – number of cooling rates.

4.2. Identification of the phase transformation model based on the control theory

Data for training the model were obtained from the dilatometric tests for the DP steels with the chemical compositions presented in Table 1. The model coefficients were determined by solving the inverse problem and using the experimental data obtained in the tests and they are given in Table 4. The full description of the phase transformation models and the relevant coefficients are given in publications (Kuziak et al., 2014) for steel A. Comparison of the CCT diagram obtained from the experiment and calculated using the model with the coefficients shown in Table 4 and in (Kuziak et al., 2014) is presented in figure 5.

Table 4. Coefficients on the phase transformation model obtained from the inverse analysis of the dilatometric tests

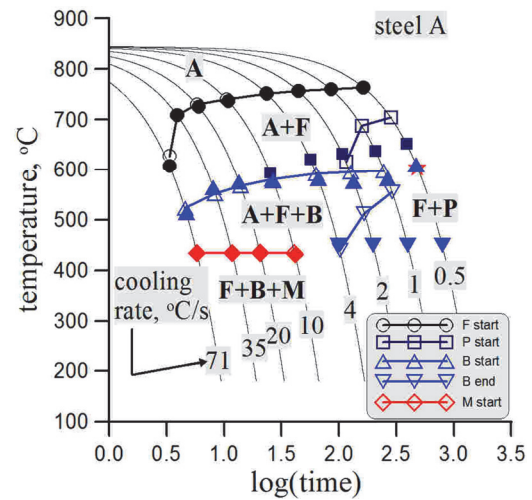| Steel	a_4	a_5	a_6	a_7	a_8
A	370.5	0.0557	0.209	736.7	15.02
B	493.3	0.0418	0.4089	701.9	30.7
C	203.2	0.084	0.572	759.8	16.38
D	342.7	0.068	0.195	663.6	44.45

Fig. 5. Comparison of the CCT diagram obtained from the experiment and calculated using the model with the coefficients shown in Table 4 for ferritic transformation and in (Kuziak et al., 2014) for remaining transformations.

5. RESULTS

Further validation of the model was performed by comparison of the measured start temperature for the ferritic transformation and the calculated one for four steels using developed model with coefficients presented in Table 4. The results of these calculations are shown in figure 6. It is seen in this figure that the model predicts ferrite start temperature with very good accuracy.

Numerical tests of the developed model were performed for the continuous annealing process. Data for the tests were taken from the paper (Pietrzyk et al., 2014), where various thermal cycles for the annealing were investigated. Two cycles from that paper were selected, number 3 and number 5. These cycles are shown in figure 7. In the cycle no. 3 heating was to the intercritical temperature between A_{c1} and A_{c3} for all investigated steels. In the second cycle no. 5 full austenitization was obtained for these steels after the heating stage.
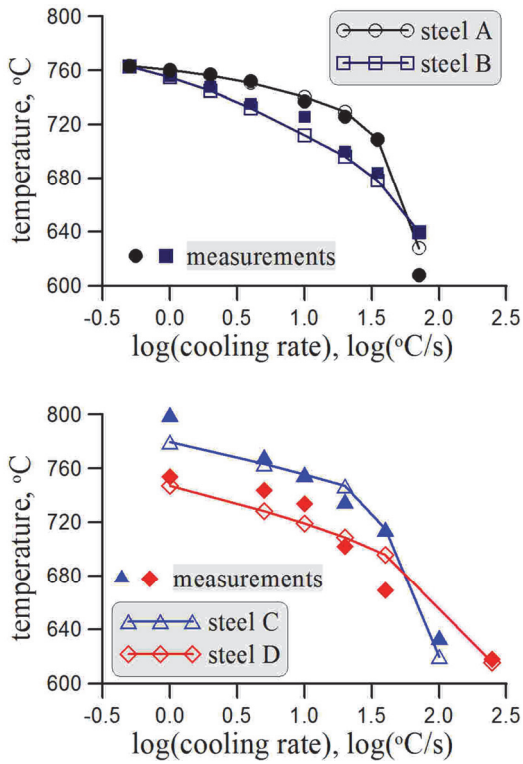
Fig. 6. Comparison of the start temperature for the ferritic transformation obtained from the experiment and calculated using the model with the coefficients presented in Table 4.
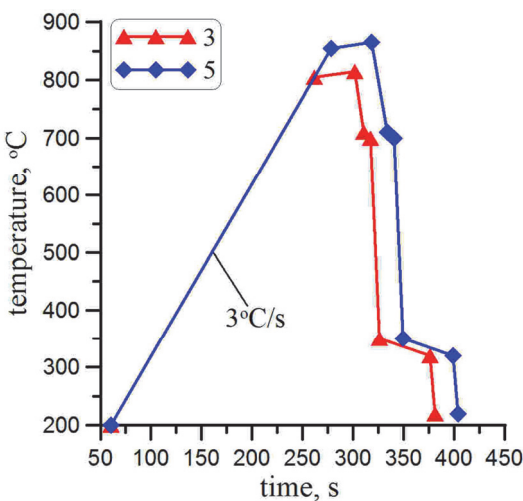

Fig. 7. Continuous annealing thermal cycles selected for the analysis – numbers refer to the paper (Pietrzyk et al., 2014).

Simulations of the two annealing cycles was performed for all steels in Table 1. Physical simulations were performed in (Pietrzyk et al., 2014) for the steel B only. Results obtained for different steels were compared between each other and the result for the steel B was compared with the experiment, see figures 8 and 9. Changes of the volume fraction of ferrite during the annealing process are shown in figure 8. It is seen in this figure that differences in the response of various steels are noticeable. They

are due to differences in the chemical composition and differences in the phase composition at the beginning of the annealing process.
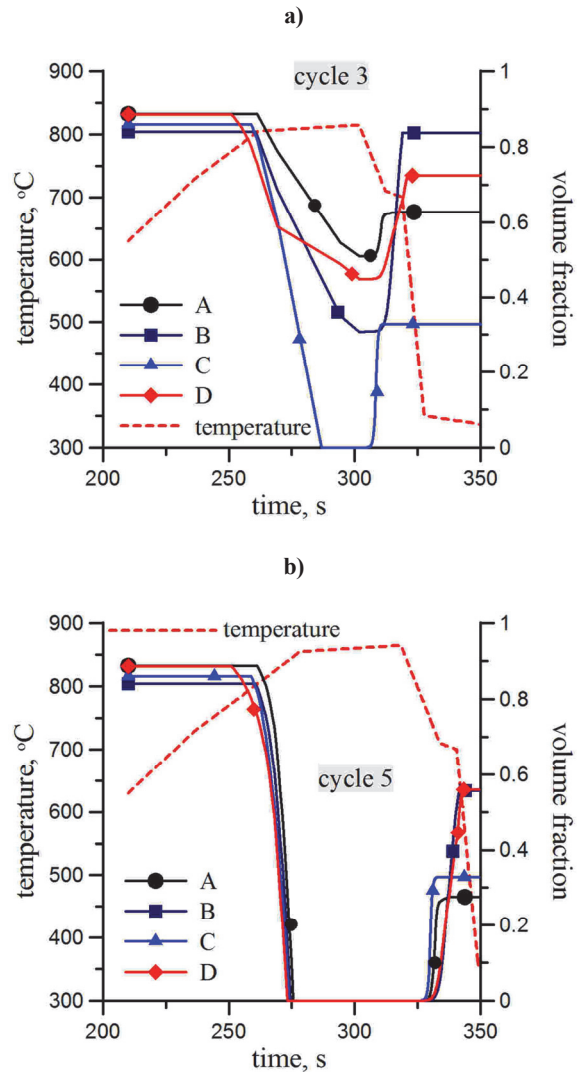

Fig. 8. Changes of the volume fraction of ferrite during the annealing process with the thermal cycles 3 (a) and 5 (b).
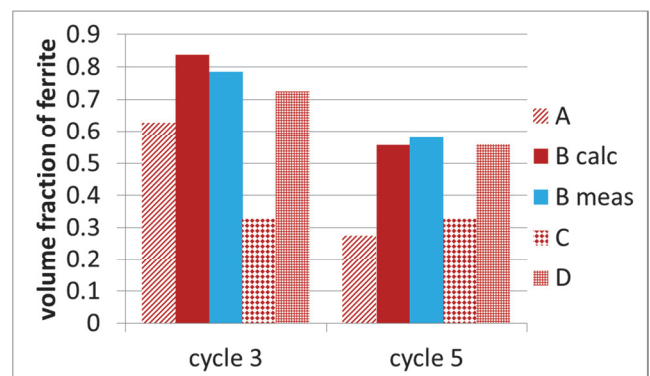

Fig. 9. Volume fraction of ferrite in the investigated steels after annealing cycles 3 and 5.

Volume fractions of ferrite in the investigated steels after annealing cycles 3 and 5 are shown in figure 9. Results for the steel B were compared with

the experimental data published in (Pietrzyk et al., 2014) and good agreement was obtained. Comparison between various steels showed again that behaviour of these steels is different.

6. CONCLUSIONS

Phase transformation model based on the control theory was developed and presented in the paper. Numerical tests of the model were performed and the following conclusions were drawn:

− Identification based on the dilatometric tests yielded coefficients in the model, which gave reasonable sensitivity of predictions to the steel chemical content and very good accuracy of calculations. Good predictive accuracy of the developed model was confirmed

− Various functions describing time constants as functions of the temperature were tested and those reproducing mechanisms of nucleation and growth were proposed.

− Simulations of the continuous annealing process confirmed good predictive capabilities of the model. Differential form of the main equation of the model makes this model particularly effective in simulations of processes characterized by varying temperatures.

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ZASTOSOWANIE TEORII STEROWANIA DO MODELOWANIA PRZEMIANY AUSTENIT-FERRYT W STALI

Streszczenie

Tematem artykułu jest modelowanie kinetyki przemian fazowych. Z obserwacji doświadczalnych wynika, że charakter odpowiedzi materiału na zmiany temperatury w zakresie przemian fazowych jest podobny do odpowiedzi elektrycznego elementu inercyjnego 2-go rzędu. Dlatego za cel niniejszej pracy postawiono sobie zastosowanie metod teorii sterowania do modelowania przemiany austenit-ferryt w stalach. Stan równowagi przedstawiono w funkcji temperatury wykorzystując program ThermoCalc. Zaproponowano opis kinetyki przemiany fazowej różniczkowym równaniem 2-go rzędu ze stałymi czasowymi zależnymi od temperatury. Identyfikację współczynników w modelu przeprowadzono stosując rozwiązanie odwrotne dla prób dylatometrycznych. Opracowany model zastosowano do wyznaczenia odpowiedzi materiału, czyli zmian ułamka objętości ferrytu, na zmiany temperatury. Przeprowadzone testy numeryczne dla czterech stali potwierdziły prawidłowość działania modelu.

COMPUTER METHODS IN MATERIALS SCIENCE