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Rafal GOLAB[1]
Lukasz MADEJ[1]
Maciej PIETRZYK[1]

THE COMPLEX COMPUTER SYSTEM BASED ON CELLULAR AUTOMATA METHOD DESIGNED TO SUPPORT MODELLING OF LAMINAR COOLING PROCESSES

The user friendly computer system that have the capability of modelling material behaviour both at the macro and micro scales was developed in this work. The system was designed to predict microstructure evolution during phase transformation in laminar cooling conditions with the use of the multi scale cellular automata finite element (CAFE) model. The finite element (FE) part is based on the conventional Fourier type equation and is used to predict macroscopic temperature distribution. This is an input for the micro scale cellular automata (CA) model of austenite-ferrite phase transformation. To facilitate the research, proposed micro scale CA model was implemented within developed universal object-oriented programming framework CAF. Description of major assumptions and functionality of the developed numerical system including efficient Graphical User Interface (GUI) is presented in the paper. The intuitive visualization of data obtained in different length scales facilitates work with the software.

1. INTRODUCTION

The main problem in computer modelling systems is to realistically describe the phenomena occurring in materials at micro scale level under the complex thermal or mechanical processing conditions and at the same time provide an easy to use, user friendly numerical tool. In recent years many different numerical approaches with varying level of complexity were developed to describe phenomena occurring in materials (e.g., using Finite Element (FE) method to predict temperature distribution in different cooling conditions or using Cellular Automat (CA) method to simulate phase transformations, etc. [1],[2],[3]). When combined together, they can describe material behaviour in different length scales. Thus, these models create very complex multi scale numerical tools, however they require an expert knowledge for appropriate use. There are various approaches to multi scale modelling, that can be generally classified into two groups: upscaling and concurrent approaches, as seen in Fig. [4].

[1] AGH University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science, Cracow, Poland, E:mail: rgolab@agh.edu.pl

In the upscaling class of methods, constitutive models at higher scales are constructed from observations and models at lower, more elementary scales. By a sophisticated interaction between experimental observations at different scales and numerical solutions of constitutive models at increasingly larger scales, physically based models and their parameters can be derived at the macro scale, what is discussed in [5]. Methods of the computational homogenisation, e.g. [6], are considered to belong to this group of methods. Since in these approaches the micro models are connected to particular integrations points, solution at the micro scale level is usually insensitive to the mesh density at the macro scale. The upscaling models, can be uncoupled or fully coupled. Thus, information is passed between scale only in one or two directions, respectively.

In the concurrent multiscale computing, one strives to solve the problem simultaneously at several scales by an a priori decomposition. Two-scale methods, whereby the decomposition is made into coarse scale and a fine scale, are usually considered [7].

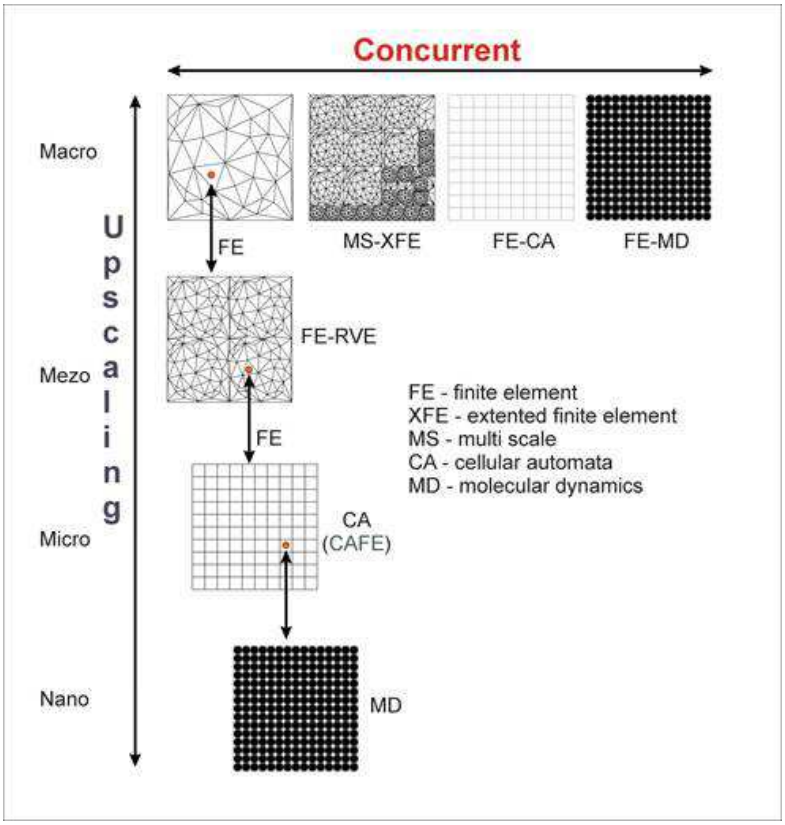

Fig. 1. Classification of the concurrent and upscaling multiscale models [4]

Multi scale numerical models are becoming increasingly more often applied to support not only scientific investigations but also applied research dedicated for industrial partners. These models provide a wide range of possibilities in analysis material behaviour under industrial conditions in subsequent length scales. However, their practical application is still limited by the fact that modelling with these methods usually requires cooperation between engineers working in industry and scientists responsible for model development and implementation. That inspired the authors to create a complex multi scale computer system,

which combines the simulation of phenomena at the macro and micro scales, but remains easy to use and user-friendly at the same time. As a case study, a multi scale numerical model of laminar cooling process often used in industry to control final microstructure and product properties was developed. Laminar cooling allows the control of the phase transformation mechanisms in the material after hot rolling. It involves the cooling of the material by spraying the top and bottom surfaces with water at the appropriate pressure using sets of cooling boxes. The proposed numerical approach is based on the cellular automata finite element (CAFE) method [8],[9],[10],[11]. At this stage of the research an uncoupled upscaling multi scale model was created. Information from the conventional macro scale finite element simulation of heat transfer during cooling is used as boundary conditions for the micro scale cellular automata model of phase transformation occurring during cooling. As a result, users obtain not only global information on temperature profile across the sample but also corresponding microstructure morphology, which is of importance to properly design the final material properties.

Basis of the macro and micro scale models developed for the purposes of this research are presented next.

2. MODELS

The finite element model is used to predict temperature gradients occurring during laminar cooling operations. The temperature changes are calculated by the FE solution on the basis of the Fourier heat transfer equation:

$$\nabla k(T)\nabla T + Q(T) = c_p(T)\rho(T)\frac{\partial T}{\partial t} \tag{1}$$

where: $k(T)$ – conductivity, $Q(T)$ – heat generation rate due to transformation, $c_p(T)$ – specific heat, $\rho(T)$ – density, T – temperature, t – time.
The following boundary conditions were used in the solution:

$$k\frac{\partial T}{\partial \mathbf{n}} = \alpha(T_a - T) \tag{2}$$

where: α – heat transfer coefficient, T_a – surrounding temperature or tool temperature, n – unit vector normal to the surface.

Discretization of the problem is performed in a typical finite element manner [12]. Heat transfer coefficient α for the air cooling was calculated using combined convection/radiation equation. Due to the influence of a number of random phenomena, determination of the heat transfer coefficient for the water cooling is a complex problem. This part takes into account influence of number of cooling boxes used during laminar cooling. In the present work this coefficient was determined on the basis of research described in [13]. Heat exchange was measured for various conditions and the following equation was proposed by approximation of the experimental data:

$$\alpha = 3.15\times10^{6}\,\dot{w}^{0.616}\left[700+\frac{T-700}{\exp(0.1T-70)+1}\right]^{-2.455}\left[1-\frac{1}{\exp(0.025T-6.25)+1}\right] \tag{3}$$

where:

$\dot{w}$ – water flux rate.

This method of calculation of the heat transfer coefficient was successfully applied in [14] to simulation and optimization of the laminar cooling of hot rolled strips, thus it was used in the present work as the basis for the user friendly multi scale model.

Results in the form of temperature distribution across the investigated sample at the macro scale in subsequent time steps are then an input for the concurrent simulation of phase transformation evolution. Data transfer protocol is based on detailed information of temperature changes, in particular locations across the sample. The microstructure evolution at the micro scale level is predicted by the developed CA model, which is designed to simulate austenite – ferrite transformation during cooling [15],[16].

In the developed model, each CA cell is described by several state and internal variables in order to properly describe physical state of the material. The cell can be in three different states: ferrite (α), austenite (γ) and ferrite-austenite (α/γ), as shown in Fig. 2. The last state is used to describe CA cells located at the interface between austenite and ferrite grains. Additionally, internal variables are defined to describe other necessary microstructure features. Cells contain information e.g. how many ferrite phase is in a particular cell $f_{i,j}$, what is the carbon concentration in each cell $C_{i,j}$, the growth length $l_{i,j}$ of the ferrite-austenite cell into the austenite cell or the growth velocity $v_{i,j}$ of the interface cell. The major governing equation that controls the phase boundary movement is a product of the phase transformation driving force and the phase boundary mobility:

$$v = MF = M_0 D(T) F = M_0 D_0 \exp\left(\frac{Q}{RT}\right) F \tag{4}$$

where:

M_0 – mobility coefficient, T – absolute temperature, D_0 – diffusion coefficient.

The driving force for the phase transformation F is a sum of the mechanical driving force F_{mech} and chemical driving force F_{chem}. The former, related with the influence of plastic deformation, is neglected in the present model. The latter is due to the differences in the carbon concentration in equilibrium conditions and actual carbon concentration in each cell:

$$F_{chem} = \beta(C_{eq}(T_i) - C_{i,j}^{\gamma}) \tag{5}$$

where:

β – model coefficient, C_{eq} – equilibrium carbon concentration calculated using Thermocalc software, $C_{i,j}$ – carbon concentration in the (i,j) CA cell.

These internal variables are used in the developed transition rules to replicate mechanisms of phase transformation. Two major parts of the model are defined to describe nucleation and growth of the ferrite grains into the austenitic matrix. The detailed

description of discussed model is available in [15],[16]. Similar solutions with different level of complexity are more often used to solve metallurgical problems, see e.g. [17].

Presented above finite element and cellular automata numerical models, are the core of the developed user friendly system that is described in the following chapter.

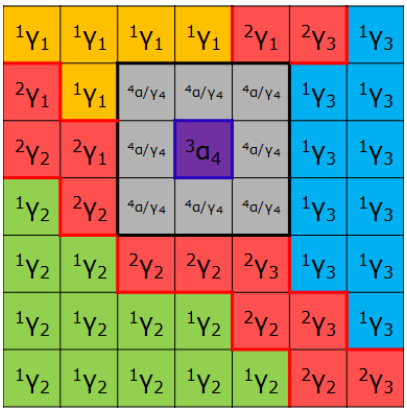

Fig. 2. Illustration of the nucleus of the ferrite phase and the surrounding cells in the ferrite-austenite (α/γ) state

3. COMPUTER SYSTEM

In order to address as wide as possible group of potential users, the proposed complex multi scale computer system was designed for computers with Windows operating system. To obtain required level of user friendliness the C++ Managed programming language was selected for the implementation purposes. The CA phase transformation model was implemented within the Cellular Automata Framework (CAF) developed in [16],[18] and available in the form of the DLL library. The CAF allows to create microstructure models with pseudo-language that is easily understood by engineers who don't have programming skills. Below is a list of basic assumptions of the framework:

- framework is to serve primarily the construction of complex physical models,
- framework should be efficient and effective,
- framework has to be easy to use for people who don't know programming,
- CA Framework should work properly on different operating systems.

The FE solution was written in the Fortran language to obtain high computing efficiency and was also compiled into the form of DLL library. Finally, mentioned models, in the form of DLL libraries, are incorporated into the developed graphical user interface (GUI) that is used to provide all the necessary parameters and process conditions for users not familiar with the implementation issues (Fig. 3). As seen in Fig. Fig. 3, the main parameters for the FE part of the system, which can be easily modified and reset, are divided into two groups in the tab *Mesh properties*. The first deals with process conditions: initial temperature prior to cooling, shape and dimensions of the investigated sample and cooling schedules. The second contains material data: emissivity coefficients, heat exchange

parameters and initial grain size. The user interface allows to design several cooling stages, to provide required level of flexibility during modelling.

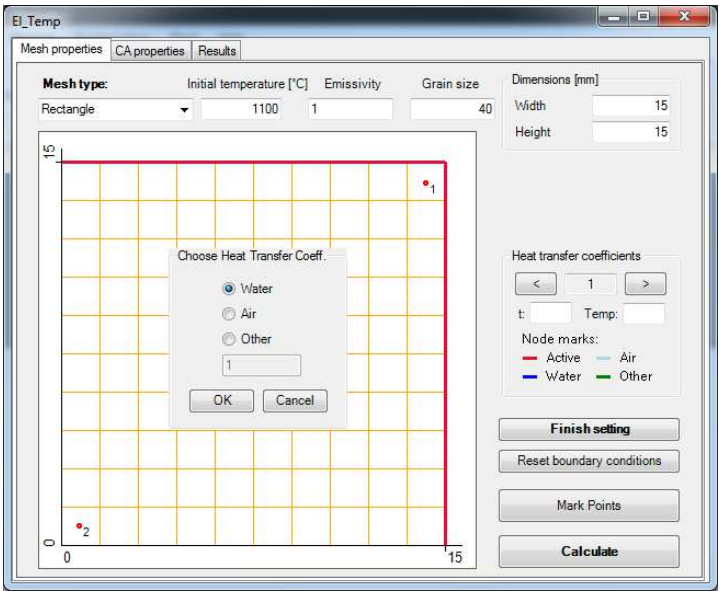

Fig. 3. Tab with setup parameters for the FE part of the system

Presently several commonly used shapes of long products subjected to laminar cooling can be preselected for further calculations (square, circle, circle with ribs) as seen in Fig. 4. Size of the finite element mesh is adjusted automatically to the prescribed sample dimensions.

a) b)

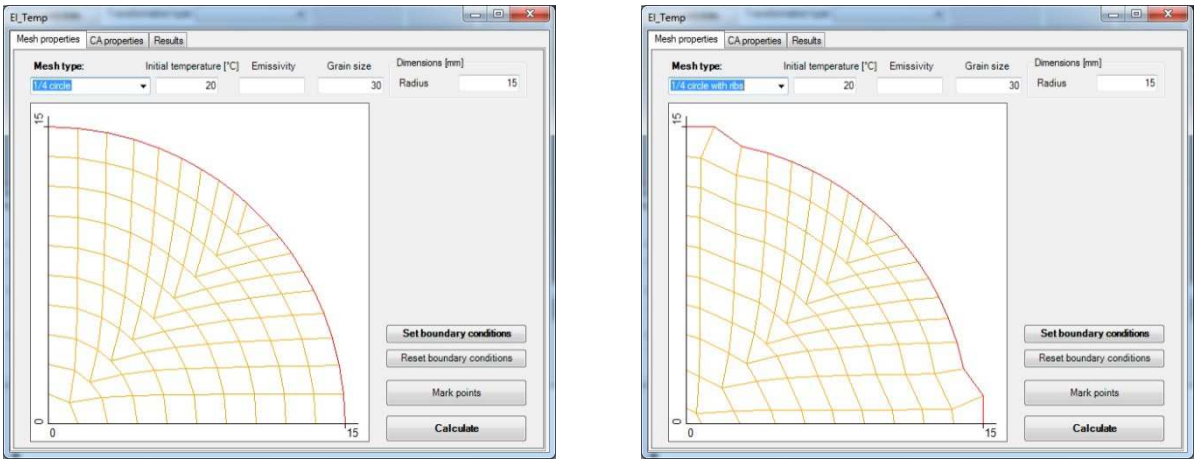

Fig. 4. Two types of meshes. a) ¼ circle b) ¼ circle with ribs

Finally, the developed user interface provides a possibility to select location at the macro scale sample, where micro scale phase transformation model will be attached to

provide corresponding information on the phase transformation during cooling. User can easily select interesting point by left-mouse button as seen in Fig. 5.

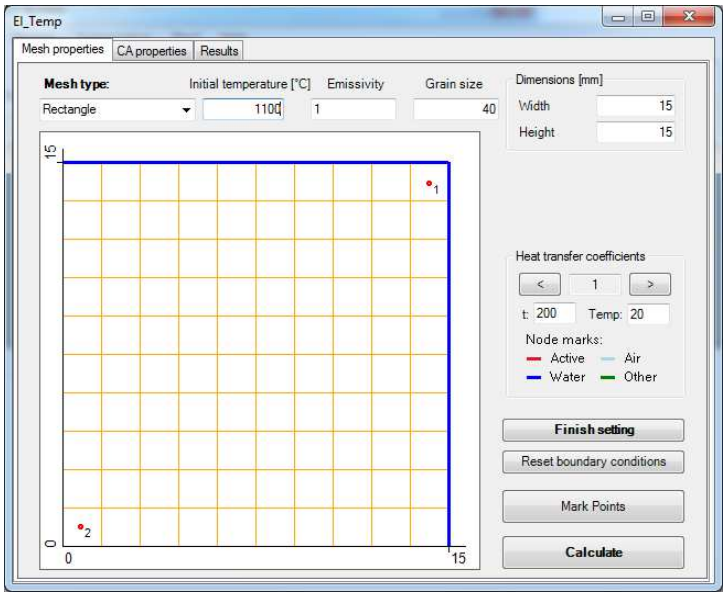

Fig. 5. Selection of locations for subsequent micro scale CA calculations

At this stage of research the maximum number of point, which can be selected for micro scale simulation, is set to 5 in order not to extend computational time. When smaller amount of micro scale points is selected then user finishes this step with the button *Stop Marking*.

The main parameters of the CA part of the system are set in the *CA properties* tab as seen in Fig. 6. Similar to the FE part, parameters in the CA tab are divided into two groups dealing with the computational space setup (CA space dimensions, physical size of each CA cell, initial temperatures etc.) and material properties (Thermocalc data, grain boundary mobility, activation energies etc.).

All the CA model parameters that are set through the interface are exported into the XML file, which is a standard input format for the simulations realized on the basis of the developed CAF, including phase transformation model. Finally after the calculations obtained results of the simulation can be easily visualized in the *Results* tab.

In order to facilitate handling of input data and obtained results a dedicated data base was developed and incorporated into the presented computer system. That way all the data regarding finite element model (mesh settings, boundary condition setting etc.) and CA settings (CA space size, neighbourhood type etc.) are stored for future references. Results obtained from the previous calculations are available for detailed investigation, as well. At present, more advanced visualization of the cellular automata results (carbon content, phase distribution, etc.) is realized in the external open source scientific visualization software ParaView. Obtained data from the proposed system are automatically exported into the required vtk format for further visualization. In the future these data will be also visualized within the *Result* tab.

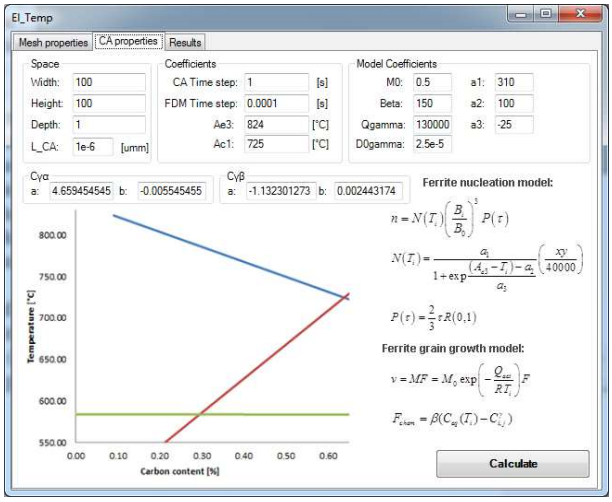

Fig. 6. Tab with setup parameters for the CA part of the system

Examples of results obtained at the macro and micro scale levels for the preselected points from Fig. 5 are shown in Fig. 7. Temperature profile obtained in particular point (Fig. 5) is used as input for the CA calculation (Fig. 7 a, 7c, 7d).

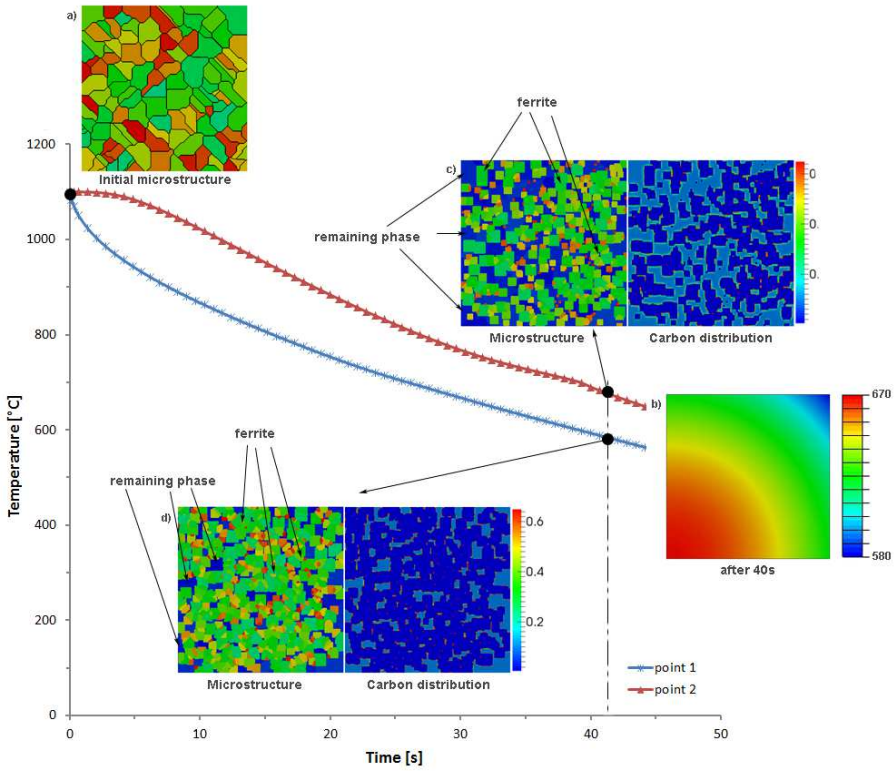

Fig. 7. Temperature changes during cooling process obtained from the macro scale model and corresponding microstructure evolution with inhomogeneous carbon distribution in investigated points

It is assumed in the model that the dimension of the CA cell in the space is L_{CA}=1μm. The CA space in the example is 400×400μm, and initially it contains 120 austenite grains.

This is equivalent to the average grain size of approximately 40μm. Comparison between the phase transformation kinetics for investigated points is presented in Fig. 8 a and 8 b.

Based on obtained results it is possible to evaluate not only differences in cooling conditions in various locations across the microstructure but also corresponding microstructure morphology. Data on phase transformation kinetics are additionally supported by detailed evolution of progressing phase transformation in subsequent time steps.

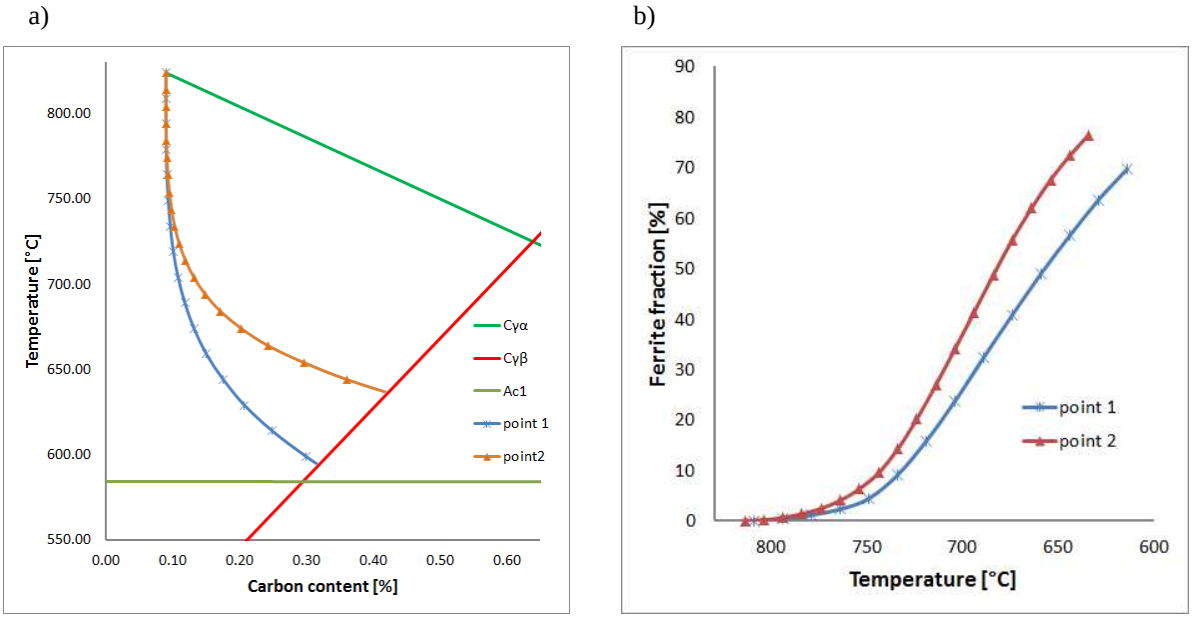

Fig. 8. Phase transformation results: a) carbon concentration change in the austenite phase, b) ferrite fraction evolution as a temperature function

As seen, the CA calculations stops when ferrite transformation is finished. Remaining austenite phase with different carbon concentration level is considered to further transform into perlite, bainite or martensite depending on cooling conditions. The CA models for subsequent transformations are under development and they will be incorporated into the developed multi scale modelling software.

4. CONCLUSIONS

The complex, but user friendly, computer system designed to support modelling of laminar cooling processes was presented in the paper. The multi scale cellular automata finite element model of the industrial laminar cooling process is the main part of the system. User friendly graphical interface facilitates use of the CAFE model and in the present form it can be a useful tool in industrial practice, providing not only global but also detailed local information on material behaviour.

The following steps are required to prepare a simulation on the basis of the developed multi scale computer system:

1) Setting initial parameters for the FE and CA.
2) Setting the required cooling schedule.
3) Selection of the points for micro scale simulation.
4) Running FE model.
5) Running CA model on the basis of input data provided by the FE solution.

Beyond this, the following functionalities of the system should be pointed out:

1. Possibility to store input and output data.
2. User-friendly interface.
3. Convenient visualization of simulation data.

Presented computer system will be further developed in order to extend its modelling capabilities towards simulation of other phase transformations (perlitic, bainitic, martensitic) occurring during laminar cooling.

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