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INTERNAL VARIABLE AND CELLULAR AUTOMATA – FINITE ELEMENT MODELS OF HEAT TREATMENT

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ABSTRACT

Heat treatment is one of the most important processes in advanced steel products manufacturing. While production processes are still being optimised, numerical modelling of heat treatment is very useful. Finite Elements Method (FEM) is widely used in these cases, due to its proved potential for modelling of continuous, macroscopic phenomena. However, its capability to simulate microscale and non-continuous processes is very limited. Introducing empirical model of phase changes into FEM, usually based on Internal Variable Method (IVM) is useful when the information about volume fraction of the phases in the domain and stresses due to phase change satisfies the requirements. Notwithstanding, it is difficult to obtain information in-depth about microstructure during heat treatment, because it requires more sophisticated description of phase change process. Those problems can be resolved with multiscale modelling. One of the current approaches in this field employs FEM for computing of temperature, stress and strain fields, while non-continuous, microscale model is based on Cellular Automata (CA) method [1]. Recently, several CA models concerning phase transformation have been proposed, e.g. [2]. In this paper Cellular Automata – Finite Elements (CAFE) is applied for modelling of both macroscopic and microscopic influence of heat treatment. It also takes into account a stochastic character of processes, which is hard to obtain in typical FEM or IVM solution.

The advantage of CAFE model ensues from direct representation of microstructure. Although the current microstructural CA model is two-dimensional, it reproduces topological and morphological relations between components of microstructure. The state of CA cells is updated synchronically in consecutive time steps. Every cell includes state vector representing fractions of all phases. Thermodynamics of phase transition is a base for a rule-based knowledge representation in the CA model. However, the nondeterministic definition of neighbourhood and probabilistic energy

transition is introduced. As a result, the distribution of grain sizes and volume fractions in FE integration points is calculated by CA model.

Implementation of the IV and CAFE methods to modelling of heat treatment of steel parts for aerospace industry is the objective of the paper. FEM model, which simulates thermal and mechanical phenomena, is based on the commercial ADINA software. In the IV based simulation, phase change model is introduced as user procedures. Empirical equations for bainite and martensite fraction, with parameters determined from dilatometric tests, are used. The microstructural CA code was developed by the Authors and is coupled with the FE solution according to the CAFE assumptions.

Comparison of macroscopic predictions of both models is discussed in the paper, as well as results of microstructure development simulation from the CAFE model. Results of the computations based on the IV model of heat treatment process (steel, starting from 820^{o}C in quenching oil) are presented below. Variations of bainite and martensite fraction in time are presented in fig. 1. Fig. 2 shows distribution of bainite and martensite in chosen time step. Effective stress and accumulated plastic strain results are presented on fig. 3.

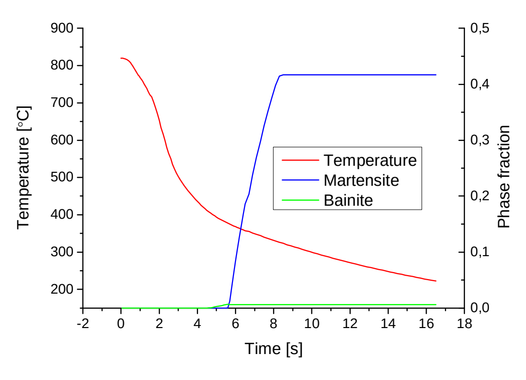
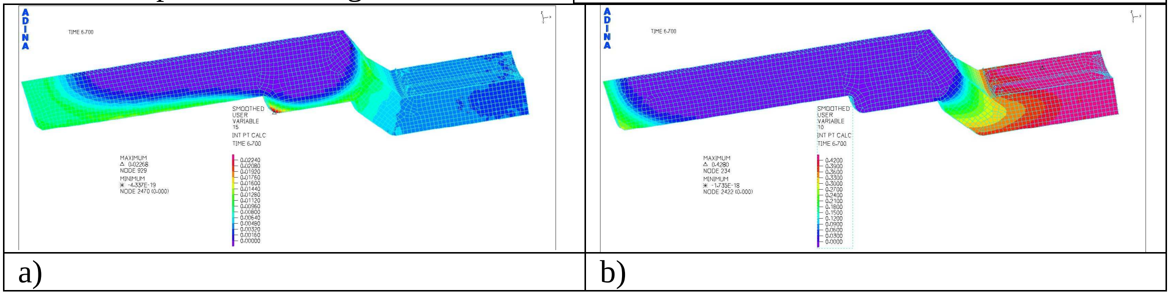


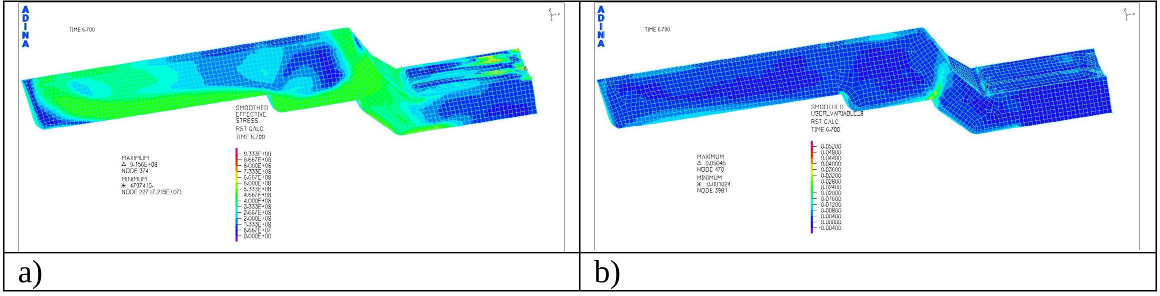
Fig. 1. Variations of bainite and martensite fraction in time



a)

b)

Fig. 2. Bainite (a) and martensite fraction at time 6.7 s



a)

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Fig. 3. Effective stress (a) and accumulated plastic strain at time 6.7 s

REFERENCES

[1] J. Gawąd and M. Pietrzyk, “Application of CAFE multiscale model to description of microstructure development during dynamic recrystallization”, *Arch. Metall. Mater.*, Vol. **52**, pp. 257-266, (2007)

[2] Y.J. Lan, N.M. Xiao, D.Z. Li and Y.Y. Li, “Mesoscale simulation of ferrite transformation from deformed austenite during continuous cooling in a C-Mn steel using a cellular automaton method”, *Comp. Mat. Sci.*, Vol. **32**, pp. 147-155, (2005)