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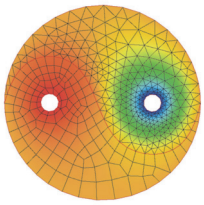

SENSITIVITY ANALYSIS AND IDENTIFICATION OF THE PHASE TRANSFORMATION MODEL BASED ON THE CONTROL THEORY

IVAN MILENIN*, KRZYSZTOF BZOWSKI, ŁUKASZ RAUCH

AGH University of Science and Technology, al. Mickiewicza 30, 30-059 Kraków, Poland
**Corresponding author: imilenin@agh.edu.pl*

Abstract

The aim of this work was to improve the previously developed model of austenite-ferrite phase transformation by its identification for selected steels and by performing sensitivity analysis. The created model allows prediction of phase transformation kinetics for non-isothermal conditions. The model is characterized by very short computing time and relatively good predictive capabilities. There are five input coefficients in the model, which should be identified for each steel on the basis of dilatometric tests. In the previous works the model was used to predict phase transformation kinetics in various DP steels for different thermal cycles. In the first part of this work sensitivity analysis of the model was performed using two methods: local sensitivity analysis and Morris method. Obtained sensitivity coefficients described how changes of the model input parameters influence the response of the model and which of these parameters are the most significant. The second part of the work was devoted to model identification for the selected steels. Identification problem was turned into optimization task which was solved using Hooke-Jeeves method. The obtained parameters of the model allowed describing austenite-ferrite phase transformation in the conditions of varying temperatures. Validation of the model was performed by comparison with the results obtained from the advanced numerical model based on the solution of the diffusion equation in the austenite. The results obtained from both models for standard thermal cycles applied to get multiphase microstructure were compared.

Key words: phase transformation model, identification, sensitivity analysis

1. INTRODUCTION

As long as phase transformation modelling is considered, a number of papers devoted to this problem can be found in literature. A variety of models are discussed by Pietrzyk et al. (2015) and classified with respect to their predictive capabilities and computing costs. The presented paper is focused on single point models, which can be efficiently implemented in the finite element (FE) programs used to simulate industrial processes. The fundamental equation proposed by Johnson and Mehl (1939), Avrami (1939) and Kolmogorov (1937), known as JMAK equation, is the leading approach in this group of models. Several upgrades of this equation have been developed during last half of the century, among which papers by Donnay et al. (1996), Farjas and Roura (2012), Pietrzyk and Kuziak (2012) and Starink (2001) could be mentioned. These modifications were in general based on introduction of the coefficient in JMAK equation as a function of the temperature. In a majority of works Aarhenius type function (Starink, 2001) or modified Gauss function (Donnay et al., 1996) were used. The problem with calculations of the kinetics of phase transformations in a varying temperature was a natural consequence of these modifications and the additivity rule (Scheil, 1935) had to be used to avoid these difficulties. Beyond this, JMAK equation gives volume fraction of the ferrite with respect to the maximum volume fraction at the given temperature. Since in

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non-isothermal processes the temperature changes, this maximum volume fraction changes as well and volume fraction calculated from the JMAL equation has to be corrected all the time at each time step of simulations (Pietrzyk & Kuziak, 2012). All these facts lead to numerical problems when JMAK equation is implemented in the FE code.

To avoid the complications ferritic phase transformation model based on the control theory was proposed in the previous paper (Milenin et al., 2015). The model makes use of the idea suggested first by Leblond and Devaux (1984). Authors propose a hypothesis that a rate of transformation is proportional to the distance from the equilibrium. Introduction of the second order differential equation by Milenin et al. (2015) was the main upgrade comparing to the original work of Leblond and Devaux (1984). The approach is based on the control theory and the material is treated as the second order inertia term. Since this new model is based on differential equation with respect to time, all problems encountered in the JMAK equations are eliminated. The main advantage of the proposed model when compared with JMAK is that it allows description of processes at varying temperatures without using additivity rules. Moreover, the solution always tends to the equilibrium state at the current temperature and no correction is needed when the temperature changes. The proposed model can substitute JMAK equation in modelling processes in varying temperature, for example in thermal treatment of steels. The aim of the present work was identification, further development and sensitivity analysis of this model. These objectives were reached by comparison with the experimental data and with the results obtained from the advanced model based on the solution of the carbon diffusion equation.

2. MODELS

Two phase transformation models were considered. The first is the model based on the control theory (Milenin et al., 2015) and this model was analysed and tested as a prospective tool for the efficient and reliable simulations of phase transformations. The second model was based on the solution of the carbon diffusion equation in the austenite (Pernach et al., 2014).

2.1. Phase transformation model based on the control theory

The idea of the previously proposed model (Milenin et al., 2015) is based on the application of the second order differential equation to describe phase transformation kinetics. Kinetics of ferritic transformation is characterized by three stages. The first stage is characterized by a delay due to time necessary for nucleation of the new phase grains. The second stage is characterized by the maximum rate of the transformation due to growth of a new phase. In the third stage The process is slowing down due to an impingement of the new phase grains. The main equation of the model is:

$$B_1^2 \frac{d^2 X_f}{dt^2} + B_2 \frac{dX_f}{dt} + X_f = \mathrm{f}(T) \qquad (1)$$

where: X_f – current ferrite volume fraction with respect to the maximum volume fraction of ferrite in steel ($F_{f\max}$), t – time, B_1 and B_2 - time constants, T – temperature in ^{o}C, f(T) – equilibrium ferrite volume fraction at the temperature T.

Function f(T) is defined as a ratio between equilibrium ferrite volume fraction (F_{f_eq}) at the temperature T and maximum ferrite volume fraction in the investigated steel ($F_{f\max}$):

$$\mathrm{f}(T) = X_{\max}(T) = \frac{F_f}{F_{f\max}} \qquad (2)$$

The equilibrium states for the model were determined using ThermoCalc software. Relation of the carbon content at the γ-α boundary ($c_{\gamma\alpha}$) and at the γ-cementite boundary ($c_{\gamma\beta}$) on the temperature was approximated by the following linear relationships:

$$\begin{aligned} c_{\gamma\alpha} &= c_{\gamma\alpha 0} + c_{\gamma\alpha 1} T \\ c_{\gamma\beta} &= c_{\gamma\beta 0} + c_{\gamma\beta 1} T \end{aligned} \qquad (3)$$

where: T – temperature in ^{o}C

In equation (2) the equilibrium ferrite fraction with respect to the whole volume of the material for the current temperature T is defined by the following equation:

$$F_{f\_\mathrm{eq}} = \frac{c_{\gamma\alpha - C_0}}{c_{\gamma\alpha - C_\alpha}} \qquad (4)$$

Then, maximum volume fraction of ferrite in steel is defined as follows:

$$F_{f\max} = 1 - \frac{(c_0 - c_\alpha)}{(c_{eut} - c_\alpha)} \tag{5}$$

where: c_0 – 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 $c_{\gamma\beta}$ on ferrite-cementite equilibrium plot.

In order to describe phenomena of nucleation and growth, the two time constants were introduced in the model and were based on the mathematical description of the second order inertia term. Time constant B_1 is responsible for the delay of the response in the initial stage of transformation, therefore, it was correlated with the nucleation rate. Since nucleation rate directly depends on undercooling below A_{c3} temperature, the following definition was assumed:

$$B_1 = x_1 \exp\left[-x_2\left(A_{e3} - T\right)\right] \tag{6}$$

where x_1, x_2 – coefficients which are fitted for the investigated material using inverse analysis algorithms.

B_2 constant is responsible for the growth of the ferrite phase, so it was correlated with mobility of the interface and diffusion coefficient. Thus it can be assumed that B_2 constant can be presented in the form of modified inverse Gauss function with a nose at the temperature of maximum transformation rate (a_4 coefficient). Finally, B_2 constant is represented by the following equation:

$$B_2 = \left\{ x_3 \exp\left[-\left(\frac{x_4 - T}{x_5} \right)^2 \right] \right\}^{-1} \tag{7}$$

where x_3, x_4, x_5 - coefficients

With the application of such an approach it is possible to model metallurgical processes in real time, unlike in case of approaches which use complicated computation methods. On the other hand, proposed model allows to model transformation in variable temperature conditions (unlike simple model such as JMAK). Current work is devoted to sensitivity analysis and identification of the model based on dilatometric tests data.

2.2. Phase transformation model based on the solution of the diffusion equation

Validation of the phase transformation model described in the previous Chapter was one of the objectives of the paper. This validation was performed in two ways. The first was comparison with the results of the more advanced model based on the solution of carbon diffusion equation in the domain representing microstructure of the austenite. The second was comparison with the experiments performed for various cooling cycles.

The austenite-ferrite transformation model based on the solution of carbon diffusion equation in the domain representing microstructure was described in detail in previous publications (Pernach & Pietrzyk, 2008; Pernach et al., 2014, Bzowski et al., 2016) Therefore, only main features of this model are given in the present work.

The phase transformation model is based on the assumption that transformation is controlled only by the rate of carbon diffusion i.e. the interface moves as fast as diffusion of carbon allows for it. Mathematical formulation is based on the solution of the Second Fick law with moving boundary conditions:

$$\frac{\partial c}{\partial t} = D(T)\nabla^2 c \qquad \text{in } \Omega_\gamma \tag{8}$$

$$\begin{aligned} c(x_{\min}, y) &= c(x_{\max}, y) \qquad \text{for } y \in (y_{\min}, y_{\max}) \\ c(x, y_{\min}) &= c(x, y_{\max}) \qquad \text{for } x \in (x_{\min}, x_{\max}) \end{aligned} \tag{9}$$

$$c(x,0) = c_0 \qquad \text{in } \Omega_\gamma \tag{10}$$

$$c(x_\xi, t) = c_{\gamma\alpha}(T) \tag{11}$$

Evolution of grain boundaries is done using Level Set Method (LSM) developed by Osher and Sethian (Osher & Sethian, 1988). A major advantage of the LSM is that merging and splitting of regions comes naturally and the grid does not have to be changed when the interface moves. In such an approach each grain has its own assigned individual level set function (multiple level set approach) initialized with the distance function. The equation of motion governing grain boundaries is then given by:

$$\frac{\partial \phi}{\partial t} + v\left|\nabla \phi\right| = 0 \tag{12}$$

Where the velocity field v is a function of carbon diffusion. Each level set function is solved on the

same grid and the coupled level set functions are corrected as:

$$\phi_i^c = \frac{1}{2}\left[\phi_i^p - \max_{i\neq j}\left(\phi_j^p\right)\right] \tag{13}$$

where ϕ_i^c is the corrector of ϕ_i^p level set function. After evolution and corrections of each interface, global level set solution $\tilde{\phi}$ are defined as a union of separated level sets, which finally determinates microstructure morphology for given time step:

$$\tilde{\phi} = \underset{x\in\Omega}{\forall} \max\left(\phi_i\right) \tag{14}$$

The model based on the solution of the diffusion equation was further used to simulate experimental thermal cycles and to validate the simple model described in section 2.1.

3. SENSITIVITY ANALYSIS

Sensitivity analysis (SA) allows to determine how model reacts to changes of various parameters (Szeliga, 2014). SA allows also to check whether model describes properly phenomena corresponding to physical laws and to find which model parameters have more influence on model response then others and which parameters are irrelevant.

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

steel	C	Mn	Si	Cr	Mo	Cu	Ni	Al	V	Nb	Ti
DP600	0.071	1.45	0.25	0.55	0.03	0.02	-	0.022	0.005	0.005	0.002
bainitic	0.23	1.52	0.98	1.51	0.14	0.01	0.07	0.023	-	-	-
AHSS	0.16	1.53	0.39	0.23	-	-	-	0.022	-	0.013	-

Analysis was performed by the two methods: local sensitivity analysis and Morris global method (Morris, 1991). The main aim of such analysis of the proposed model is to determine whether equations assumed for *B* time constants, which define physical properties in the model, can ensure proper description of the process. The whole analysis was performed for model identified in (Milenin et al., 2015) for the steel DP600 with chemical composition given in table 1. Coefficients of the model are shown in table 2.

Table 2. *Coefficients of the model for the DP600 steel determined in (Milenin et al., 2015) and for the bainitic and AHSS steels determined by the inverse analysis in the present work.*

steel	x_1	x_2	x_3	x_4	x_5
DP 600	370.5	0.0557	0.209	736.7	15.02
bainitic	486.75	0.0107	0.53	698.8	11.025
AHSS	98.33	0.0993	0.184	643.6	176

3.1. Local sensitivity analysis

Local sensitivity analysis algorithm defines sensitivity coefficients which show how influent individual parameters are on the output only in a narrow surrounding of the initial values. Let us assume that it can be described by the following equation:

$$y = y(\mathbf{x}, t) \tag{15}$$

where **x** – vector of model parameters, *t* – time. Then, the influence of parameters change at the moment of time *t* on the model output can be written in a form of Taylor series:

$$y(t, x+\Delta x) = y(t,x) + \sum_i \frac{\partial y}{\partial x_i}\Delta x_i + \frac{1}{2}\sum_i\sum_j \frac{\partial^2 y}{\partial x_i \partial x_j}\Delta x_i \Delta x_j + \ldots \tag{16}$$

Partial derivatives $\frac{\partial y}{\partial x}$ in equation (16) are introduced as first-order sensitivity coefficients, $\frac{\partial^2 y}{\partial x_i \partial x_j}$ – as second-order sensitivity coefficients etc. First-order coefficients define sensitivity matrix **S**:

$$\mathbf{S} = \left[s_{ij}\right] = \left[\frac{\partial y_j}{\partial x_i}\right] \tag{17}$$

Index *j* under *y* is introduced because the model can have more than one output

The best way to compute sensetivity matrix are analytical calculations. But in the case of complicated nonlinear problems like phase transformation modelling, the following finite difference approximation is used:

$$\frac{\partial y_j}{\partial x_i} = \frac{y_j(x_i + \Delta x_i) - y_j(x_i)}{\Delta x_i} \tag{18}$$

Elements of sensitivity matrix (17) are computed for different parameters x_i and are expressed in units connected with selected parameter x_i and output *y*, so

it is impossible to compare values of such coefficients. In order to solve this problem, coefficients should be normalized according to the equation:

$$\overline{\mathbf{S}} = \left[\overline{s_{ji}}\right] = \left[\frac{x_i}{y_j}\frac{\partial y_j}{\partial x_i}\right] \tag{19}$$

Table 3. *Sensitivity coefficients for the ferrite transformation model for the DP600 steel*

	S_1	S_2	S_3	S_4	S_5
Start	-0.31686	0.979647	0.812769	194.6614	6.564959
End	0.009422	-0.11855	0.054561	-0.65064	0.042716

In equation (19) coefficients $\overline{s_{ji}}$ represent relative changes of the output y_j after introducing relative change of the parameter x_i to the model.

Matrix $\overline{\mathbf{S}}$ was computed for the investigated model for two characterictic time moments: the start of transformation and its end. Ferrite volume fracture at the end of transformation was considered as a model output in that case. The values of the components of $\overline{\mathbf{S}}$ matrix are given in table 3.

Calculated sensitivity coefficients made it possible to clonclude that model is much more dependent on parameters variations at the starting stage of transformation. Besides, the coefficients x_5 and especially x_4 have the largest influence on the model output. The difference between values of sensitivity coefficients can be explained with the fact that at the starting stage the transformation rate is much higher than at the final stage.

3.2. Morris method

Morris method (Morris, 1991) belongs to the group of screening methods. Such methods treat sensitivity of the parameters as a global index and search through the whole domain of posiible values of the parameters. The main idea of such methods is defining which coefficients have the most significant influence on model response.

One-At-a-Time (OAT) approach created by Morris was chosen for the proposed model. This technique investigates the influence of each parameter separately. OAT technique is called global sensitivity analysis method because algorithm explores the whole parameters domain. This algorithm introduces main effect concept, the value of which is defined by computations of local measures in various points in the domain. After this, the main effect is calculated from mean and standard deviation values. Mean values of main effects show influence degree of the parameter and standard deviation values describe whether parameters are dependent on each other and whether parameter influence on the model output is linear or not.

The results of Morris analysis are given below. The analysis was performed for two cooling rates: c_{r1} = 1°C/s and c_{r2} = 0.5°C/s. A ferrite phase volume fraction was selected as a model response. Assumed boundaries of parameters domains and computed main effects for both cooling rates are shown in tables 4, 5 and 6. Mean values and standard deviation values are also presented graphically in figures 1 and 2.

Table 4. *Assumed parameter domains boundaries*

	x_1	x_2	x_3	x_4	x_5
Upper boundary	400	0.1	1	850	40
Lower boundary	250	0.01	0.05	650	5

Table 5. *Calculated mean and standard deviation values for c_{r1} = 1°C/s*

	Mean	Standard deviation
x_1	0.1011	0.1147
x_2	0.6237	0.9545
x_3	0.5378	0.7918
x_4	1.9450	2.0840
x_5	0.6045	0.6321

Table 6. *Calculated mean and standard deviation values for c_{r2} = 0.5°C/s*

	Mean	Standard deviation
x_1	0.0714	0.0675
x_2	0.4337	0.6804
x_3	0.44	0.8064
x_4	1.2642	1.55655
x_5	0.435	0.4954

The results of the analysis approved and specified the conclusions obtained from the local sensitivity analysis. Coefficient a_4 definitely exerts major influence on the model response. At the same time, influence of a_1 parameter is negligible. The influence of other parameters is comparable. Relatively high values of standard deviation show that parameters influence on the model is nonlinear.

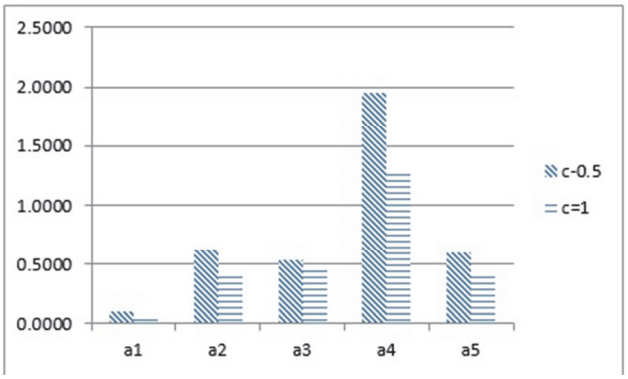

Fig. 1. *Mean values of main effects with respect to individual model parameters.*

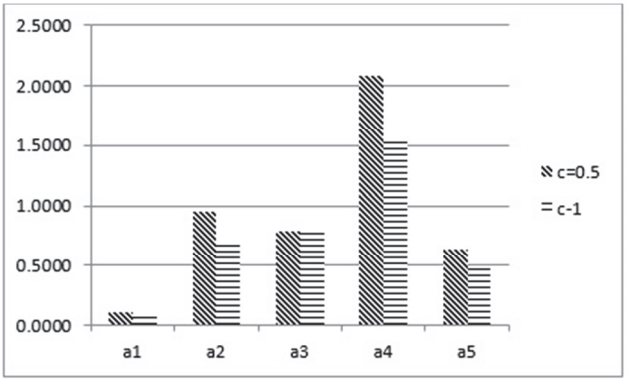

Fig. 2. *Standard deviation values of main effects with respect to individual model parameters.*

4. IDENTIFICATION OF THE MODEL

Identification of the model was performed by inverse analysis method composed of three basic stages (Szeliga et al., 2014):

- Performing physical experiment and gathering results.
- Numerical simulation of performed experiment in chosen physical conditions.
- Using optimization procedure, which minimizes the difference between measured and computed results.

Such algorithm was applied for identification of coefficients $a_1 - a_5$. Any phase transformation model can be written in a form:

$$\mathbf{y} = f(\mathbf{a}) \tag{20}$$

where $\mathbf{y}$ - vector of model response parameters, $\mathbf{a} = \{\mathbf{p}, \mathbf{x}\}$ - vector of model inputs constructed from process parameters vector $\mathbf{p}$ and model coefficients vector $\mathbf{x}$.

Identification of the coefficients vector $\mathbf{x}$ for the known inputs $\mathbf{p}$ and outputs $\mathbf{y}$ is called an inverse problem:

$$\mathbf{x} = f^{-1}(\mathbf{y}, \mathbf{p}) \tag{21}$$

Inverse function f^{-1} can be found analytically only for simple linear problems. Phase transformation problem is nonlinear. Therefore, the problem of identification of coefficients vector $\mathbf{x}$ is transferred into the following optimization task:

$$\Phi(a) = min\|y^c(x) - y^m\|^2 \tag{22}$$

where: $\mathbf{y}^c(\mathbf{x})$ - model responses vector, $\mathbf{y}^m$ - vector of measured output data, $\mathbf{a} = \{\mathbf{p}, \mathbf{x}\}$ - vector of model inputs.

It was proved (Szeliga, 2014) that minimum of the goal function (22) with respect to $\mathbf{x}$ coefficients is a solution of the inverse problem (21). In particular case of phase transformations goal function takes a form (Pietrzyk & Kuziak, 2012):

$$\Phi(\mathbf{x},\mathbf{p}) = \sqrt{\frac{1}{Ncr}\sum_{i=1}^{Ncr}\left\{\left[\frac{T_i^c(\mathbf{x},\mathbf{p}) - T_i^m}{T_i^m}\right]^2 + \left[\frac{F_i^c(\mathbf{x},\mathbf{p}) - F_i^m}{F_i^m}\right]^2\right\}} \tag{23}$$

where: $\mathbf{x} = \{x_1, \ldots, x_5\}^T$ - vector of model coefficients, T^c, T^m - calculated and measured temperatures of transformation start, respectively, F^c, F^m - calculated and measured volume fractions of ferrite, respectively, N_{cr} - the number of cooling rates.

In the current study the model was identified for two steels. The first was a bainitic steel with different chemical composition comparing to previously investigated DP steels. The second was an industrial AHSS grade, which allows to obtain either DP or CP microstructure, depending on the cooling cycle. Chemical compositions of both steels are given in table 2.

In order to solve optimization task the Hooke-Jeeves (Kusiak et al., 2009) method was used. Dilatometric tests were performed in the Institute for Ferrous Metallurgy in Gliwice. It should be mentioned that for the bainitic steel for the cooling rate 2°C/s the ferritic transformation is practically absent. Therefore it is impossible to estimate start temperature for this rate. Estimated coefficients in the model for bainitic and AHSS steels are given in the rows 2 and 3 in table 2. Comparisons of measured and calculated model outputs are shown in figure 3.

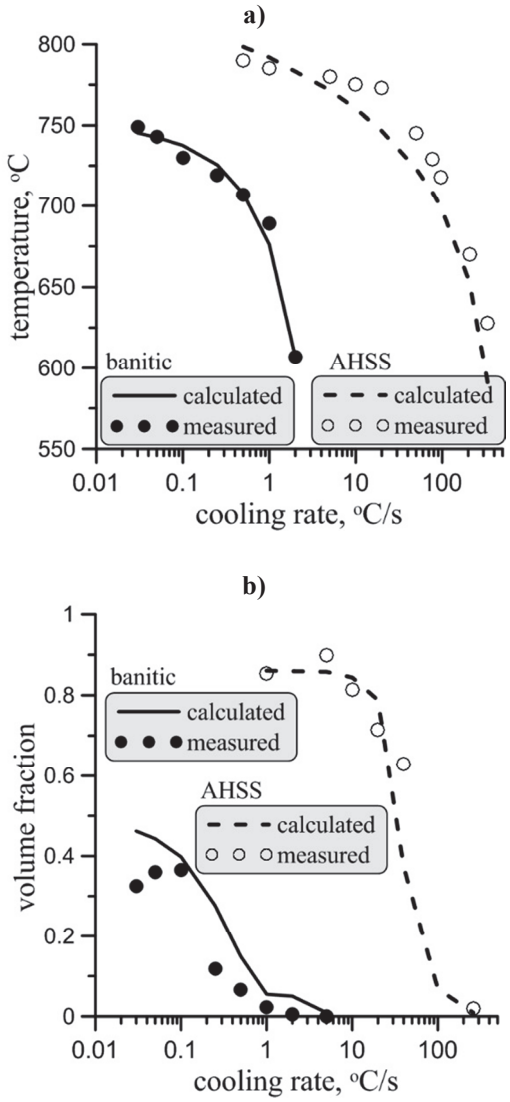

Fig. 3. *Comparison of measured and calculated ferrite start temperatures (a) and ferrite volume fractions (b) for bainitic steel and for ASSH.*

Computed results prove that the proposed model is able to predict temperature for the start of transformation and final ferrite volume fraction with good accuracy. The differences between measured and calculated data are growing with cooling rate growth. It may be caused by the fact that for investigated steel ferritic transformation does not go completely for low cooling rates, so for cooling rates over 0.5°C/s for bainitic steels and over 50°C/s for ASSH steels the determination of start temperature can be complicated.

5. NUMERICAL EXPERIMENT AND MODEL VALIDATION

The objective of the numerical experiment was to provide the data for validation of the model based on the control theory. Two tests described in literature (Kwiaton, 2016) were considered. The AHSS steel with the chemical composition in table 2 was subjected to two cooling thermal cycles to obtain DP and CP microstructures, respectively. These cycles are shown schematically in figure 4. Ferrite volume fraction growth in both cycles calculated with model based on control theory and coupled diffusion-level set method is shown in figure 5.

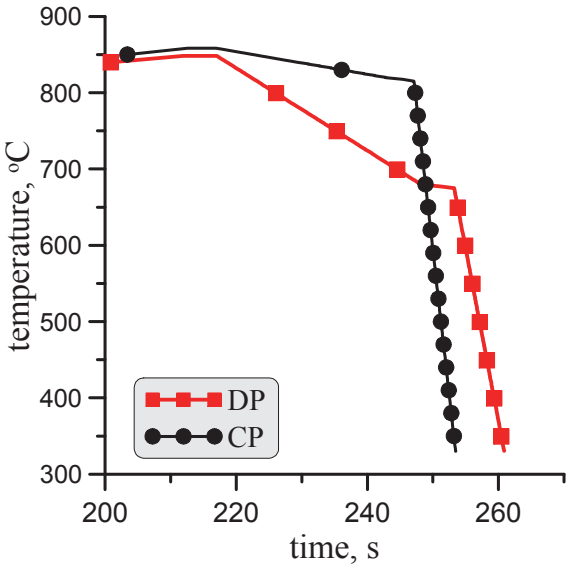

Fig. 4. *Cooling thermal cycles to obtain DP and CP microstructures (Kwiaton et al., 2016).*

Presented results show good agreement between the two models. Additionally, the models predicted properly phase compositions for DP (75-80% of ferrite) and CP (45-50% of ferrite). It can be concluded that in simulation/optimization of industrial processes fast model based on the control theory (Milenin et al., 2015) can be used. Model is able to give results for a problem compared to presented in a, literally, few moments. This model can be implemented into the FE codes and will not cause significant increase of the computing costs. Computation time based on diffusion equation solution model is much higher. Depending on the solution size it can reach a few hours. However, when advanced features of the microstructure have to be calculated, the model based on the solution of the diffusion equation has to be applied. Predictive capabilities of this model are seen in figure 6, when results of calculations of carbon distribution during transformation are shown. Typical austenite microstructure generated using cellular automata approach was used as an initial data. Nucleation sites were set randomly in triple points. DP thermal cycle was applied in the presented example.

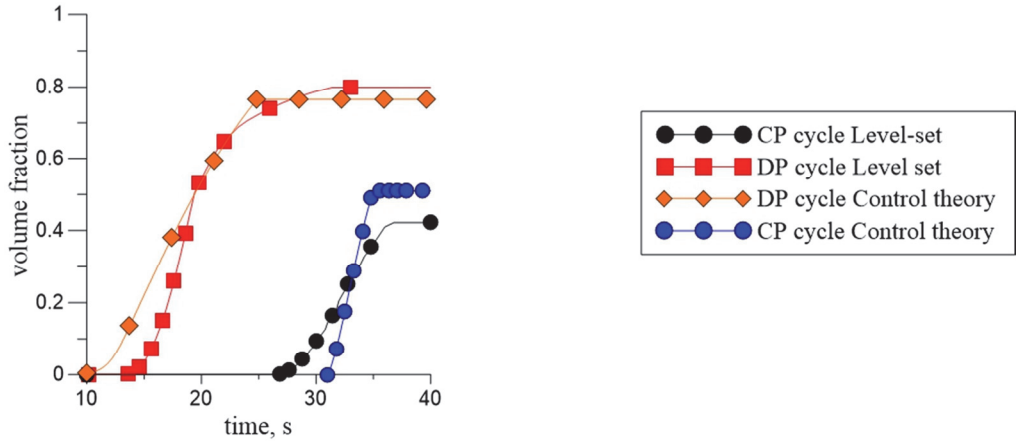

Fig. 5. Ferrite phase growth kinetics in DP and CP cycles calculated with model based on control theory (orange and blue) and coupled diffusion-level set method (red and black).

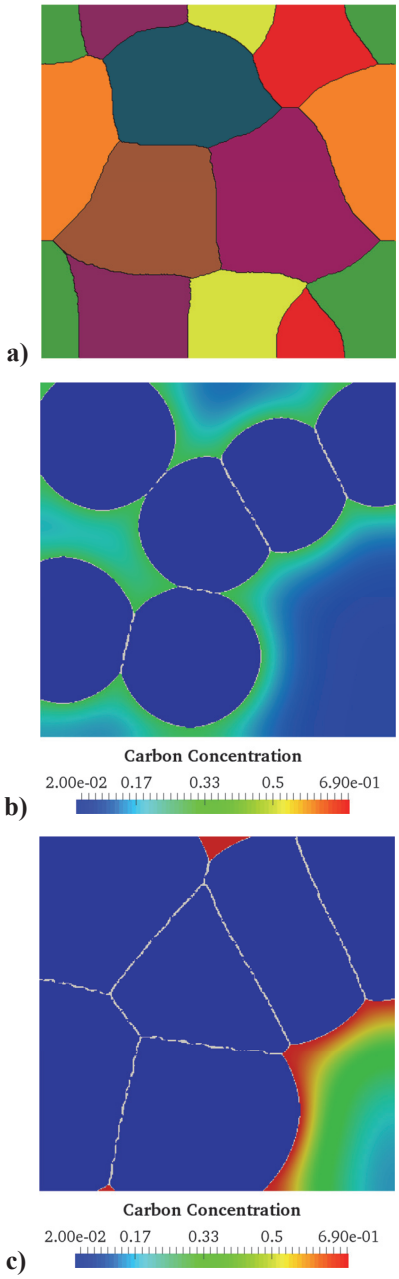

Fig. 6. Austenite microstructure used as a starting point for simulation (a), carbon concentration distribution in front of growing ferrite grains: after 20 s (b) and after 40 s (c).

The knowledge of carbon distribution in the austenite allows for further prediction of local martensite start temperatures and carbon distribution in martensite. This is a complete information needed to predict properties of the DP or CP steels.

6. CONCLUSIONS

1. Previously proposed phased transformation model was developed, tested an validated. Sensitivity analysis was performed. Both local algorithm and Morris method had shown the same result for time constants' coefficients. SA showed that coefficient a_4, which determines the nose in the Gauss function describing time constant B2, has the largest influence on both kinetics of transformation and ferrite volume fraction
2. The model based on the control theory was identified using dilatometric tests data for three steels with different chemical compositions. The model with optimized coefficients showed reasonable accuracy for prediction of both final ferrite volume fraction and transformation start temperature.
3. Numerical experiments for AHSS were performed. Results were compared to the results given by coupled diffusion-level set method and good agreement between the two models was obtained.
4. Both the model based on the control theory and the model based on the solution of diffusion equation predicted phase compositions for DP and CP thermal cycles with good qualitative accuracy.
5. The model based on the control theory is fast and predicts accurately transformation temperature and ferrite volume fraction. It can be efficiently used with FE codes describing tempera-

tures in macro scale and in optimization of technological processes. Predictive capabilities of the model based on the solution of diffusion equation are much larger and they include shape of grains and carbon distribution in the austenite. On the other hand, computing costs for this model are very high.

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REFERENCES

Avrami, M., 1939, Kinetics of phase change. I. General theory, *Journal of Chemical Physics*, 7, 1103-1112.

Bzowski, K., Bachniak, D., Pernach, M., Pietrzyk, M., 2016, Sensitivity analysis of phase transformation model based on solution of diffusion equation, *Archives of Civil and Mechanical Engineering*, 16, 186-192.

Osher, S., Sethian, J. A., 1988, Fronts propagating with curvature-dependent speed: Algorithms based on Hamilton-Jacobi formulations, *Journal of Computational Physics*, 79, 12-49.

Donnay, B., Herman, J.C., Leroy, V., Lotter, U., Grossterlinden, R and Pircher, H., 1996, Microstructure evolution of C-Mn steels in the hot deformation process: The STRIPCAM model, *Proc. 2nd Conf. Modelling of Metal Rolling Processes*, eds, Beynon, J.H., Ingham, P., Teichert, H., Waterson, K., London, 23-35.

Farjas, J., Roura, P, 2012, Isoconversional analysis of solid-state transformations: A critical review. Part III. Isothermal and non isothermal predictions, *Journal of Thermal Analysis and Calorimetry*, 109, 183-191.

Johnson, W.A., Mehl, R.F., 1939, Reaction kinetics in processes of nucleation and growth, *Transactions AIME*, 135, 416-442.

Kolmogorov, A., 1937, A statistical theory for the recrystallisation of metals, *Akademia Nauk SSSR, Izviestia, Ser. Matematica*, 1, 355-359.

Kwiaton, N., Kuziak, R., Pietrzyk, M., 2016, Comparison of numerical simulation and experiment for the microstructure development of a cold-rolled multiphase steel during annealing, *Materials Science Forum, Production and further processing of flat products*, eds, Kawalla, R., Ullmann, M., Neh, K., Trans Tech Publications, 167-173.

Leblond, J.B., Devaux, J., 1984, A new kinetic model for anisothermal metallurgical transformations in steel including effect of austenite grain size, *Acta Metallurgica*, 32, 137-146.

Milenin, I., Pernach, M., Pietrzyk, M., 2015, Application of the control theory for modelling austenite-ferrite phase transformation in steels, *Computer Methods in Materials Science*, 15, 327-335.

Morris, M.D., 1991, Factorial sampling plans for preliminary computational experiments, Technometrics, 33, 161-174.

Pernach, M., Pietrzyk, M., 2008, Numerical solution of the diffusion equation with moving boundary applied to modeling of the austenite-ferrite phase transformation, *Computational Materials Science*, 44, 783-791.

Pernach, M., Bzowski, K., Pietrzyk, M., 2014, Numerical modelling of phase transformation in DP steel after hot rolling and laminar cooling, International *Journal for Multiscale Computational Engineering*, 12, 397-410.

Pietrzyk, M., Kuziak, R., 2012, Modelling phase transformations in steel, *Microstructure evolution in metal forming processes*, eds, Lin, J., Balint, D., Pietrzyk, M., Woodhead Publishing, Oxford, 145-179.

Kusiak J., Danielewska-Tułecka A., Oprocha P., 2009, *Optymalizacja. Wybrane metody z przykładami zastosowań*, Wydaw. Nauk. PWN, Warszawa, 310.

Pietrzyk, M., Madej, Ł., Rauch, Ł., Szeliga, D., 2015, *Computational Materials Engineering: Achieving high accuracy and efficiency in metals processing simulations*, Elsevier, Amsterdam.

Scheil, E., 1935, Anlaufzeit der Austenitumwandlung, *Archiv für Eissenhüttenwesen*, 12, 565-67.

Starink, M.J., 2001, On the meaning of the impingement parameter in kinetic equations for nucleation and growth reactions, *Journal of Materials Science*, 36, 4433-4441.

Szeliga, D., 2013, *Identification problems in metal forming. A comprehensive study*, Publisher AGH, no. 291, Kraków.

ANALIZA WRAŻLIWOŚCI I IDENTYFIKACJA MODELU PRZEMIAN FAZOWYCH OPARTEGO O TEORIĘ STEROWANIA

Streszczenie

Celem pracy była poprawa modelu przemian fazowych poprzez jego identyfikację dla wybranych gatunków stali oraz przeprowadzenie analizy wrażliwości. Opracowany model pozwala przewidywać kinetykę przemian fazowych w warunkach zmiennej temperatury. Model charakteryzuje się bardzo krótkim czasem obliczeń i dobrymi możliwościami obliczeniowymi. W modelu jest pięć współczynników, które muszą być wyznaczone dla badanej stali na podstawie badań dylatometrycznych. We wcześniejszych pracach model został wykorzystany do przewidywania kinetyki przemian fazowych w wybranych stalach DP poddawanych różnym cyklom cieplnym. W pierwszej części niniejszej pracy przeprowadzono analizę wrażliwości modelu wykorzystując dwie metody: lokalną analizę wrażliwości i metodę Morrisa. Wyznaczone współczynniki wrażliwości opisują w jakim stopniu parametry modelu wpływają na jego wyjście oraz które z tych parametrów mają największe znaczenie. W drugiej części pracy przeprowadzono identyfikację współczynników modelu. Zadanie identyfikacji jest problemem odwrotnym, który przekształcono w zadanie optymalizacyjne. Optimum poszukiwano metodą Hooke-Jeevesa. Wyznaczone współczynniki modelu pozwoliły na opisanie kinetyki przemiany austenite-ferryt w warunkach zmiennej temperatury. Walidację modelu przeprowadzono poprzez porównanie uzyskiwanych wyników z rezultatami symulacji zaawansowanym modelem numerycznym wykorzystującym rozwiązanie równania dyfuzji węgla w austenicie. Analizowano standardowe cykle cieplne stosowane dla uzyskania mikrostruktur wielofazowych i uzyskano dobrą zgodność między modelami.

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