NEW TRENDS IN EFFICIENT MODELLING OF PHASE TRANSFORMATIONS

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Abstract

Classification of the phase transformation models with respect to computing times and predictive capabilities was the objective of the paper. Selection of the best model for a particular application was discussed and three models were chosen for the analysis. The first was an upgrade of the JMAK model, the second was an extension of the Leblond model the third was a solution of the carbon diffusion equation in the austenite. Capabilities of the models regarding prediction of microstructure after transformation were evaluated. Accuracy of predictions and efficiency of the models were compared. Results of dilatometric tests were used to validate the models. Finally, the models were applied to simulations of the industrial process and their predictive capability and efficiency were compared.

Keywords: Phase transformation, modelling, computing costs, multiscale methods

1. INTRODUCTION

Large number of phase transformation models are available in the literature, from the simplest ones based on the JMAK equation [1] through more advanced models based on solution of differential equation [2] phase field [3] or to discrete models based on the Cellular Automata method [4]. All these models are characterized by various complexity of mathematical formulation and various predictive capabilities. Two aspects decide about accuracy and effectiveness of the phase transformation modelling: i) selection of a relevant model for a particular application, ii) proper identification of models. In metals processing the problem of identification of models using inverse analysis was widely investigated and application of this approach to the identification of phase transformation models presented in [5] was used in the present work. Showing new trends in modelling phase transformations and evaluation of the phase transformation models with respect to their predictive capabilities and computing costs was the general objective of this paper. The selection of the best model for particular application has to be made by searching for a balance between these two features. A primary classification of the models with respect to these criteria was made in [6]. The following objectives of the paper compose case studies of the application of the selected models to industrial processes and comparison of the performance of these models.

2. CLASSIFICATION OF PHASE TRANSFORMATION MODELS

Historically, JMAK type equations [1] were commonly used for simulations of phase transformations. In this approach, all attention is focused on the kinetics and microstructural aspects are essentially ignored. However, several upgrades of this model were proposed and it is still commonly used. More advanced model was proposed in [2], where rate of the transformation is assumed to be proportional to the distance from the equilibrium state. The proposition of [2] was extended by the Authors of the present paper by introduction of the second order differential equation [7]. More refined transformation models incorporate relevant features of the parent microstructure. The simplest approach considered the austenite grain as a sphere and the ferrite to nucleate uniformly along the outer surface. Geometrically more-refined models, in which the austenite grain is assumed to be a more complex geometrical figure, were proposed in [8]. In recent years, the phase field approach has emerged as one of the most powerful methods for modelling many types of microstructure-evolution processes, including the austenite decomposition [3]. Since early 1970-ies, finite element (FE)

method has become the most popular simulation technique. In modelling phase transformations this method was applied to simulations of carbon distribution in austenite and became an alternative for the phase field models, see eg. [9]. FE solution of the diffusion equation with a moving boundary (Stefan problem) was performed in that work for various shapes of austenite and ferrite grains. In the late 1990-ies such discrete methods as cellular automata (CA), molecular dynamics (MD) or Monte Carlo (MC) begun to be applied to modelling recrystallization and phase transformations during materials processing. The general idea of the CA phase transformation model was presented in [10]. Classification of phase transformation models with respect to predictive capabilities and computing costs is presented in **Fig. 1**. The first group (bottom left corner in **Fig. 1**) contains models commonly used for fast simulations of industrial processes and they are generally limited to description of the kinetics of transformations and volume fractions of phases. Additivity rule [11] has to be applied in these models to account for the temperature changes during transformations. In the second group (the centre in **Fig. 1**) there are differential equations or phase field technique models, usually applied to technology design and optimization of processes. Models based on the FE solution of the diffusion equation with moving boundary [10] are further right top. All these models accurately describe transformations in varying temperatures. The next group (far right in **Fig. 1** includes multiscale models. The last two groups of models are capable to predict distribution of carbon concentration in austenite and resulting hardness of bainite and martensite.

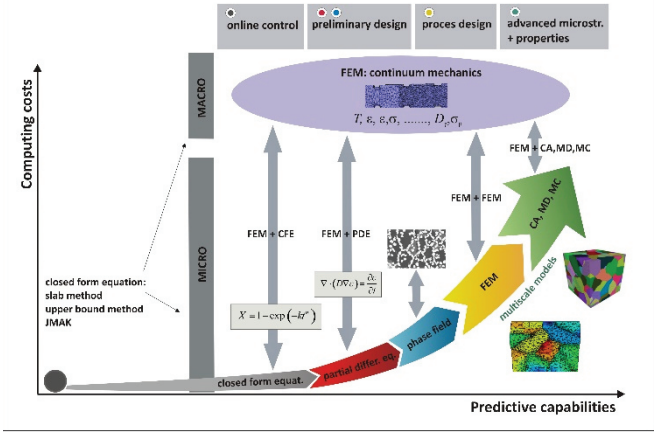


Fig. 1 Classification of selected phase transformation models: computing costs versus predictive capabilities

Starting from the late nineties, microstructural models, both phenomenological and physically-based, have been implemented into the FE codes making possible to carry out fully coupled thermal-mechanical - microstructural simulations, giving raise to new challenges in modelling materials processing. As it is shown in **Fig. 1**, while the computing times of the FE method remain at approximately stable level (increase of the complexity of models is compensated by the increase of the computing power), the computing costs at micro scale increase rapidly when more complex methods are applied.

3. MODELS

Three models developed by the Authors were analysed. Detailed information regarding the models is given elsewhere and only brief information is given below. The first model (JMAK) is an upgrade of the equation:

$$X = 1 - \exp\left(-kt^n\right) \tag{1}$$

where: X - transformed volume fraction, k, n - coefficients. In equation (1) coefficient k was introduced as a function of the temperature [5]. In the next model assumption is made that response of the steel subjected to temperature changes is similar to the response of the 2nd order inertia term in the control theory [7].

Temperature is an input and ferrite volume fraction is an output of this term. Therefore, similarities between materials response and control theory (CONT) is the second order differential equation describing kinetics of transformation:

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

where: B_1, B_2 - time constants representing nucleation and growth, T - temperature. The 3rd model (DIFF) assumes that growth of the new phase is controlled by carbon diffusion in the austenite. Kinetics of the transformation is calculated by the FE solution of the diffusion equation with moving boundary (Stefan problem). Details of this model are described in [12]. The following equations are solved

$$\nabla \cdot (D \nabla c) = \frac{\partial c}{\partial t} \tag{3}$$

where: D - diffusion coefficient, c - carbon concentration, t - time. Equation (3) was solved with the following initial and boundary conditions:

$$c(\mathbf{x},0) = c_0 \qquad \frac{\partial c}{\partial t} = \nabla \cdot D \nabla c \qquad c(\mathbf{x}_\xi, t) = c_{\gamma\alpha} \tag{4}$$

where: c_0 - carbon concentration in steel, $c_{\gamma\alpha}$ - equilibrium carbon concentration at the austenite-ferrite boundary, $\mathbf{x}$ - vector of coordinates, $\mathbf{x}_\xi$ - position of the interface, $\mathbf{n}$ - unit vector normal to the boundary.

4. EXPERIMENT

Dual phase (DP) steel containing 0.095%C, 1.51%Mn 0.0039%N, 0.005%Nb, 0.045%V, 0.006%Ti, 0.23%Si, and 0.41%Cr was investigated. Dilatometric tests for various cooling rates were performed results were subjected to the inverse analysis and were used for identification of JMAK and CONT models, see publication [5] for the former and [7] for the latter model. In the present work the tests aiming at validation of the models were performed. The samples measuring 15x20x35 mm were deformed in 6 passes of plane strain compression (PSC) on the Gleeble 3800 with reductions and temperatures typical for the hot strip rolling. Two thermal cycles shown in **Fig. 2** were applied after the deformation. Microstructure and mechanical properties of the samples cooled to the room temperature were investigated.

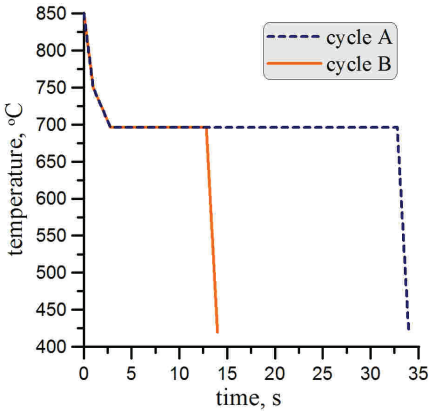
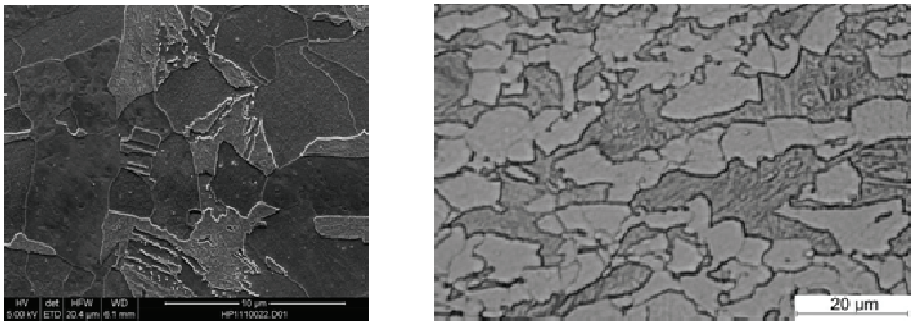


Fig. 2 Thermal cycles applied after PSC hot deformation on the Gleeble 3800

Microstructures of samples are shown in **Fig. 3**. Microstructure of the sample subjected to the cycle A is mainly ferritic with some martensite islands. Microstructure composed of ferritic matrix with bainitic and martensitic islands was obtained after the cycle B.



A) B)

Fig. 3 Microstructures of samples subjected to the cooling cycles A and B

5. RESULTS

5.1. Verification and validation of models

The models were verified by comparison calculated start and end temperatures of phase transformations with measurements in dilatometric tests. Upgrade of the JMAK model has been extensively used by the Authors for various steels, see publications for AHSS [5] or bainitic steels [14] where good predictive capability of that model was confirmed. Beyond this, the model predicts changes of the average carbon concentration in the austenite during ferritic transformation and accounts for the influence of this concentration on start temperatures of the bainitic and martensitic transformations. Model DIFF was verified and validated in [12] and its good accuracy was confirmed, as well. Advanced information, such as morphology and hardness of martensite islands, can be predicted by that model, which supplies data for prediction of the steel properties depending on the cooling cycle and predicts areas of possible occurrence of the retained austenite. Model CONT has been recently developed [7] and its verification was performed for the steel investigated in the present work. This model describes ferritic transformation only and JMAK model of the remaining transformations [5] were used. **Fig. 4** shows comparison of the measured and calculated start and end temperatures for phase transformations.

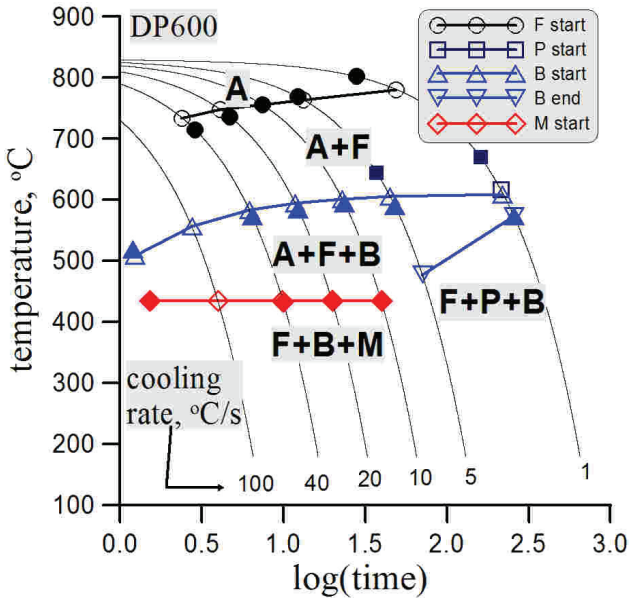


Fig. 4 Comparison of the start and end temperatures for phase transformations measured in dilatometric tests and calculated using model CONT. Empty symbols show results obtained from model, filled symbols obtained from experiment

Recapitulating, all models were verified by comparison prediction with the results of dilatometric tests. Good accuracy of the models was confirmed. Validation of the models showed much larger predictive capabilities of the DIFF model comparing with the remaining two models. Predictive capabilities of JMAK and CONT models are similar. They describe with good accuracy kinetics of transformation and volume fraction of phases. Model CONT accounts directly for changes of temperature, while JMAK model has to be combined with the additivity rule [11].

5.2. Comparison of models performance and predictive capabilities

Thermal cycles shown in **Fig. 2** were simulated using three models. Typical austenite microstructure created using Digital Material Representation (DMR) technique with periodic boundary conditions was used in DIFF model to generate initial data (**Fig. 5 left**). Mesh was generated and ferrite nuclei were placed in selected triple points. **Fig. 1** centre shows results for the thermal cycle A, and **Fig. 5** right for the thermal cycle B. Both show shapes of martensite islands as well as carbon distribution at the end of cooling.

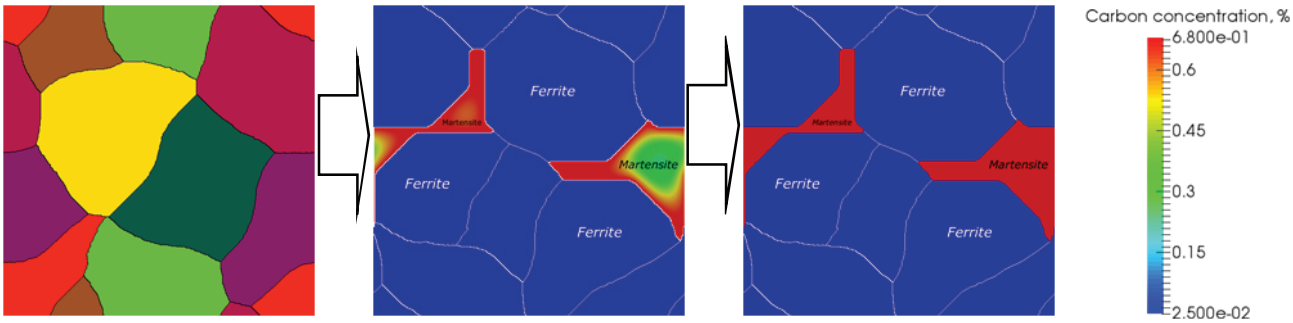


Fig. 5 Selected results obtained using DIFF model, from left: initial austenite microstructure, DP microstructure after thermal cycle A and DP microstructure after thermal cycle B

Calculated volume fraction of phases are shown in **Fig. 6a**. It is seen that model JMAK predicts similar volume fractions for both cycles. It means that ferritic transformation is completed after 10 s of maintaining at constant temperature, what is seen in **Fig. 7a** where kinetics of transformations is shown. Contrary, different volume fractions of phases for the two cycles were obtained from models CONT and DIFF. Comparison of the kinetics of the ferritic transformation predicted by JMAK and DIFF models is shown in **Fig. 6b**, while **Fig. 7b** shows carbon concentrations during cycles A and B calculated by JMAK and CONT models.

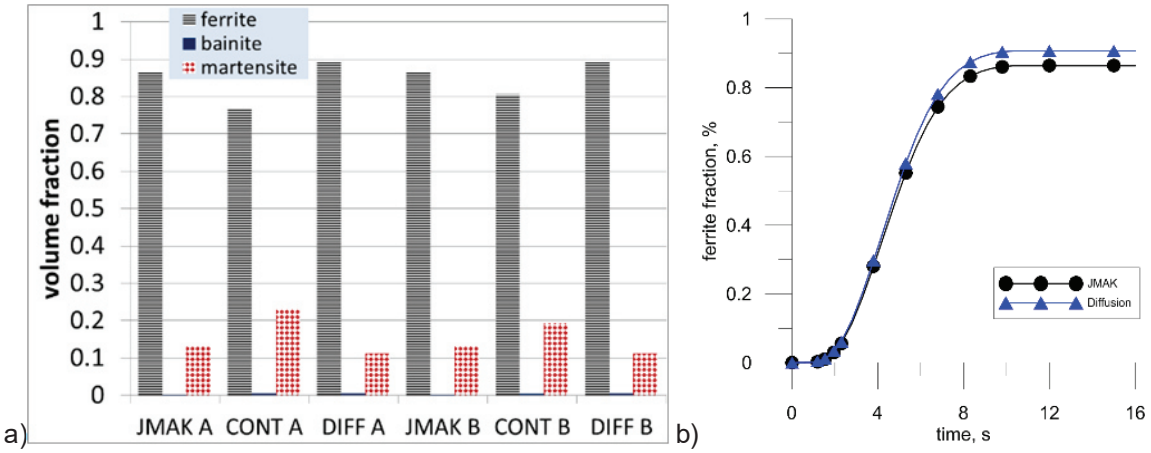


Fig. 6 Volume fractions of phases (a) and comparison of kinetics of transformations obtained by JMAK and DIFF models for the cycle A

Differences between models JMAK and CONT are well seen in **Fig. 7b**, where changes of the average carbon concentration in the austenite during the tests are shown. Model JMAK predicts that during the isothermal part of the cycle carbon concentration reaches the maximum value $c_{\gamma\beta}$.

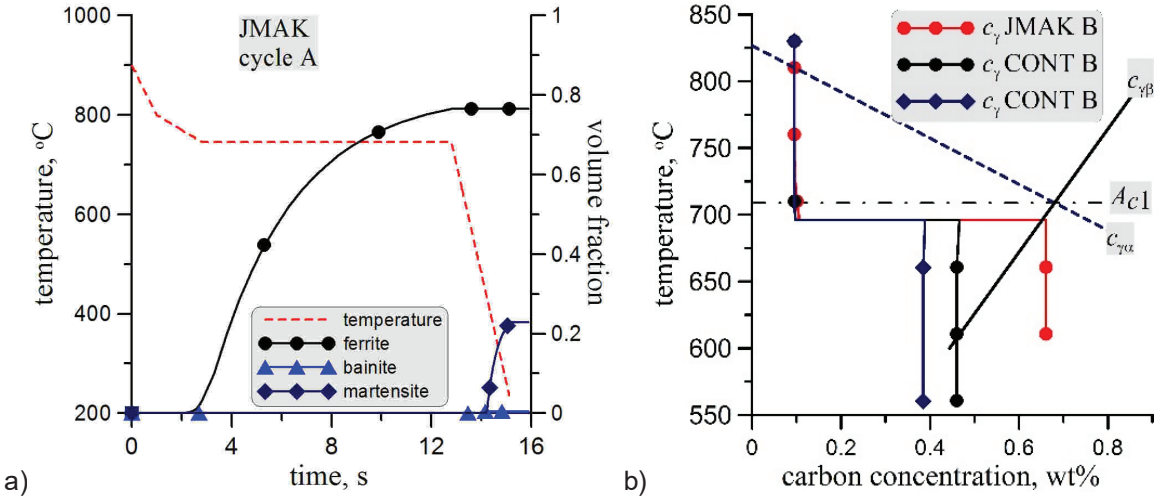


Fig. 7 Kinetics of phase transformations calculated using JMAK model for the cycle (A) and changes of carbon concentrations during cycles A and B calculated by JMAK and CONT models (b)

6. CONCLUSIONS

Classification of phase transformation models was performed following [14] and three models of various complexity of mathematical formulations and various predictive capabilities were selected for the analysis. Performed validation and numerical tests have shown that all models predict kinetics of transformation reasonably well, although slight differences in final volume fractions of phases were observed. Model based on the solution of the diffusion equation predicted well global parameters (kinetics) and, additionally, it predicted carbon distribution in the remaining austenite.

ACKNOWLEDGEMENTS

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