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Development and evaluation of data transfer protocols in the fully coupled random cellular automata finite element model of dynamic recrystallization

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ABSTRACT

Development and application of the hybrid fully coupled, random cellular automata finite element (RCAFE) approach to modelling dynamic recrystallization phenomenon, during a high temperature deformation is the overall goal of the paper. The finite element (FE) solver provides information on equivalent stress, equivalent strain, temperature fields as well as on geometry of deformed computational domain after each time step. These data are transferred to the developed random cellular automata (RCA) model, which is responsible for evaluation of corresponding microstructure morphology evolution and dislocation density changes under dynamic recrystallization (DRX) conditions. Finally, a set of data from the RCA part is send back to the FE solver and used as an input for the next time step. As a result, the fully coupled RCAFE model for simulation of a DRX progress is established. Crucial developments of the RCA model related to the space deformation and efficient neighbors selection are presented within the paper. However, particular attention is put on the development of efficient communication algorithms and methods for input/output data transfer between the FE and RCA modules. The communication protocols based on text files and sockets have different levels of complexity but both are based on the Abaqus VUMAT subroutine. Their capabilities and limitations are evaluated within the paper. Finally, an application of the proposed RCAFE method to simulation of a dynamic recrystallization progress at the level of single grains is presented and discussed to highlight capabilities of the model.

1. Introduction

A set of sophisticated final exploitation properties of metallic materials can be achieved during controlled sequence of a thermo-mechanical treatment, such as: hot rolling, forging, extrusion, annealing, heating, cooling etc. During the treatment even small modifications of e.g. a deformation rate or a temperature can result in significant changes in material microstructure morphologies and eventually obtained properties. There are in general three phenomena responsible for this behavior. The first is a texture evolution, the second is a group of phase transformations, and finally the third is a group of recrystallization phenomena including static, dynamic and meta-dynamic ones. All of them are also closely related to basic deformation mechanisms including deformation slip, twinning, shear banding etc.

Recrystallization along with recovery are two groups of phenomena, which take place under hot deformation conditions and have crucial impact on a microstructure evolution. Thus, from experimental point of view, it is crucial to understand all physical mechanisms controlling mentioned phenomena in a wide range of metallic materials and processing conditions. A lot of works are focused on this matter see e.g. [1,2]. At the same time, an increased computational power, which is now even available in every day work stations, gave a possibility to numerically investigate more advanced and complex material systems as well as to predict materials behavior in a wide range of processing condition. As a result, these numerical approaches can be a valuable support for extensive experimental investigations.

Nowadays, five so called full field methods are usually used in microstructure evolution modelling: Phase Field (PF) [3], Level Set (LS) [4], Cellular Automata (CA) [5–7], Monte Carlo (MC) [8,9] and Vertex models [10]. They have an ability to include not only kinetics of the process but also a microstructure morphology changes based on different crystallographic orientations, grains boundaries shapes or a heterogeneous dislocation density distribution. This

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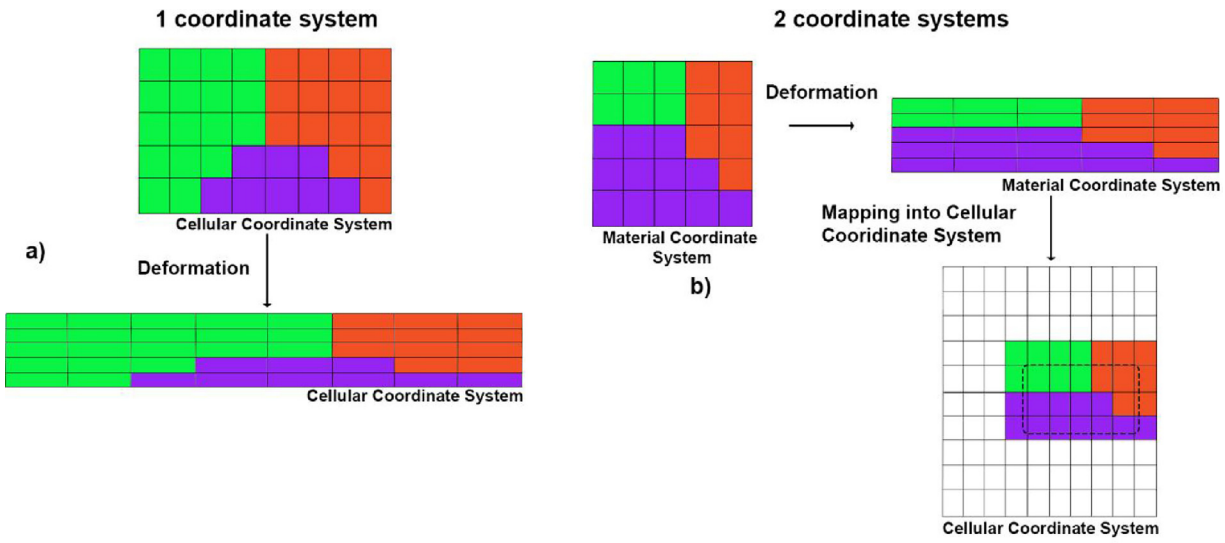

Fig. 1. Different CA space deformation mechanisms: a) the simple elongation technique, b) the space mapping technique.

is especially important when the dynamic recrystallization (DRX) is considered, because geometrical changes of deformed grains directly influence for example mechanisms of nucleation of new recrystallized grains.

Authors of the paper have previously gained a broad experience in application of the CA approach to modelling recrystallization phenomena [11–14]. Unfortunately, due to the discrete nature of the cellular automata, this method has some major disadvantages when DRX simulations are considered. Particularly proper description of a computational domain deformation under plastic forming conditions is a limitation. In many recent papers different simplifications of a space deformation mechanism or even its total omission have been presented [6,15–19]. Up to now, only few works dealt with the CA space deformation issue in a more complex manner. The simplest solutions to trace material deformation in the CA space were presented in [20–22]. In these works authors proposed the CA space elongation algorithm along selected axis (Fig. 1a). This approach is based on a simple geometrical elongation of CA cells, what changes their aspect ratio and affects proper interactions with neighboring CA cells. As a result, after simulation new recrystallized grains are elongated but in an unphysical, artificial manner. Recently, more advanced space deformation algorithms have also been proposed see e.g. [22]. In this case the CA space mapping technique between two defined coordinate systems was proposed, as seen in Fig. 1b. That way, some of mentioned disadvantages have been eliminated, however the approach still considers a set of geometrical assumptions.

Currently the most advanced mechanism of the CA space deformation was presented in [23], where authors associated a regular FE mesh geometry with a classical regular CA space and then carried out deformation based on the FE simulation results. Moreover, the model was based on the crystal plasticity simulations to provide additional information on a texture evolution (CACPFE—cellular automata in crystal plasticity finite element). The proposed information exchange diagram is presented in Fig. 2. As seen, the CA simulations are realized on a regular space and the geometrical movement of each cell is possible. The limitation of the approach is associated with the regular CA space, which may limit further FE remeshing operations required at the higher deformation degrees.

To eliminate disadvantages of mentioned solutions and create an efficient CA space deformation algorithm authors of the paper has recently proposed a hybrid concurrent approach, which is based on combination of random CA (RCA) and finite element (FE) methods [24].

The concept of the concurrent RCAFE (random cellular automata finite element), in contrast to the classical upscaling CAFE method, lies in the assumption that the cellular automata cells directly correspond with finite element integration points. Thus, such superposition of the particular CA cell with the particular Gaussian point allows different types of FE meshes, not only regular ones, to be used during calculations. As a result, the microstructure evolution during a nucleation and subsequent growth is modelled by the RCA algorithm and the deformation of investigated computational domain is predicted by the finite element model.

However, the key aspect in the proposed model is development of the information exchange mechanism between the two computational techniques in order to obtain fully coupled concurrent RCAFE solution. This issue is addressed in the present paper.

2. Assumptions of the data transfer module

As mentioned, the proposed RCAFE model provides solution to one of the major disadvantages related to reliable description of the CA space deformation during metalforming operations and its influence on the DRX progress. A conventional channel die compression test of St3S steel sample was selected as case study to explain developed data transfer mechanisms. Such case study will be used to point out all modifications that have to be introduced into the RCA and FE modules to perform an effective coupling.

It has to be pointed out that different colors are used to distinguish groups of FE elements representing subsequent grains in the investigated microstructure. Presently, colors are not directly related to crystallographic orientations, but are used primarily to distinguish different grains behavior during a deformation. As a result, different flow curves, diversified according to the Gauss distribution function can be assigned to each grain.

The isotropic hardening model based on a simple flow rule, identified by the inverse analysis [25], was used during the FE simulation. The approach is often used when the digital material representation (DMR) model is being developed see e.g. [26].

The key difficulty in the present research is associated with the fact that commercial finite element software do not provide sufficient algorithmic solutions to combine the two computational techniques, namely the RCA and the FE. Thus, authors have designed and implemented an in-house communication protocols