THE STRATEGY FOR EFFICIENT MODELLING OF PHASE TRANSFORMATIONS IN MATERIALS PROCESSING

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1. Introduction

Computer aided design of materials processing is common now. Beyond one step processes, whole manufacturing chains are simulated [1]. 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 to calculate 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 [2]. Moreover, when objective function is composed of microstructural parameters or product properties, application of multi scale modelling is needed and computational costs are further increased. In the present paper the possibilities of decreasing the computation costs for optimization of materials processing were explored. The particular emphasis is put on processes, in which phase transformations are used to control properties of steel products.

2. Computing costs in modelling of materials processing

Problems of computing costs in modelling of materials processing has been in the field of interest for scientists for a few decades now. It is due mainly to the fact that usually multiscale models require, which describe multiphysical phenomena. Among methods of reduction of computing costs the following should be mentioned: i) reduced order modelling (ROM), ii) Simplification of the microstructure by using statistically similar representative volume element – SSRVE, iii) metamodelling, iv) variant optimization, which uses knowledge of experts to reduce the search domain in optimization, v) high performance computing (HPC) and distributed computing.

The present work is focused on processes, in which modelling of phase transformations is essential. Five industrial processes were analysed: i) laminar cooling of strips, ii) intercritical continuous annealing, iii) forging of heavy forgings, iv) heat treatment of gear wheels, v) controlled cooling of rails. Computing times for phase transformations models differ significantly, sometimes few orders of magnitude. Therefore, a reduction of the computing costs can be obtained by carefully considered selection of the model adequately to the investigated optimization task.

3. Phase transformation models.

Three phase transformation models were investigated. The first is based on the control theory and kinetics of transformation is calculated by a solution of the second order differential equation:

(1)
$$B_1^2 \frac{d^2 X}{dt^2} + B_2 \frac{dX}{dt} + X = \frac{F_{f\max T}}{F_{f\max}}$$

where: $F_{f\max T}$, $F_{f\max}$ – maximum volume fraction of ferrite in temperature T and A_{e1}, respectively. Equation (1) describes second order inertia term. Time constant B_1 is responsible for the delay of the response (nucleation) and B_2 for the rate transformation [3]. The second model (called DIFF in the paper) was based on the solution of the diffusion equation in the domain representing microstructure of steel and the third model was the cellular automata (CA) approach. The two latter models are described in [4]. Figure 1 shows possibilities of connections between FE thermal-mechanical code and the phase transformation model.

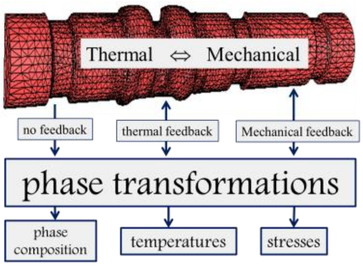

Fig. 1. Possible roles of phase transformation models

The role of this model determines its selection. Thus, since mechanical part is not needed for laminar cooling or continuous annealing, computationally costly CA or DIFF models could be used. If the thermal feedback is needed, then transformation model has to be solved at each FE node and CA or DIFF models involve long computing times. Using of CONT model is advised in modelling of heat treatment of gear wheel or manufacturing of heavy crank shafts. Simulations for all considered processes were performed in this work but the results for heat treatment of gear wheels only are presented. Selected results for other investigated processes can be found elsewhere, see case studies in [4].

Modelling of heat treatment of gear wheels is the most computationally demanding. It is due to very complex geometry which requires large number of elements (few millions) and to necessity of calculations of thermal and dilatometric stresses. The latter requires solution of the thermo elastic problem at each node and, additionally, calculation of dilatation due to phase transformations. Calculated temperatures after 600 s and plastic strains are shown in Figure 2. Comparison of computational costs for all investigated processes is shown in Figure 3.

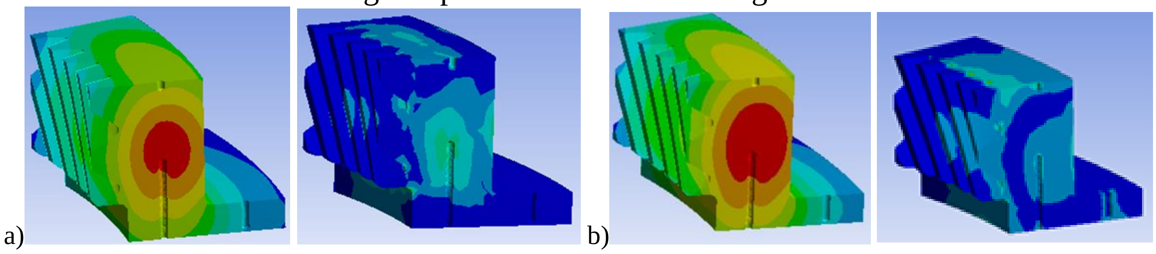

Fig. 2. Temperatures (left) and plastic strains (right) for calculations not accounting (a) and accounting (b) for phase transformations.

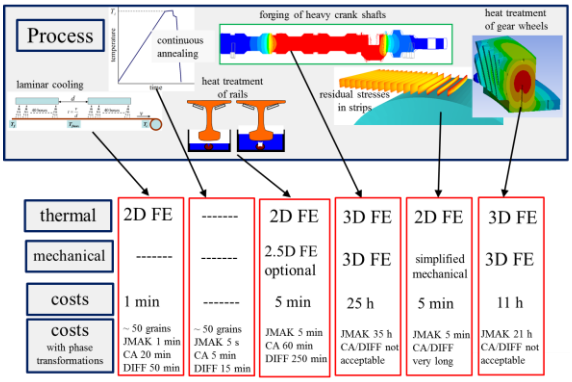

Fig. 2. Computational costs for the investigated processes.

5. Conclusions

Modelling phase transformation is crucial in simulations of manufacturing of steel products. Multiscale approach has to be applied with FE or alternative method in macro scale. Feedback from micro to macro scale is a criterion for the selection of the micro scale model. When feedback is needed (dilatometric strains, heat of transformations) then application of discrete micro scale models becomes extremely costly. When it is not needed, micro scale calculations can be performed as post processing. CONT model appeared very efficient for optimization with respect to phase composition.

6. References

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