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RCAFE BASED NUMERICAL MODEL OF DYNAMIC RECRYSTALLIZATION

The main goal of the paper is dedicated to proper arrangement of the Finite Element (FE) and Random Cellular Automata (RCA) methods in order to develop numerical model of dynamic recrystallization (DRX) and therefore to simulate microstructure morphology changes during plastic deformation at elevated temperatures. In the approach, Finite Element solver provides information on equivalent stress and strain fields after subsequent time steps. Then these data are transferred to RCA model, which is responsible for evaluation of corresponding microstructure morphology evolution and dislocation density changes. Finally, information from the CA part is send back to the FE solver as an input for the next time step. As a result, a fully coupled RCAFE model to simulate progress of DRX is established. The present paper is directly focused on development of algorithms and methods to transfer input/output data between both FE and RCA models. The developed communication protocol is based on the Abaqus VUMAT subroutine. Examples of obtained results from the developed model are also presented to highlight its potential.

1. INTRODUCTION

Desired shape and properties of metallic components can be obtained in production processes by use of various thermo-mechanical treatment operations. Recovery and recrystallization are two groups of phenomena, which take place under hot deformation conditions and have crucial impact on microstructure evolution. Thus, a lot of research has been carried out from experimental point of view to understand physical mechanisms controlling mentioned phenomena in a wide range of metallic materials [13]. At the same time, the investigation is supported by advanced numerical simulations broadening predictive capabilities of experimental analysis.

Nowadays, three usually main methods are used in microstructure evolution modelling: Phase Field (PF), Cellular Automata (CA) and Monte Carlo (MC). The reason for this, is their ability to include not only kinetics of the process but also microstructure

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morphology changes in an explicit manner. This is especially important when dynamic recrystallization (DRX) is considered, because geometrical changes of deformed grains directly influence e.g. mechanisms of nucleation of new recrystallized grains. Authors of the paper has previously gained broad experience on application of CA approach to modelling recrystallization phenomena [5],[9],[10]. Unfortunately, due to the discrete nature of cellular automata method it has some disadvantages when DRX simulations are considered. Particularly proper description of deformation of computational domain is a limitation. In the scientific literature different approaches with different levels of complexity were proposed to deal with CA space deformation issue. The simplest solution to reflect material deformation in the CA space were presented in e.g. [4],[7],[12,]. In these works authors proposed CA space elongation algorithm along selected axis Fig. 1a. However, in the approach many simplifications of material flow were introduced. Recently, more advanced space deformation algorithm was proposed [2], [3]. In this case authors developed CA space mapping technique between two defined coordinate systems as seen in Fig. 1b. The approach is promising, however it is still based on geometrical assumptions.

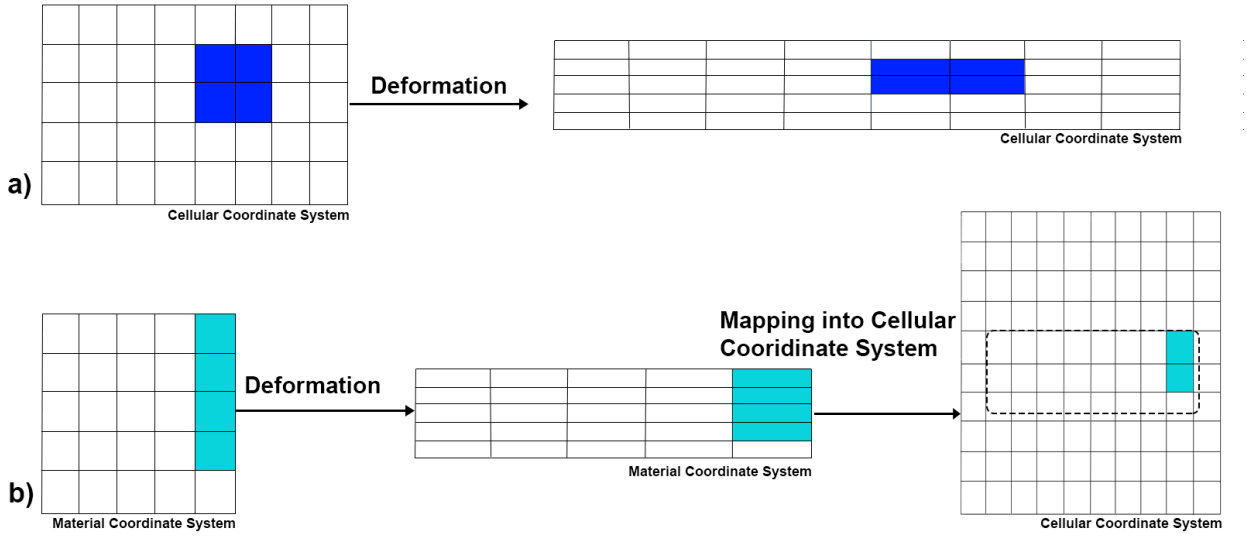

Fig. 1. Different CA space deformation mechanism: a) simple elongation technique, b) space mapping technique

Thus, to eliminate disadvantages of mentioned solutions and create an efficient CA space deformation algorithm authors has recently proposed a hybrid approach, which is based on combination of Random CA (RCA) and finite element (FE) methods [10]. The concept of the RCAFE (random cellular automata finite element) method lies in the assumption that the cellular automata cells directly correspond with finite element integration points. As a result, the microstructure evolution during nucleation and subsequent growth is modelled by the CA algorithms and deformation of investigated domain is predicted by the finite element model. However, the key aspect of the proposed model is development of the information exchange mechanisms between the two computational techniques in order to obtain fully coupled RCAFE solution. This is the subject of the present paper.

2. FE MODEL AND DATA TRANSFER ASSUMPTIONS

As mentioned, the proposed RCAFE model provides solution to one of the major disadvantages related to reliable description of the CA space deformation during plastic deformation and its influence on DRX progress. As a case study during RCAFE model development, authors used a simple channel die compression of St3S steel sample (Fig. 2). Different colours of grains are used to distinguish groups of FE elements representing subsequent grains, and presently, are not directly related to crystallographic orientations.

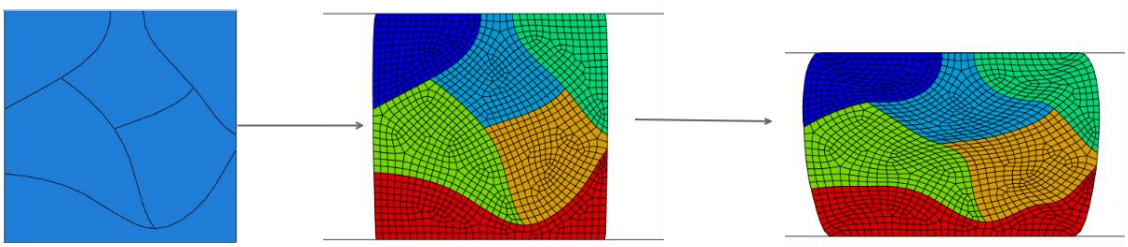

Fig. 2. Case study of the finite element channel die compression of microstructure with 6 grains

The isotropic hardening model based on simple flow rule, identified during the inverse analysis [8], was used during FE simulation. However, to implicitly capture differences in the grain behaviour related to different crystallographic orientations, flow stress values for each grain were additionally diversified according to the Gauss distribution function. The approach is often used when digital material representation (DMR) models are being developed see e.g. [11].

The commercial finite element software does not provide sufficient algorithmic solutions to combine the two computational techniques, namely RCA and FE. Thus, authors has designed and implemented an in-house communication protocols for the developed system as seen in Fig. 3.

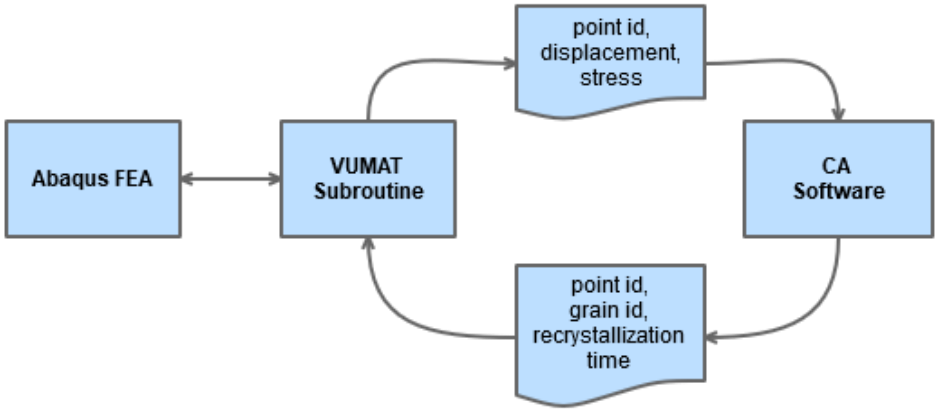

Fig. 3. System communication diagram

Interaction between FE solver and RCA model is realized by the developed Abaqus user subroutine VUMAT and implemented with c++ and Python programming languages. In each time increment information from FE model regarding positions of integration points, their ID as well as calculated stress values are send to the RCA model as input data. The RCA model, which is described below, based on provided data predicts nucleation as well as growth of new grains. Eventually information on DRX progress is send back to the FE solver and is used to modify the flow stress value for particular integration point during the next time step. Such data transfer is realized in fully coupled mode until the end of simulations.

In order to allow such fully coupled communication between the two models, following components were designed and implemented:

- Input file parser, which allows to obtain information about integration points IDs, their coordinates and list of their neighbours. Parser is a simple Python script, which automatically opens Abaqus input file and collects information about mesh nodes. Next coordinates of integration points are calculated and proper IDs are assigned. Finally, the script creates adjacency matrix for all investigated integration points. Generated data is then saved to text file for further use.
- VUMAT user subroutine, which allows to define the constitutive behaviour of material. In presented solution, the VUMAT subroutine contains not only material model, which depends on data from RCA model, but also implemented mechanisms to read and write data files used in communication between parts of the developed system.
- Text files generated by the VUMAT, which contain necessary data associated with specific integration point that are then used by the RCA model e.g. integration point ID, displacements in x and y axes or equivalent stress values.

Proposed communication protocols are used to simulate progress of dynamic recrystallization presented in next chapter.

3. RCAFE MODEL FOR DYNAMIC RECRYSTALIZATION

As a case study, a simple channel die compression test at elevated temperature (900^{o}C) was selected. To evaluate RCAFE model behaviour and test robustness of developed communication protocols following assumptions were introduced at the present state of the research:

- Only 3 new grains can appeared during recrystallization, after reaching the critical dislocation density.
- Both simulation time frames in the FE and CA models are the same and equal 1s.

At the beginning of RCA simulation the initial CA space corresponding with FE mesh is generated. CA cells position, ID and size are assigned based of each integration point location with respect to the size of each FE element. During a CA time step, positions of CA cells are updated based on algorithm presented in previous chapter. The concept of the RCA space creation is illustrated in Fig. 4. As seen, in the proposed RCAFE model, each FE integration point exactly corresponds to unique CA cell within the cellular automata space.

Due to the irregular nature of the cellular automata space in the random CA method, classical definitions of neighbourhoods cannot be used. Thus, authors developed and implemented specific algorithm based on radius neighbourhood to evaluate CA cells contributing to the cell changes via transition rules.

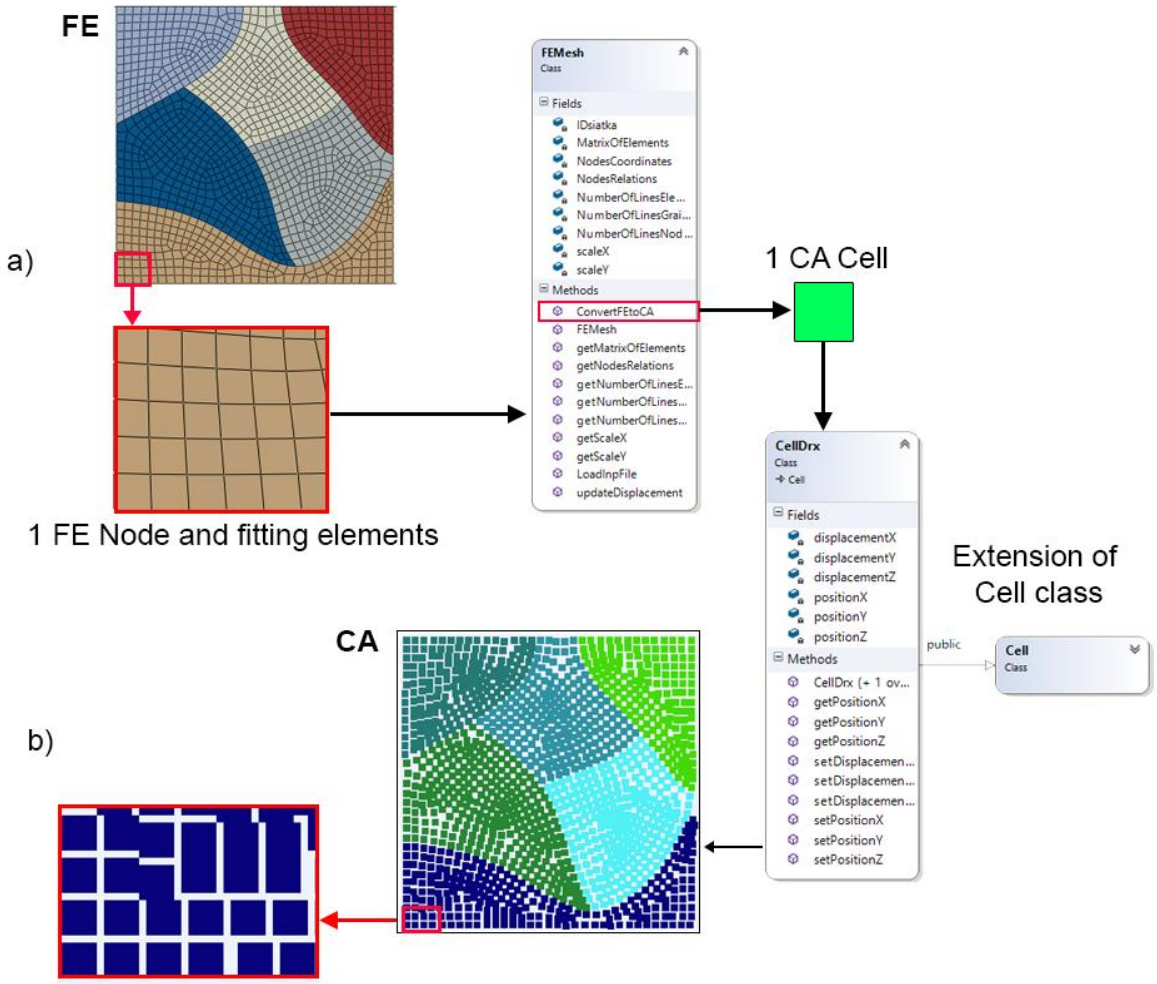

Fig. 4. Information flow diagram: a) FE mesh and corresponding FEMesh class, that contains converter function, b) CA cells class extension and CA space with square cells

Thus, as presented, during the RCAFE DRX simulation, information on displacement of each CA cell as well as equivalent stress values in subsequent cells are updated from the previously realized FE time step. This interaction between FE and CA leads to deformation of the CA space during subsequent simulation stages as seen in Fig. 5.

As can be seen in Fig. 5, the CA space geometry of investigated sample changes in exactly the same way as in the FE simulation. Additionally, not only CA space elongation is predicted but also all irregularities in deformation and final shape of the computational domain are replicated in detail, what was not possible with the presented earlier simplified CA space deformation algorithms.

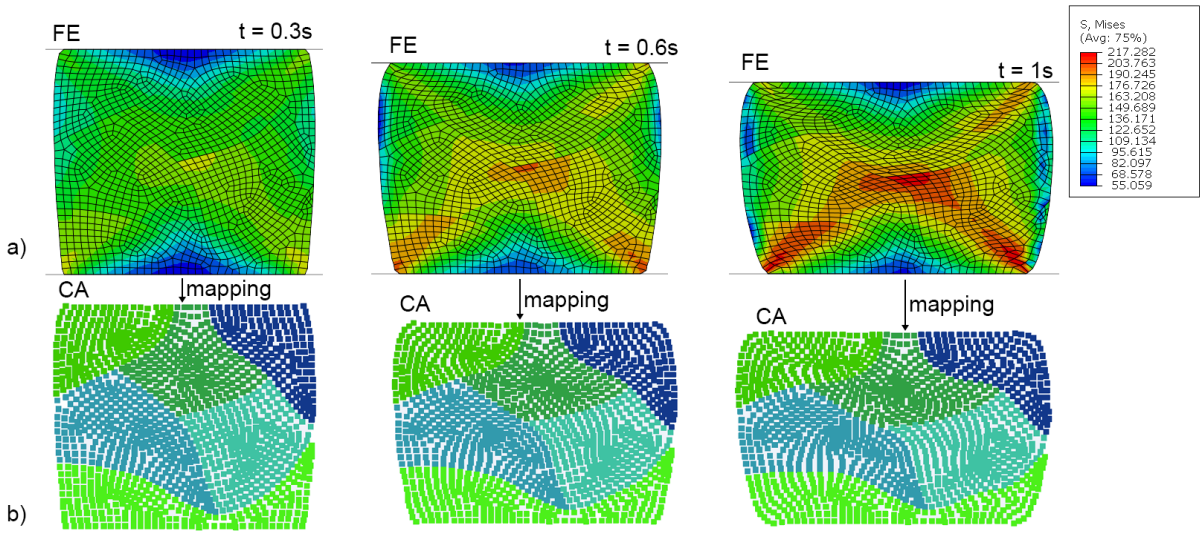

Fig. 5. Illustration of the CA space deformation in partially coupled model at different simulation time steps: a) stress field from the FE, b) corresponding CA space visualized as square cells.

In the DRX model, during each CA iteration dislocation density is updated based on information from the FE simulation:

$$\bar{\rho} = \frac{1}{\rho_0}\left(\frac{\sigma_i}{a_6 G b}\right)^2 \tag{1}$$

where: G – shear modulus, σ_i – equivalent stress value received from Abaqus, a_6 – constant, b – magnitude of burgers vector, ρ_0 – initial dislocation density.

After recalculation and distribution of dislocations, two major phases of CA DRX model take place, nucleation and grain growth, respectively. The first, is controlled by nucleation rate per unit of grain boundary area:

$$\dot{N} = c\dot{\varepsilon}\exp\left(-\frac{Q_n}{RT}\right) \tag{2}$$

where: c – constant, $\dot{\varepsilon}$ – strain rate, Q_n – the activation energy for nucleation, T – temperature, R – universal gas constant.

Nucleon can appear only in cells located along grain boundaries, when dislocation density within the cell exceeds critical value ($\rho_{(i,j)} > \rho_c$) [10].

After the nucleation, grain growth takes place and is controlled by energy stored along the dislocation lines. The grain boundary velocity is calculated as:

$$V = M_0 \exp\left(-\frac{Q_m}{RT}\right) 2\alpha\tau\left(\rho_{(k,l)} - \rho_{(i,j)}\right) \tag{3}$$

where: M_0 – initial grain boundary mobility, Q_m – activation energy for grain boundary motion, α – coefficient from the range (0,1), $\rho_{(k,l)}$ – dislocation density of k - neighbour cell,), τ – energy required for dislocation movement.

The defined transition rule, is based on recrystallized volume fraction in particular cell with the surface area S_{CA}:

$$\gamma_{i,j}^{t+1} = \begin{cases} DRX \; if \; \Delta\alpha_{RX} \geq 1.0 \\ \gamma_{i,j}^{t} \quad if \; \Delta\alpha_{RX} < 1.0 \end{cases} \tag{4}$$

where:

$$\Delta\alpha_{RX} = \frac{V\Delta t}{\sqrt{S_{CA}}} \tag{5}$$

When the cell changes its state to recrystallized, the dislocation density value is reset to reference value $\rho_{(i,j)} = \rho_0$. The CA model coefficients used during the present investigation were previously identified and validated in [9], [10].

Finally in a fully coupled system behaviour of the FE part is updated based on feedback from the RCA model of DRX controlling changes in CA cell states with defined transition rule. At the beginning of each FE step information on recrystallized cells and actual flow stress values calculated based on local dislocation densities in the CA cells are updated. Examples of obtained results from such a fully coupled model are presented in Fig. 6.

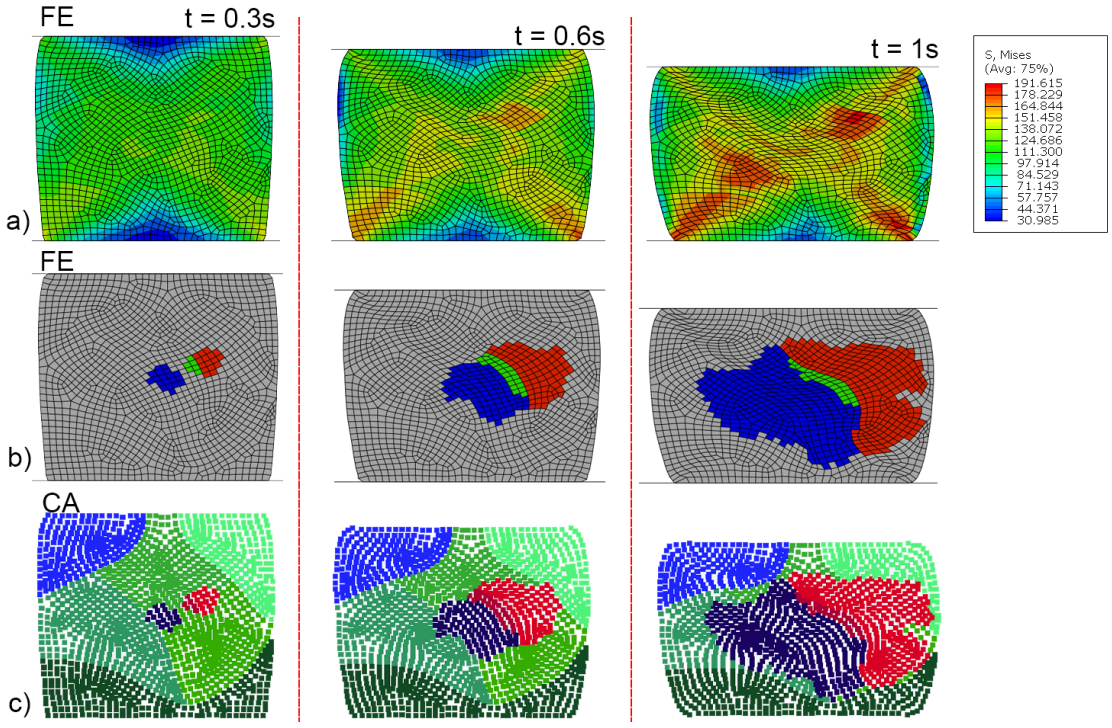

Fig. 6. Simulation results after time steps 0.3s, 0.6 s and 1 s: a) equivalent stress, b) recrystallized grain IDs, c) CA space morphology

As seen in Fig. 6 when FE and CA parts are connected, microstructure deformation, grain growth and equivalent stress evolution can be predicted. The maximum stress value in the coupled model was lower over 25MPa, in comparison to partially coupled simulation without recrystallization from Fig. 5a. Also stress distribution in coupled model is significantly different. As can be seen in in Fig. 6c, recrystallized grains appears at higher deformation levels. During simulation new recrystallized grains grow into areas with higher stresses but at the same time are subjected to elongation due to proceeding deformation. Thus, no artificial elongation typical for classical CA models is observed.

4. CONCLUSION

Based on presented results following conclusion can be made:

- Fully coupled model of recrystallization based on FE and RCA models can be developed.
- Application of the VUMAT and c++ language to develop communication protocols between CA and FE part seems to be an efficient approach.
- CA space deformation mechanism provide reliable behaviour of the CA part of simulation.
- Artificial elongation of new recrystallized grains was eliminated.

More advanced case studies including practical multi scale calculations will be investigated in further research on that topic.

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