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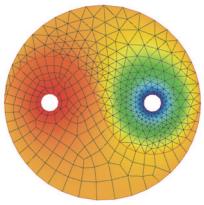
AKAPIT

COMPUTER METHODS IN MATERIALS SCIENCE

Informatyka w Technologii Materiałów

Vol. 16, 2016, No. 4



STRATEGY FOR THE SELECTION OF THE BEST PHASE TRANSFORMATION MODEL FOR SIMULATION OF METALS PROCESSING

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Abstract

Connection of the finite element program with phase transformation models is often needed when prediction of distribution of phase composition in the product is of interest. Depending on the type of the phase transformation model this connection may involve long computing times. Moreover, when the optimization task has to be formulated and solved, the computing costs may radically increase. It is particularly troublesome when the objective function is composed of advanced microstructural parameters or product properties, evaluation of which requires an application of multiscale modelling techniques. In the present paper the possibilities of decreasing of the computing costs for optimization of metals processing were explored. Several case studies, which require connection of the FE code with phase transformation models, were analysed and computing times were compared. Efficiency of modelling depending on the complexity of the macro scale FE mesh was evaluated.

Key words: modelling, phase transformations, computing costs, materials processing

1. INTRODUCTION

Computer aided design of materials processing is common now. Beyond one step processes, whole manufacturing chains are simulated (Pietrzyk et al., 2008). Typical optimization problems for manufacturing chains are based on simulations of various variants of several processes according to the applied optimization technique. In industrial materials processing problems finite element (FE) simulations are usually used for calculations of the objective function, which often consists of the in use properties of products. Thus, solution of the optimization task is costly and there is a continuous search for alternative methods (Behrens et al., 2011). Moreover, when objective function is composed of advanced microstructural parameters or product properties, application of multiscale modelling is needed and computational costs are further increased. In the present paper we explored the possibilities of decreasing the computation costs for optimization of materials processing. The particular emphasis is put on processes, in which phase transformations are used to control properties of steel products.

2. MODELS

Finite element (FE) is commonly used to describe thermal and mechanical phenomena in the macro scale. Conventional model based on Sellars fundamental works (1980) is used to describe microstructure evolution during hot forming. Finally, a variety of phase transformation models is used to describe kinetics of phase transformations and phase composition of products. All these models are described briefly in the following Sections.

ISSN 1641-8581

2.1. Finite element model

The FE solution is based on the rigid-plastic thermo-mechanical finite element approach proposed by Lee and Kobayashi (1973). Detailed description of the algorithm and the program, which was used in this work, is given by Pietrzyk (2000). The solution assumes that the material obeys Huber-Mises yield criterion and associated Levy-Mises flow rule. The velocity field is calculated by searching for a minimum of the power functional:

$$J = \int_{\Omega} \left(\sigma_i \dot{\varepsilon}_i + \lambda \dot{\varepsilon}_V \right) d\Omega - \int_{\Gamma} \mathbf{f}^T \mathbf{v}_s d\Gamma \qquad (1)$$

where: σ_i - effective stress, which is equal to the flow stress σ_p, $\dot{\varepsilon}_i$ - effective strain rate, V - volume, S - contact surface, $\dot{\varepsilon}_V$ - volumetric strain rate, λ - Lagrange multiplier, $\mathbf{f}$ - vector of boundary tractions, $\mathbf{v}_s$ - vector of velocities.

Mechanical solution is coupled with the thermal part of the model, see Lenard et al. (1999) for details.

2.2. Computing times for multiscale models

There are several factors which determine computing times for multiscale models. Some of these factors are listed below:

- Complexity of the macro scale model. Usually it is finite element (FE) model. If simpler approach can be used, a significant decrease of the computing time can be achieved (see section 4.2.2). 3D solution would require few order of magnitude longer computing times than a 2D one. Solutions of thermal problems are much faster than mechanical or thermo-mechanical ones.
- Complexity of the micro scale model. Depending on the needs, a variety of models ranging from simple JMAK (Johnson-Mehl-Avrami-Kolmogorov) equation to discrete (e.g. Cellular Automata (CA)) models can be used. See section 2.3 for classification of micro scale models.
- Type of coupling between the scales. Fully coupled models (with feedback from micro to macro scale) will require much longer computing times than semi coupled. The former requires micro scale calculations to be performed on-line at each Gauss point in the macro scale. The latter can be often performed during post processing at selected points only.
- Thermal feedback (eg. effect of the heat generated due to transformation on the temperature) will be much faster than mechanical feedback (eg. the effect of the strain due to dilatation on residual stresses).
- Capability of the models for distributed computing using modern computer architectures.

All these aspects are considered in the present paper using six industrial processes as an example. Modelling of phase transformation in the micro scale is the common feature of all these processes. Models of various complexity are used in the macro and micro scales and computing costs are compared.

2.3. Microstructure evolution model

This mode is based on equations describing kinetics of recrystallization, recrystallized grain size and grain growth during dynamic, metadynamic and static recrystallization, as proposed in the works of Sellars (1980). In the present work the coefficients in the model for the investigated steel were determined on the basis of the experimental tests, see for example (Kuziak & Pietrzyk, 2011). Since in the present work the focus is on phase transformations and properties of products and the microstructure evolution model is needed only to determine the grain size at the beginning of phase transformations, the latter is not described here.

2.4. Phase transformation models

A variety of phase transformation models of various complexity of mathematical description and of various predictive capabilities were investigated by the Authors. An attempt of classification of these models in the coordinate system computing costs vs. predictive capabilities was presented in (Rauch et al., 2014). Upgraded version of this classification is shown in figure 1. Four of these models were investigated in the present work, these are JMAK upgrade, 2nd order differential equation, diffusion based model and Cellular Automata model. Two of these models are described in earlier publications and they are not discussed in the present paper. These are upgrade of the JMAK model described by Pietrzyk and Kuziak (2012) and Cellular Automata model described by Halder et al. (2014) for heating and by Gołąb et al. (2014) for cooling.

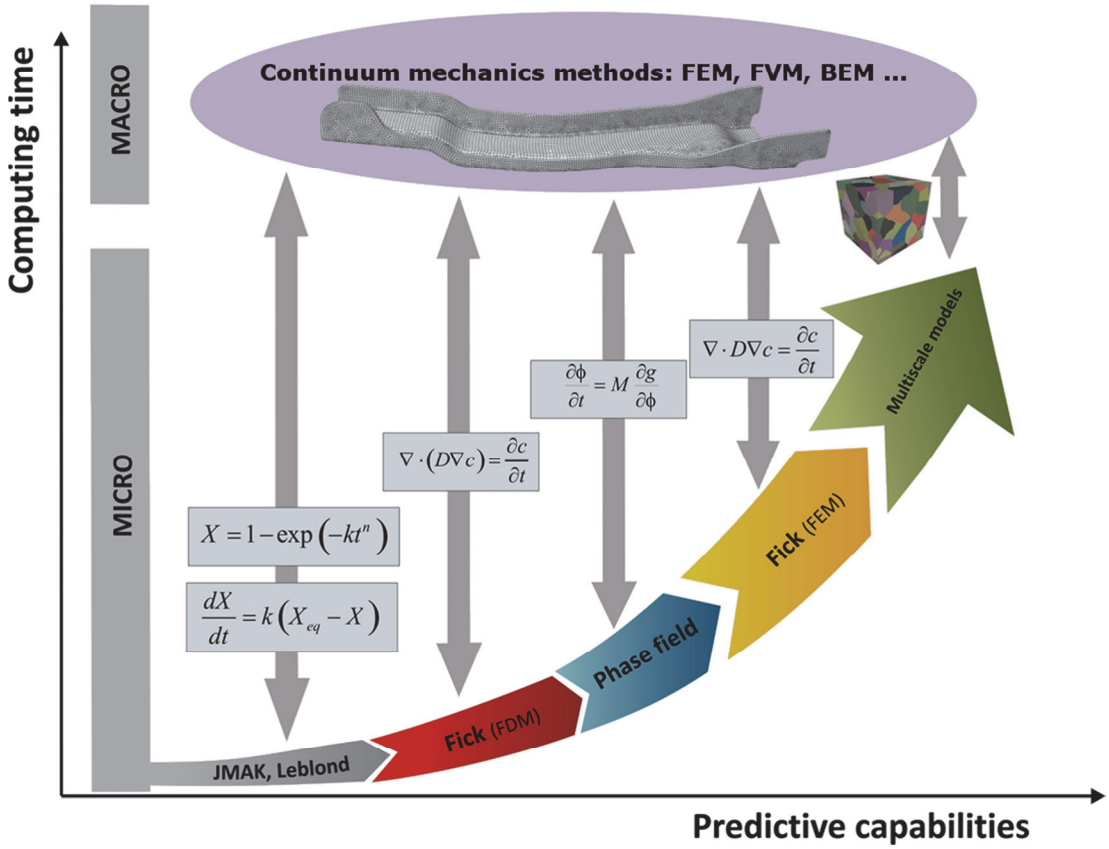


Fig. 1. *Classification of phase transformation models with respect to their predictive capabilities and computing time*

2.4.1. Model based on the control theory

The idea of this model is based on the Leblond equation (Leblond & Devaux, 1984). The main assumption of Leblond was that the rate of the transformation is proportional to the distance from the equilibrium:

$$\frac{dX}{dt} = k\left(X_{eq} - X\right) \tag{2}$$

where: X – volume fractions of a new phase, X_{eq} – equilibrium volume fractions of a new phase in the current temperature, k – coefficient.

In the present paper the model was applied for the ferritic transformation only. 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. Since equation (2) describes the first order inertia term, it is not capable to account for the delay of the response. Thus, the second order equation was proposed by Milenin et al. (2015) to eliminate this constraint. The following equation was proposed:

$$B_1^2 \frac{d^2X}{dt^2} + B_2 \frac{dX}{dt} + X = \mathrm{f}\left(T\right) \tag{3}$$

where: B_1, B_2 - time constants defined as functions of the temperature..

Right hand side of equation (3) is a function of temperature, as well. This function has to be equal to the equilibrium volume fraction of ferrite at the considered temperature:

$$\mathrm{f}\left(T\right) = \frac{F_{fT}}{F_{f\max}} \tag{4}$$

where:

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

$$F_{fT} = \frac{c_{\gamma\alpha} - c_0}{c_{\gamma\alpha} - c_\alpha} \tag{6}$$

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 $c_{\gamma\beta}$ determined from the ThermoCalc software. $c_{\gamma\alpha}$ is the carbon concentration at the γ/α interface and $c_{\gamma\beta}$

is the carbon concentration at the γ/*cementite* interface.

Volume fraction X in equation (3) is calculated with respect to the maximum volume fraction F in the steel defined by equation (5). Time constants B_1 and B_2 in this equation are responsible for the delay of the response and for the rate of the response, respectively. Thus, 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, which is directly connected with the undercooling below A_{c3}. The following definition of B_1 was assumed in the first approach:

$$B_1 = a_4 \exp\left[-a_5\left(A_{e3} - T\right)\right] \tag{7}$$

where: a_4, a_5 - coefficients.

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 (coefficient a_7 in the model). In consequence the following relation was proposed:

$$B_2 = \left\{ a_6 \exp\left[-\left(\frac{a_7 - T}{a_8} \right)^2 \right] \right\}^{-1} \tag{8}$$

where: a_6, a_7, a_8 – coefficients.

Modelling of the ferrite phase transformations begins with equation (3) when the temperature drops below A_{c3}. As it has already been mentioned, 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. This maximum value is determined by the line $c_{\gamma\alpha}$. This maximum value of X is equal to the right hand side of equation (3). Thus, the current volume fraction of ferrite with respect to the whole volume of the material is $F_f = XF_{f\max}$. Since F_{fT} changes when the temperature changes, the following correction of X has to be introduced in each time step of calculations:

$$X\left(T_{i+1}\right) = X\left(T_i\right)\frac{F_{fT}\left(T_i\right)}{F_{fT}\left(T_{i+1}\right)} \tag{9}$$

where: i – iteration number, T_i – temperature in i^{th} iteration.

In the present work equation (3) was solved using the finite difference method. During continuous cooling simulation continues until the transformed volume fraction X achieves 1. However, when carbon content in austenite exceeds the limiting value $c_{\gamma\beta}$, the austenite-pearlite transformation begins in the remaining volume of the austenite.

2.1.2. Model based on the solution of the diffusion equation

The idea of this model is described by Pernach and Pietrzyk (2008) and examples of its applications can be found in (Pernach et al., 2014). The model assumes that diffusion is the main phenomenon, which controls rate of the ferrite transformation. Mathematical formulation is based on the solution of the second Fick law:

$$\nabla \cdot \left(D \nabla c\right) = \frac{\partial c}{\partial t} \tag{10}$$

where: D – diffusion coefficient, c – carbon concentration, t – time.

Equation (10) was solved with the following initial and boundary conditions:

$$\begin{aligned} c\left(\mathbf{x}, 0\right) &= c_0 \quad \mathbf{x} \in \Omega_\gamma \\ D\nabla c \cdot \mathbf{n} &= 0 \quad \mathbf{x} \in \Gamma_{GB} \\ c\left(\mathbf{x}_\xi, t\right) &= c_{\gamma\alpha} \quad \mathbf{x} \in \Gamma_{IF} \end{aligned} \tag{11}$$

where: c_0 – carbon concentration in steel, $c_{\gamma\alpha}$ – equilibrium carbon concentration at the γ/α interface, $\mathbf{x}$ – vector of coordinates, $\mathbf{x}_\xi$ – position of the interface, $\mathbf{n}$ – unit vector normal to the boundary, Ω_γ – domain of the solution, which is the austenite grain, Γ_{GB} – boundary between austenite grains, Γ_{IF} – γ/α interface.

Equation (10) was discretized in a typical FE manner (13). Application of the variational principle gives (Zienkiewicz et al., 2005):

$$\mathbf{Hc} + \mathbf{C}\frac{\partial}{\partial t}\mathbf{c} = \mathbf{p} \tag{12}$$

where: $\mathbf{c}$ – vector of nodal values of concentration, $\mathbf{H}$ – diffusion matrix, $\mathbf{C}$ – geometrical matrix.

Matrices $\mathbf{H}$ and $\mathbf{C}$ and vector $\mathbf{p}$ are calculated as:

$$H_{ij} = \int_{\Omega_\gamma} (\nabla n_i)^T D(\nabla n_j) d\Omega_\gamma$$
$$C_{ij} = \int_{\Omega_\gamma} n_i^T n_j d\Omega_\gamma \qquad p_i = 0 \qquad (13)$$

where: n_i – shape functions in the FE method.

Application of the Galerkin time integration scheme results in a set of equations:

$$\hat{\mathbf{H}}\mathbf{c} = \hat{\mathbf{p}} \qquad (14)$$

where:

$$\hat{\mathbf{H}} = \left[2\mathbf{H} + \frac{3}{\Delta t}\mathbf{C}\right] \quad \hat{\mathbf{p}} = \left[-\mathbf{H} + \frac{3}{\Delta t}\mathbf{C}\right]\mathbf{c}_i \qquad (15)$$

Δt – time step.

Solution of equations (14) allows to calculate distribution of the carbon concentration in the austenite grain at the end of the time step Δt when this distribution at the beginning of the time step is known.

of the interface is controlled by the mass balance, assuming constant carbon concentration in ferrite:

$$\int_{\Omega_\gamma} \left[c(x) - c_0\right] d\Omega_\gamma > (c_0 - c_\alpha)\Omega_\alpha + \Delta c \qquad (16)$$

where: Ω_γ, Ω_α – domain of the austenite and ferrite grain, respectively, c_α – carbon concentration in ferrite, Δc – increment of the concentration, which determines when the interface should be moved.

Value of the Δc is chosen that way, that realistic motion of the boundary is obtained. When the inequality (16) is true, the boundary is moved to a new position located along the concentration isoline close to this boundary. The isoline is selected by the programmer.

The volume fraction of the ferrite F_f is calculated as the ratio of the area covered by the ferrite to the area of the primary austenite grain. The fraction of austenite–ferrite transformation X is defined as:

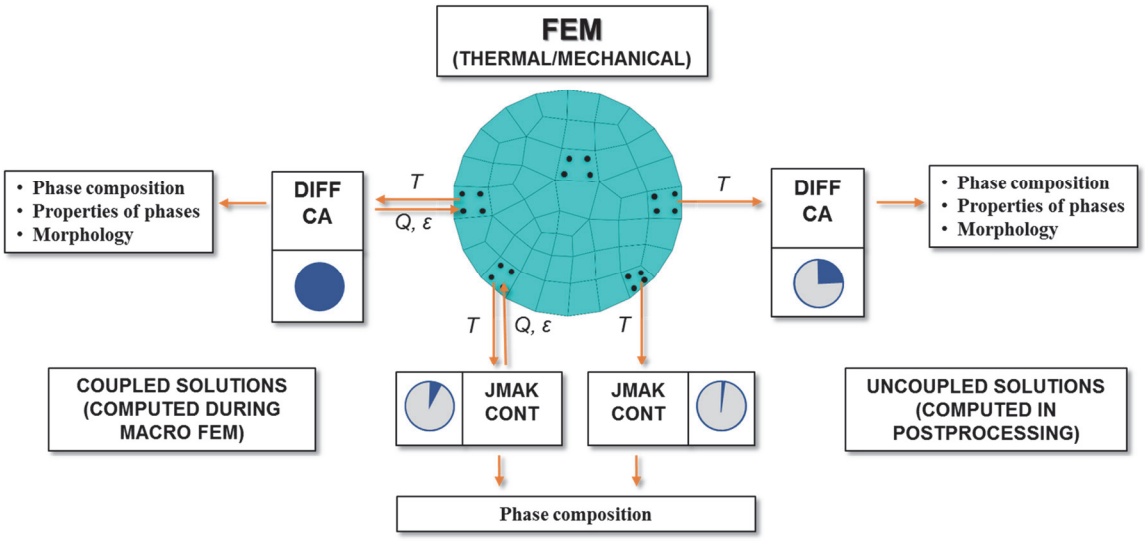


Fig. 2. *Schematic illustration of the computing costs of multiscale models depending on the connection between scales.*

Determination of the position of the interface boundary, which varies in time, is defined as Stefan problem. The front-tracking method was used by Pernach and Pietrzyk (2008) to solve numerically the Stefan problem and it resulted in unrealistic shape of resulting ferrite grains. Therefore, the method based on concentration isolines was proposed by Pernach et al. (2014) and was used in the present work. In this approach diffusion is solved on the stationary mesh and the mass balance is checked at each time step. In a numerical solution a motion

$$X = \frac{F_f\left(c_{\gamma\alpha} - c_0\right)}{\left(c_{\gamma\alpha} - c_\alpha\right)} \qquad (17)$$

When the temperature drops below bainite start temperature B_s, bainite transformation is simulated Following this, martensite transformation is simulated below the martensite start temperature M_s. Equations describing bainite and martensite transformation in the present model are presented by Pietrzyk and Kuziak (2012).

3. COMPUTING COSTS IN MODELLING OF MATERIALS PROCESSING

Problems of computing costs in modelling of materials processing have been in the field of interest for scientists for a few decades now. It is due mainly to the fact that simulations of processing of materials usually require multiscale models, which describe multiphysical phenomena (Pietrzyk et al., 2015). Accounting for various dimensional scales may have significantly different influence on computing costs, depending on the type of the connection between the scales, what is schematically shown in figure 2. Feedback from the micro scale to the macro scale is the main factor influencing the computing costs.

Uncoupled solutions, which do not need feedback from micro to macro scales, do not require long computing times. Micro scale calculations can be usually performed as post processing, what fosters application of the distributed computing methods. Thus, application of discrete micro scale models (CA, DIFF) does not lead to very long computing times. Contrary, when feedback from micro to macro scale is needed (coupled solutions), micro scale calculations have to be performed on-line at each Gauss point of the macro scale. It leads to very long computing times. Increase of the computing times in fully coupled solutions depends on whether only thermal or also mechanical feedback is needed. In the former case an increase of the computing time is acceptable and application of the discrete models in the micro scale (CA, DIFF) leads to long but reasonable computing times. In the case of mechanical feedback (dilatometric strains) the computing times raise to not acceptable level and only very simple micro scale models can be used.

Discussion presented above shows that computing costs of multiscale modelling can vary significantly. In fully coupled solution these costs may increase to an unacceptable level. Therefore, an extensive research on possibilities of reduction of costs of multiscale modelling have been performed and numerous papers in this field have been published. Among various methods of reduction of computing costs the following should be mentioned:

- Reduced order modelling (ROM) techniques (Quarteroni & Rozza, 2014). High performance reduced order modelling (HPROM) techniques have been proposed recently (Pereira et al., 2014).
- Simplification of the microstructure by using statistically similar representative volume element – SSRVE (Schroeder et al., 2011).
- Metamodelling (Pietrzyk et al., 2016).
- Variant optimization, which uses knowledge of experts to reduce the search domain in optimization (Skóra & Pietrzyk, 2014).
- Reduction of multidimensionality by application of sensitivity analysis and methods based on principal component analysis (Bachniak et al., 2016).
- High performance computing (HPC) and distributed computing (Krol et al., 2016).

4. CASE STUDIES

Three optimization tasks, which require multiscale models, were considered. These tasks differed significantly as far as application of feedback in multiscale models is needed.

4.1. Intercritical continuous annealing

This is the simplest process regarding the macro scale. It is applied to thin strips (below 1 mm), in which through thickness temperature variations are negligible. Beyond this, the strip temperature is controlled by the continuous annealing equipment. Therefore, macro scale calculations are not needed and optimization of the process can be effectively performed using advanced micro scale models. The results obtained using DIFF and CA models are presented below and they are compared with the optimization based on the JMAK and CONT models.

4.2. Laminar cooling and coiling

Laminar cooling is performed after hot rolling for strips with the thickness of few millimetres. Therefore, through thickness temperature variations are of importance and FE calculations of temperature in the macro scale have to be performed. Beyond this, when calculations of residual stresses are needed, thermal-mechanical FE model has to be used. Two case studies for laminar cooling were considered in the present paper. The first was prediction of phase composition in products. The second was prediction of residual stresses after cooling and coiling. Multiphase advanced high strength steel (AHSS) was investigated in the former case.

4.2.1. Optimization of phase composition

Typical laminar cooling system is presented schematically in figure 3. Number of boxes in each zone is given in this figure. Each box is 1 m long what gives the ength of each section of 40 m. Notation in figure 3: T_f – finishing rolling temperature, T_{fmax} – temperature of the maximum rate of the ferrite transformation, T_c – coiling temperature, d – distance between the sections of the laminar cooling (20 m in the present work), v_6 – exit velocity from the last stand, t_p – time between the two sections of the laminar cooling, Numbers of boxes and maximum water flux (W) in the subsequent zones of the laminar cooling system are given in table 1. Parameters of the laminar cooling were taken from one of the existing modern hot strip mills.

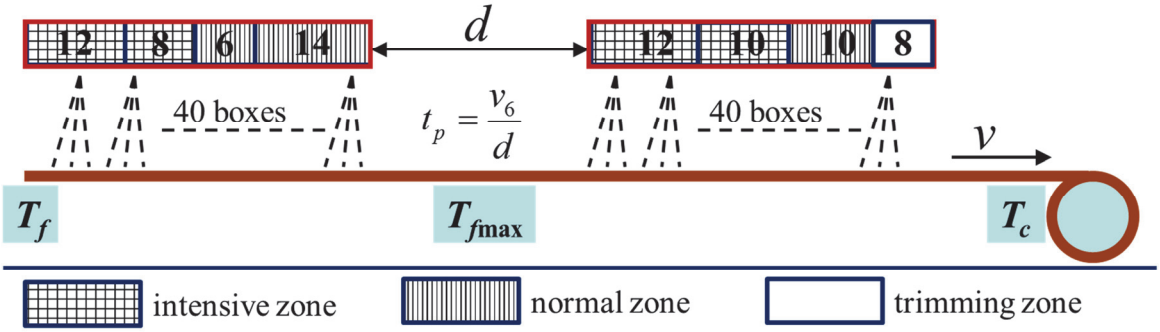


Fig. 3. *Schematic illustration of a typical laminar cooling system.*

Table 1. *Number of boxes and maximum water flux in the subsequent zones of the laminar cooling system (I – intensive zone, N – normal zone, T – trimming zone)*

Zone	1 I	2 I	3 N	4 N	5 I	6 I	7 N	8 T
Boxes	12	8	6	14	12	10	10	8
W, m^3/h	860	580	300	680	860	860	340	250

Multiphase structure is obtained by control of the ferritic transformation. Accelerated cooling is applied to the temperature of the lowest stability of austenite (about 670-720ºC). Slow cooling proceeds until the required volume fraction of ferrite is obtained. Once this is achieved, fast cooling is applied to transform the remaining austenite to bainite and/or martensite. Practical realization of this scheme in laminar cooling is difficult. Cooling rates depend on the thickness of the strip after the last stand (h_6) and on the strip velocity (v_6) what complicates selection of water fluxes in subsequent zones of the laminar cooling. Therefore, application of the optimization techniques to design laminar cooling schedule for DP steels is a part of the simulations of the manufacturing chain for these steels, what was the objective of the work (Kuziak & Pietrzyk, 2011). Three approaches to simulation of laminar cooling were used in the present work. In all approaches 2.5D FE code was used to calculate temperatures at the cross section of the strip. In this model 2D thermal problem is solved at the cross section, which is moving with the actual strip velocity. Relevant boundary conditions are applied to the surface of the strip depending on the current location of the cross section, see Lenard et al. (1999).

Optimization task for the laminar cooling was formulated by Pietrzyk et al. (2014) and it is also discussed in book publication (Pietrzyk et al., 2015). In the present work the optimization was performed for the strip with the thickness of 4 mm and for the exit velocity of 7.5 m/s and 6 m/s. Steel composition was 0.095%C, 1.51%Mn, 0.23%Si, 0.41%Cr and 0.05%Mo. The objective function was to obtain 73% of ferrite and as low as possible amount of bainite:

$$\Phi = \sqrt{w_f \left(F_f - 0.73\right)^2 + w_m \left(F_m - 0.27\right)} \quad (18)$$

where: Ω_γ, Ω_α – domain of the austenite and ferrite grain, respectively, F_f, F_m – volume fractions of ferrite and martensite, respectively, w_f, w_m – weights.

Water fluxes in subsequent zones of the laminar cooling were the design variables. Optimization performed using simplex method yielded the results in table 2. Changes of the temperature and kinetics of transformation for the optimal cycles are shown in figure 4. It is seen that exactly 73% of ferrite was obtained in both cases and that the volume fraction of bainite was below 4%. Maximum water flux in the second section had to be applied in both considered cases.

Table 2. *Optimal water flux [m^3/h] in the subsequent zones of the laminar cooling system for the strip velocity 7.5 m/s and 6 m/s.*

velocity	1 I	2 I	3 N	4 N	5 I	6 I	7 N	8 T
v_6 = 7.5 m/s	430	174	30	68	860	860	340	250
v_6 = 6.0 m/s	344	104	30	68	860	860	340	250

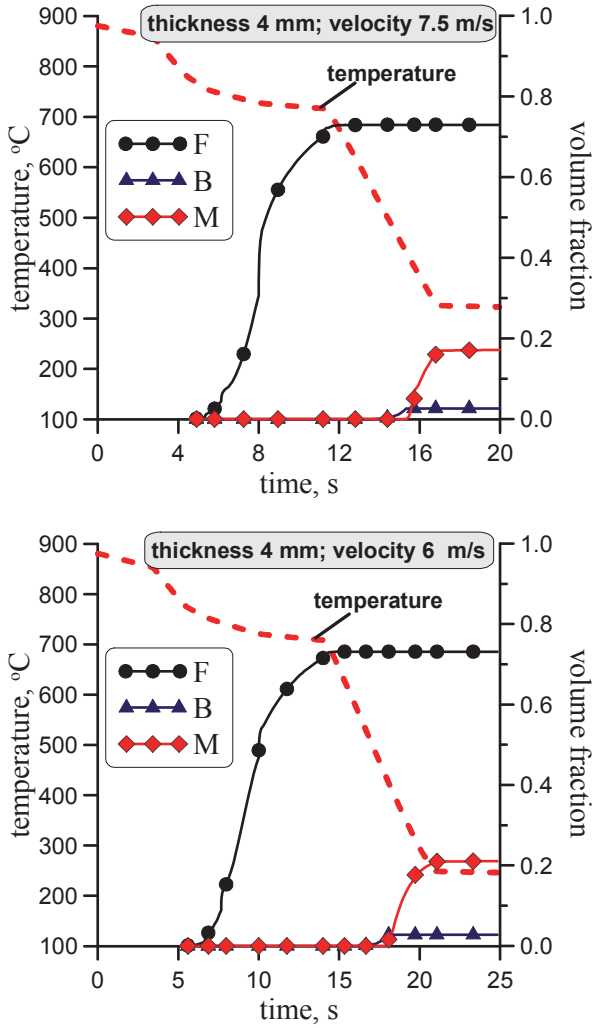


Fig. 4. *Kinetics of transformations for the optimal laminar cooling schedules for the exit velocity 7.5 m/s (up) and 6 m/s (down).*

4.2.2. Optimization of residual stresses

Residual stresses in strips after hot rolling may cause different problems during manufacturing of steel products. These stresses become of practical importance when the laser cutting of strips is applied. The stresses are caused by inhomogeneous temperatures and phase transformations during cooling, therefore, the laminar cooling parameters should be optimized with the minimum of residual stresses being the objective function. To reach this goal a model of residual stresses in hot-rolled strips was developed and validated (Milenin et al., 2016b). The model was based on thermo-elastic-plastic FE calculation of deformations in hot rolled strips during laminar cooling and in the coil. Elastic-plastic properties of the material were determined experimentally using tests on GLEEBLE 3800. Industrial testing of residual stress in strips after cooling in coil was performed and measurement of these stresses in strips was carried out using the X-ray diffraction method

To solve this optimization task 3D thermal-mechanical FE calculations have to be performed in the macro scale and phase transformations have to be simulated in the microscale. Dilatometric strain due to phase transformation has to be returned as feedback to the FE macro code. It led to extremely large computing task. Two actions were made to reduce the computing cost. The first was selection of the simple JMAK model of phase transformation. The second was substituting the FE model by simplified approach, in which the strip is represented as a set of bars (Milenin et al., 2013). This approach is based on the assumption that all components of the stress tensor except tension along the length of the strip are zero and the strip can be presented in the form of the set of the rods, which are fixed at the ends (figure 5). In addition to the thermal deformation of each rod, all the rods are exposed to the average strain of the strip that is a result of the changing length of the strip in the cooling process. Thus, if in the rod i an increment of temperature and the corresponding increment of thermal deformation appear, the total increment of the deformation of the rod will be equal to $\Delta\varepsilon_i = \Delta\varepsilon_{mi} - \Delta\varepsilon_{ti} + \Delta\varepsilon_{di}$, where: $\Delta\varepsilon_m$ – strain increment due to mechanical deformation, $\Delta\varepsilon_t = \alpha\Delta T$ – strain increment due to thermal expansion, α – heat expansion coefficient, $\Delta\varepsilon_d$ – strain increment due to dilatometric effect caused by phase transformations (Wang et al., 2008). The average strain increment in the strip is:

$$\varepsilon_{av} = \sum_{i=1}^{N} \Delta\varepsilon_i \qquad (19)$$

where: N – number of rods.

The current stress increment in the rod i is determined by the difference between strain in this rod $\Delta\varepsilon_i$ and the average strain increment ε_{av}. Proposed beam model allowed to decrease the computing time by an order of magnitude.

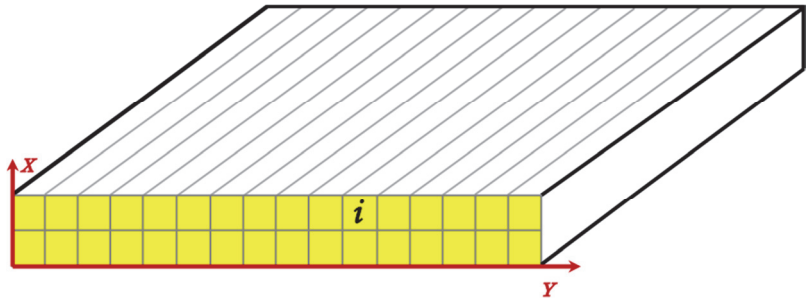


Fig. 5. Scheme of beam model of residual stresses in hot-rolled strips.

4.3. Controlled cooling of rails

When only optimization of the microstructure and properties of rails is needed, 2.5D FE calculations of the temperature distribution in the macro scale are satisfactory. The idea of this approach (Lenard et al., 1999) is similar as for the strip cooling in section 0. Detailed description of the controlled cooling system and formulation of the optimization task for this system are given by Szeliga et al. (2015) and are repeated in book publication (Pietrzyk et al., 2015). Briefly, a cyclic immersion hardening of the rail head, which enables more homogenous hardness to be achieved in the rail head, without the necessity of accurate control of the total time of heat treatment, was proposed by Kuziak and Zygmunt (2013). The rail head is inserted in the tank with the coolant directly after rolling, and initially the level of the solution is kept below the running surface level. The process of accelerated cooling starts when the rail head temperature reaches about 820°C. Then the pumps supply the solution to the tank, which leads to gradual immersion of the rail head. Keeping the head immersed for a longer period of time would lead to occurrence of the bainite in the microstructure. Therefore, the head is immersed cyclically into the polymer solution for short periods of time, after which part of the solution is removed from the tank, which brings its level below the running surface of the head and the rate at which heat is transferred to the environment from the head is substantially reduced. At this stage the heat is transferred from the hotter rail head centre to the surface and the temperature of the running surface increases. For the proper performance of the head hardening process, it is critical for the running surface temperature not to increase above 570°C. To prevent this, the coolant level is raised in the tank again and accelerated cooling stage is repeated. Sequence "accelerated cooling – cooling in still air can be repeated many times until the pearlite transformation is completed in the entire head. Proper selection of times is crucial to maintain low temperature of pearlitic transformation and to avoid danger that the running surface is cooled below the start temperature of the bainitic transformation (B_s) prior to the pearlitic transformation completion. The objective of the optimization is to design the cooling cycle, which allows to meet the conditions described above. The following objectives were formulated in the present work: i) maximum hardness and lack of bainite in the microstructure, ii) The uniform distribution of hardness at the head cross section.

$$\Phi_1 = \sqrt{\sum_{i=1}^{n_{gp}} \left(w_s S_{01}^2 + w_f F_{bi}^2 \right)}$$
$$\Phi_2 = \sqrt{\sum_{i=1}^{n_{gp}} \left(\frac{HB_i - HB_{ave}}{HB_i} \right)^2} \qquad (20)$$

where: S_0 – interlamelar spacing, n_{gp} - number of Gauss integration points in the rail head, w_s , w_f – weights, HB_{ave} – average hardness in the rail head, HB_i –hardness in the i^{th} Gauss point.

Kinetics of the phase transformations was determined using JMAK equation and interlamellar spacing was calculated using experimental model, see (Szeliga et al., 2015) for details. The micro scale calculations were performed at each Gauss points in the macro scale but due to simplicity of the models the increase of the computing time was negligible. Simulation of one case took about 2 – 5 min, depending on the number of immersions of the rail head. Optimization was performed using simplex method and the results are shown in table 3. Changes of the temperature calculated in the three locations at the cross section are shown in figure 6.

Table 3. *Optimal times of cooling in air (white) and in polymer solution (grey) for the objective functions in equation (20).*

cycle	1	2	3	4	5	6	7
times for Φ_1, s	30	15	17	14	10	11	the rest
times for Φ_2, s	30	32	15	12	15	8	the rest

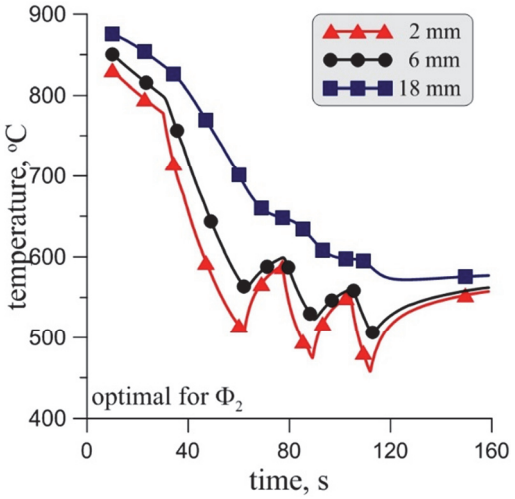


Fig. 6. *Changes of the temperature calculated in the three locations at the cross section: 2 mm, 6 mm and 18 mm from the top surface.*

Using the pearlitic transformation model based on the solution of the diffusion equation (Pernach, 2014) is an alternative for the JMAK equation. This model has much larger predictive capabilities, including possibility of determination of carbon distribution in front of the growing cementite plates. On the other hand, since the finite difference method was used to solve carbon diffusion equation, the computing times for this model are significantly larger and using this model at each Gauss iteration point is practically not justified. The best solution is performing optimization using JMAK micro scale model and then to calculate advanced microstructural parameters as post processing at few selected Gauss points, as it is shown by Pernach (2014).

Modelling of rail cooling in the present paper was constrained to prediction of microstructure and properties of the rail head, what needed thermal FE model only in the macro scale. It is, however, possible to extend the model and include predictions of thermal and dilatometric strains and stresses. Since it would require 3D FE thermal-mechanical solution in the macro scale, the computing costs would be very high. It should be pointed out that Aboauf et al. (1983) have proposed application of the 2D model to predictions of thermal and dilatometric strains and stresses in long products at much lower costs.

4.4. Forging and heat treatment of heavy crankshafts

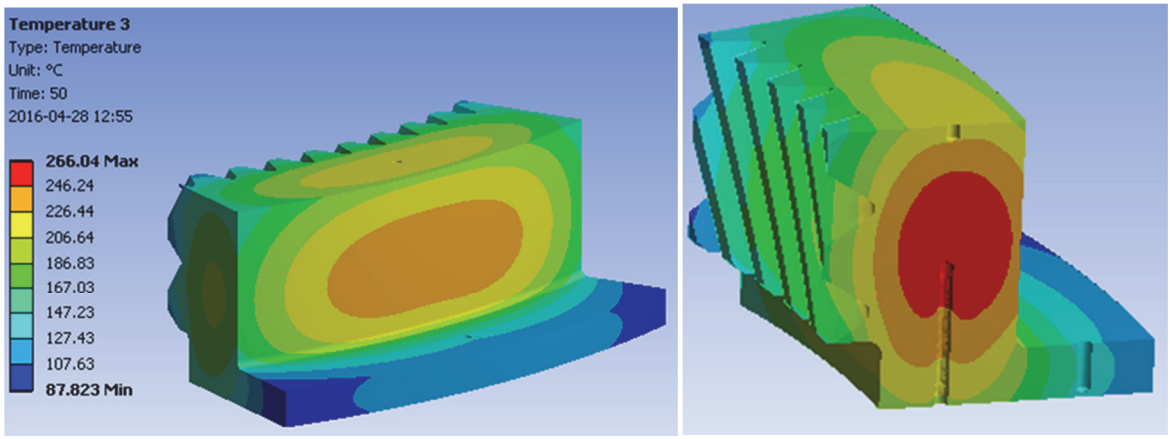
The manufacturing process for heavy crank shafts is composed of hot forging and heat treatment. Simulation of this process require complex 3D solution and is extremely time consuming. To perform optimization of this process Sztangret et al. (2011) developed metamodel of hot forging. Since it was assumed that microstructure does not influence the metal flow during forging, the uncoupled multiscale model was used and microstructural parameters were calculated at few Gauss points only during post processing. In consequence, optimization with respect to the two design variables (trajectories of tools) could be performed in a reasonable time. However, the manufacturing of large crankshafts can be affected by bending of the shaft during heat treatment, as well as at the forging step. Straightening of crankshafts is expensive and it affects organization of the production. For this reason, analysis of the curvature of the shaft at various stages of the technology is needed. Bending can occur during forging and heat treatment after forging. The aim of modelling is accounting for the elastic-plastic deformation of the shaft due to thermal expansion and dilatometric effect caused by phase transformations. Details of the model and several results of calculations are presented by Milenin et al. (2016a). In the present work this model was used to evaluate computing costs of multiscale simulation of manufacturing of crankshafts. Shaft material model was developed and the elastic-plastic characteristics were implemented in the FE code. Heat exchange with the cooling medium, dependence of thermal properties on temperature and heat of phase transformations were accounted for in a solution of the thermal problem. Dilatometric tests were performed to supply data for identification of the phase transformation model. The method of estimation of the curvature of the shaft with one design variable was proposed. Since calculations of the curvature required feedback from the micro scale to each Gauss point in the 3D FE in macro scale, the multiscale model had to be fully coupled and it was not possible to used more complex phase transformation model. Thus, JMAK model was used, see (Pietrzyk & Kuziak, 2012) for details of the numerical implementation of this model. This allowed performing optimization of

heat treatment in order to reduce the curvature of the shaft. The calculations were performed for several modes of the heat treatment. It was shown (Milenin et al., 2016a) that in the presence of phase transformations, cooling process is accompanied by a three-time changing of stress sign and the direction of bending of the crankshaft, which is due to the non-linearity of thermal deformation during the phase transformations. Variant optimization was applied to improve the forging and heat treatment technology. Few variants proposed by experienced technologists were simulated and the best variant was selected.

cific shape, requires a number of expensive laboratory tests. To support the design of the process, in the present work numerical simulations of the quenching process for gear wheels were performed. Details of the technological process as well as the description of the models are given in (Perzyński et al., 2016). Brief description of the model is given below.

Quenching is the most important heat treatment process for steel products used within jet engines. During these operations required microstructure is obtained. Unfortunately, these processes involve thermal strains and dilatometric strains and they

a)



b)

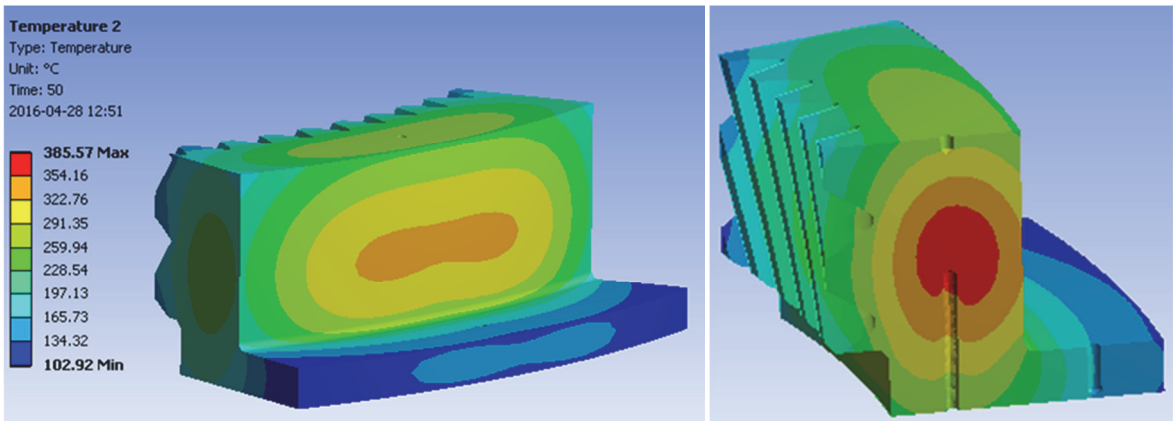


Fig. 7. *Temperature distribution in the gear wheel after 50 s of quenching calculated using model with (a) and without (b) phase transformation.*

4.5. Heat treatment of gear wheels

Metallic components manufactured by the airplane industry are often subjected to series of complicated thermo-mechanical treatments to obtain required in-use properties. These manufacturing cycles are subjected to very strict control defined by the world standards. Thus, designing a process that will lead to the expected product properties and specific shape, requires a number of expensive laboratory tests. To support the design of the process, in the present work numerical simulations of the quenching process for gear wheels were performed. Details of the technological process as well as the description of the models are given in (Perzyński et al., 2016). Brief description of the model is given below.

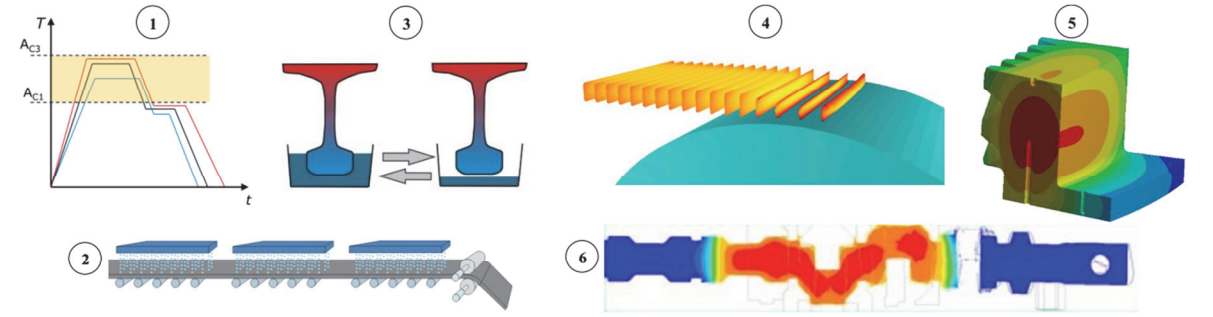
Quenching is the most important heat treatment process for steel products used within jet engines. During these operations required microstructure is obtained. Unfortunately, these processes involve thermal strains and dilatometric strains and they influence the final shape of the product. The objective of simulations was to design the process, which involves minimum of strains and allows to obtain components which meet strict geometrical requirements.

Due to complex shape and to sophisticated cooling in press, quenching of gear wheels is very complicated and it requires 3D thermal-mechanical FE model with a large number of elements. Both ther-

mal (heat due to transformation) and mechanical (dilatation strains) feedback is needed. Therefore, simple JMAK equation had to be used in the micro scale to obtain the solution in a reasonable time. Figure 7 shows temperature distribution in the gear wheel after 50 s of quenching calculated using model with and without phase transformations. It is seen that neglecting transformations leads to much lower temperatures at the cross section. Analysis of mechanical results showed that full model with phase transformations predicts larger strains and stresses. It is due to the fact that phase transformations in various parts of the wheel occur at different time and differences in dilatometric strains involve local plastic deformation.

5. DISCUSSION AND CONCLUSIONS

Six manufacturing processes based on metal forming and heat treatment were investigated. Accounting for phase transformations was common feature for these processes and multiscale models were used in all cases. Results of the analysis of the computing costs are presented schematically in figure 8. Comparison of various approaches shows that single point microstructure evolution models like JMAK do not cause a noticeable increase of the computing costs. Fully coupled simulations of very complex processes like forging of the crankshaft or heat treatment of the gear wheal were possible and



Process	1. Continues annealing	2. Laminar cooling	3. Heat treatment of rails	4. Residual stresses in stripps	5. Heat treatment of gear wheels	6. Forging of heavy crank shafts
Thermal	——	2D FE	2D FE	2D FE	3D FE	3D FE
Mechanical	——	——	2.5D FE (optional)	simplified	3D FE	3D FE
Simulation costs	——	1 min	5 min	5 min	11 h	25 h
Simulation costs (with phase transformations) — JMAK	5 s	1 min	5 min	5 min	21 h	35 h
Simulation costs (with phase transformations) — CA	5 min	20 min	60 min	very long	not acceptable	not acceptable
Simulation costs (with phase transformations) — DIFF (50 grains)	15 min	50 min	250 min	very long	not acceptable	not acceptable

Fig. 8. *Comparison of computing costs for various optimization tasks.*

Results of all simulations showed that quenching is sensitive to applied cooling conditions. The faster the cooling is the more inhomogeneous material behaviour is. This is related to occurrence of phase transformation in different regions of the ring at different times, what affects its mechanical response. Slow cooling provides more uniform material response, however inappropriate properties are obtained. Future work will be focused on application of the developed model to design a special cooling equipment that will provide a possibility to properly cool different sections of the investigated ring to minimise geometrical defects and to provide required properties.

distributions of phase composition in the final product were calculated.

Contrary, when RVE models of phase transformation are needed, full coupling with the FE codes leads to very long computing costs. Such phase transformation models as Cellular Automata or solution of the diffusion equation (phase field) when attached to each node of the FE mesh would lead to not acceptable computing times. Selection of the neuralgic points in the domain and performing micro scale calculation in these points only is an option, which is commonly used.

In the case of processes, which do not require complex 3D solutions, RVE models can be efficiently connected with the FE codes. Laminar cooling of

strips or controlled cooling of rails can be accurately simulated using reasonably simple 2D mesh at the cross section of products. In the continuous annealing process strip thickness is small and there is no need to calculate temperature distribution through the thickness. Therefore, complex RVE phase transformation models can be used efficiently.

ACKNOWLEDGEMENTS

Financial support of the NCN, project no. 2014/15/B/ST8/00187, is acknowledged.

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STRATEGIA WYBORU NAJLEPSZEGO MODELU PRZEMIAN FAZOWYCH W SYMULACJACH PRZETWÓRSTWA METALI

Streszczenie

Połączenie programu z metody elementów skończonych (MES) z modelem przemian fazowych jest niezbędne, kiedy potrzebna jest informacja o rozkładzie składu fazowego w wyrobie gotowym. W zależności od rodzaju modelu przemian fazowych takie połączenie może pociągać za sobą bardzo długie czasy obliczeń. Ponadto, kiedy dodatkowo musi zostać sformułowane i rozwiązane zadanie optymalizacyjne, koszty obliczeń mogą jeszcze radykalnie wzrosnąć. Jest to szczególnie kłopotliwe, kiedy funkcja celu zawiera zaawansowane parametry mikrostruktury lub własności wyrobu, których obliczenie wymaga zastosowania modelowania wieloskalowego. W niniejszej pracy analizowano możliwości skrócenia czasów obliczeń związanych z optymalizacją procesów przetwórstwa metali. Porównano czasy obliczeń dla symulacji różnych procesów, w których potrzebne jest połączenie MES z modelami przemian fazowych. Oceniono efektywność modelowania w zależności od złożoności siatki MES w skali makro.

Received: March 20, 2017
Received in a revised form: April 13, 2017
Accepted: April 17, 2017