Journal of Computational Science 16 (2016) 98–113

Contents lists available at ScienceDirect

Journal of Computational Science

journal homepage: www.elsevier.com/locate/jocs

Time and length scale issues in numerical modelling of dynamic recrystallization based on the multi space cellular automata method

Mateusz Sitko*, Maciej Pietrzyk, Lukasz Madej

Department of Modelling and Information Technology, AGH University of Science and Technology, Al. Mickiewicza 30, 30-059, Krakow, Poland

ARTICLE INFO

Article history:
Received 9 December 2015
Received in revised form 9 May 2016
Accepted 11 May 2016
Available online 19 May 2016

Keywords:
Time scale
Length scale
Cellular Automata method

ABSTRACT

Critical evaluation of influence of time step length and cell size on cellular automata models behavior during microstructure evolution simulations is the subject of the present work. Dynamic Recrystallization was selected as a case study for CA model application. First, general information on CA model assumptions are presented. Then series of advanced modifications including different dislocation generations schemes, multi space concept and scaling of nuclei sizes is presented. As a result, a robust numerical CA model was established and it was used to highlight importance of proper selection of time step length and cellular automata cell size. The work revealed that there is a clear relation between the two investigated factors and they have to be properly defined in order to reach the threshold values where CA model is becoming insensitive to the technical parameters.

1. Introduction

Thermo-mechanical treatment of processed metallic materials provides wide range of possibilities to control final microstructure morphology and in-use properties of products. Combination of deformation and varying process temperatures can be used to initiate and control three groups of phenomena responsible for the microstructure evolution. The texture evolution is the first one. The second group involves phase transformations in metallic materials both during heating and cooling stages and the last group is represented by thermally activated phenomena of recrystallization (static, dynamic and metadynamic). The later, has been experimentally and numerically investigated for many decades, increasing the level of understanding of interactions between processing conditions and microstructural changes. From the numerical point of view, progress in models complexity is directly related with the increasing resolution of experimental techniques providing knowledge on local heterogeneities, as well as, with the progress in computational recourses with multi core processors, computer clusters or efficient graphical processors. First numerical models for recrystallization were based on mean field approaches like simple closed form Avrami type equations. They provided general information on flow stress variations during recrystallization. Then more sophisticated models based on differential equations were developed. They may be considered as precursors of multiscale solutions, as information on micro scale features e.g. dislocation densities was used to evaluate macroscopic flow stress values. However, both approaches can provide quite general information on microstructure morphology e.g. the average grain sizes, or its distribution. Thus, again, more advanced full field models, which directly take into account microstructure morphology with all its features during modelling were proposed [1]. Phase Field (PF) [2], Level-Set (LS) [3], Monte Carlo (MC) [4] or Cellular Automata (CA) [5,6] methods can be classified into this category.

Authors of the work investigated possibilities of application of the CA to simulate microstructure evolution during both static and dynamic recrystallization. The method provides a possibility to directly link physical mechanisms leading to particular phenomenon with the basic assumptions of the algorithm. Thus, capabilities of the CA approach have been investigated in the material science applications for almost 30 years.

First research works on practical application of the CA models to microstructure evolution simulations are related to the static recrystallization [7–9,4]. This was followed by numerical investigation of dynamic recrystallization in [10] and flow stress behavior analysis with respect to initial grain size prior deformation. Development of new CA neighborhood types provided a possibility to obtain reliable grain shapes during and after growth of newly recrystallized grains [11], while incorporation of internal variable models gave the possibility to consider also hardening and recovery prior initiation of dynamic recrystallization [6,12,13]. Subsequent CA models, along with the wide range of applications of

* Corresponding author.
E-mail address: msitko@agh.edu.pl (M. Sitko).

http://dx.doi.org/10.1016/j.jocs.2016.05.007
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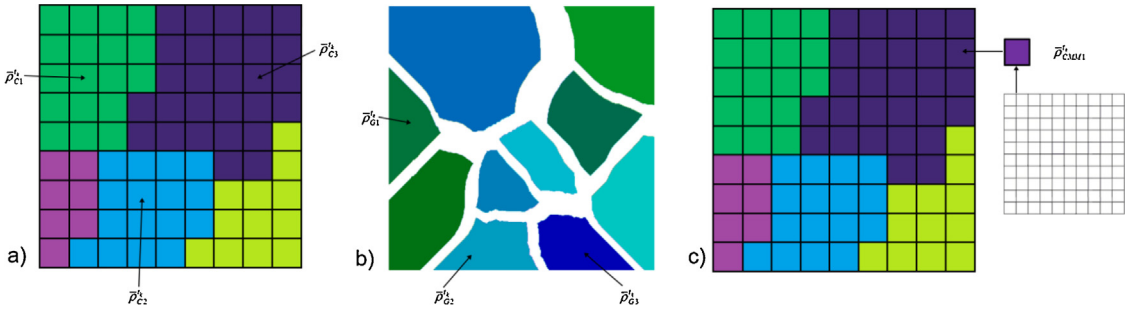

Fig. 1. Different dislocation distribution schemes: (a) cells, (b) grains, (c) sub-cells multi-space.

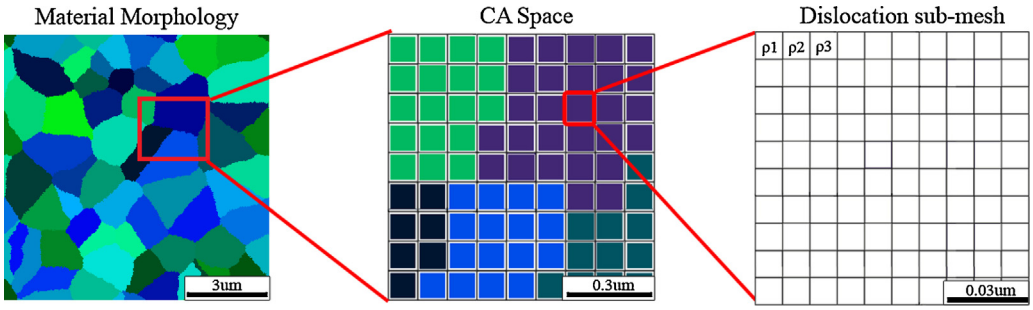

Fig. 2. Multi-space concept where each CA cell is additionally described by a set of sub-cells.

SEM/EBSD techniques, became more refined and introduced information on crystallographic aspects [14–16]. Then, the problem of solute drag effect was considered in [17] where authors used multi-scale concept based on combination of cellular automata and finite element method to describe macro and micro scale deformation of copper. An important breakthrough in CA model development was related with possibility to deform the CA space during simulations [18–20]. This subject is still addressed in the scientific literature and more advanced approaches are being developed see e.g. [21,22]. Recently, to increase predictive capabilities of cellular automata models other computational techniques are employed and interlinked e.g. crystal plasticity finite element method [23], mathematical statistics theory [24] or adaptive response surface method [25].

Thus, due advantages of the CA technique and recent progress, the method is often applied in many scientific institutes to investigate dynamic recrystallization in wide range of engineering metallic materials: stainless steels [26], C–Mn micro alloyed steel [27], titanium [23], copper [17], nickel based alloys [28].

As presented, the CA technique applications are broad, however, in most research works aspects related with the accuracy of the method in relation to time and length scales used within CA spaces during calculations seem to be neglected. Although, both parameters have significant influence on microstructure morphology as well as recrystallization kinetics. Thus, authors decided to develop a cellular automata model for dynamic recrystallization that will be insensitive to mentioned changes in the time step length and CA cell size. Initial works on the matter have already been published in [29,30], where basic assumptions of the DRX model were proposed. Present paper is devoted to advanced model modifications that were required to reach the mentioned goal. Detailed study on model robustness is also presented to highlight negative influence of time step length and cell size on quality of obtained results, as such an investigation is missing in the scientific literature devoted to the CA technique.

2. The dynamic recrystallization cellular automata model

The cellular automata model for dynamic recrystallization is divided into four interconnected stages, including:

- generation of the initial microstructure,
- evaluation of average dislocation density due to hardening and recovery occurring during deformation,

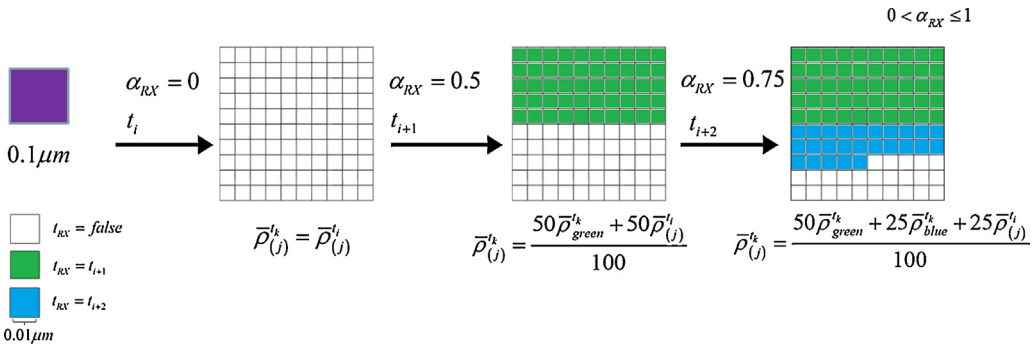

Fig. 3. Dislocation increase in one cell during multi-space calculation.