Modelling of Recrystallization and Grain Boundary Migration by Cellular Automata

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Abstract. Within past ten years, the importance of cellular automata (CA) models of both recrystallization and grain boundary migration has been recognized. It can be shown that CA provides a computationally efficient mathematical framework for simulations of physically relevant models of the above processes. Generally, CA works in such models with a vast number of identical copies of several generic processes – as recrystallization, nucleation, grain boundary migration, etc. – which interact locally and results in a complex global response. The attention is focused to some important aspects of recrystallization, grain growth and CA modelling. Finally, possible future development of more physically relevant models are briefly outlined.

1 Introduction

Mathematical and computational models have a long and successful history in modelling and description of mechanical behaviour of metallic materials. It is well known that they answered a lot of deep questions in the field of materials science. Despite such success, there are still problems that are not tractable by classical approaches. The aim of this work is to explain why some processes and material responses are not solvable by classical approaches as, for example, finite element method or the Monte Carlo simulations.

Situation in modelling of mechanical behaviour of metallic materials becomes rather complex when we enter deeper levels of description. Once we leave the macroscopic level of mean values of variables and approach the microscopic level then we enter the world of complexity. On one hand, it is impressive how nature easily "compute" or solve mechanical responses of a metallic material having any size. On the other hand, we are unable to correctly explain behaviour of it does not matter how tinny piece of the same metal with the most powerful supercomputers. It is irritating any time when we start to think about it.

A very natural question arises after all those questions: "Where we do an error?" or "What is wrong in our way of solving those problems?" This paper will try to show one of possible and as we believe the best way how to formulate and understand modelling and simulation of mechanical behaviour of metallic materials. It is far beyond the scope of this paper to discuss all aspects of this problem. Therefore we propose a general concept that will be explained on simple cases related to modelling of dynamic recrystallization (DRX) and grain boundary migration (GBM). A thorough review of all contributions of CA in material science and solid state physics is beyond the scope of this work.

2   Cellular Automata Theory

The discovery of CA-theory is related to names J. von Neumann, S. Ulam, and A. Turing. The concept had been developed in the forties of 20th century. Briefly, von Neumann had been thinking about two computer paradigms; namely, sequential one that we use in our computers so far, and parallel one as it is used in CA. The state of art of physics those days enabled to build sequential computers only. The use of sequential computers distorted our way of understanding and solving the problems.

CA–model discretize space in our case into two–dimensional (2D) lattice of squares – in general, it could be an arbitrary number of dimensions. The squares, i.e. elements of this lattice, are called cells. A neighbourhood is defined to every cell, usually a list of the nearest neighbouring cells and the cell itself, that is uniform through the whole lattice. Every cell contains a list of variables, e.g. dislocation density, orientation, etc. The evolution of the system is driven by a transition rule (a function) that computes new values of variables of an updated cell using the values of the cells laying in the neighbourhood of the cell from the previous CA–step. General information about the CA simulation technique can be found in [1, 2].
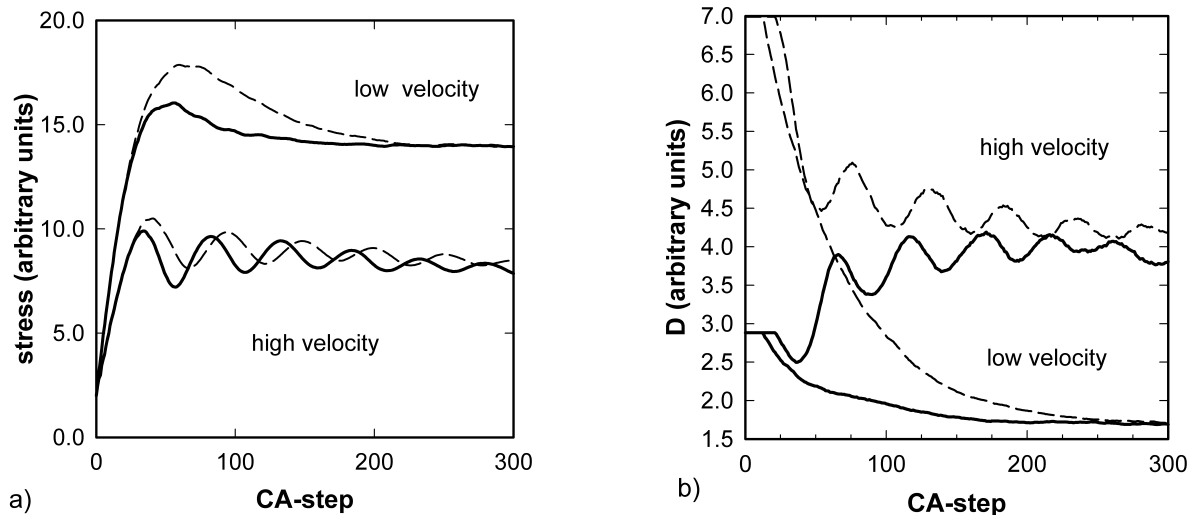

Fig. 1. (a) Flow stress curves for two different velocities, representing deformation at constant strain rate for two different initial grain sizes $D_0 = 2.9$ (solid lines) and 7.0 (dashed lines). Sensitivity of the curves on initial grain sizes is apparent. (b) Corresponding dependences of grain size on CA–steps [7].

CA transition rules can be understood from a certain point of view as finite difference scheme but it has to be stressed out that CAs are much richer than this. The number of all possible rules for a two state CA with nine neighbours is s^{s^n} where s is the number of states and n the number of neighbours, i.e. $2^{2^9} \cong 1.34 \times 10^{154}$. It is a large number of rules for one of the simplest possible CA. Therefore, there is plenty of space to build physically relevant models.

The theory of complex systems is a relatively new field that enable us to formulate and to solve problems ranging from biology through physics to pure mathematics resembling complex behaviour. A complex system is usually defined as an ensemble of vast number of identical copies of several generic processes. The processes are interacting locally and they produce a global response which is richer than any of generic processes. In our case, the elementary processes could be, for example, grain boundary (GB) movement, nucleation event or recrystallization event. The most important mathematical paradigm used to solve complex systems are CAs. Both DRX and GBM will be treated in this paper as complex systems. This approach gives us a great flexibility in definition of models and possibility to approach the way how the nature

thinks, i.e. the parts of materials response just locally to surrounding information and change their behaviour according to such information.

3   Dynamic Recrystallization

Recrystallization is split into two distinct cases, i.e. static, and dynamic one with recrystallization after and during the deformation, respectively. CA-models of static recrystallization started in [3] and were reviewed in [4]. We focuss our attention into DRX [5] in this paper.

A CA-model [6, 7] of DRX is carried out by the sequential realization of three steps representing microstructural evolution of each cell during each CA-step: (a) evolution of the dislocation density, (b) recrystallization realized by the growth of grains when driving force exceeds a critical value at GB, and (c) the nucleation of embryos of new grains. Three variables, defined for every cell separately, are used in the CA–model: dislocation density ρ, grain orientation θ, and waiting time t_w, defining GB velocity $v = d/(t_w + 2)$ where d is cell width and t_w is given by a number of CA-steps.
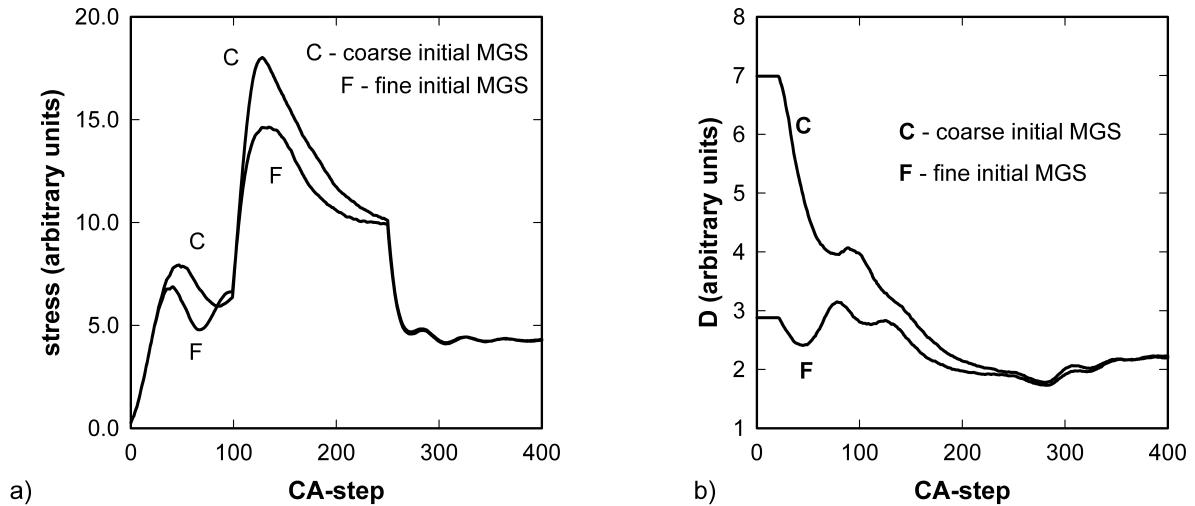

Fig. 2. (a) Flow stress curves in the case of the strain rate jump test for two different initial grain sizes $D_0 = 2.9$ and 7.0 (curve C) carried out under identical initial deformation conditions as in Fig. 1. (b) Dependences of corresponding mean grain size (MGS) curves on CA–steps.

For example, recall definition of recrystallization event from the local rule [6, 7]. A recrystallization event will occur at a cell C under consideration with 50% probability when the following conditions are fulfilled simultaneously: (i) the cell C is situated at GB, (ii) the difference in dislocation density between the cell C and neighbouring cell belonging to different grain is greater than a critical value $\Delta\rho_{cr}$, (iii) the potential new configuration of GB is not an excluded one (e.g. one cell wide re–entrant bulges are not allowed), (iv) the waiting time t_w is zero, (v) a grain with lower dislocation density grows into a grain with a higher one.

Detailed description of the CA-model of DRX with definition of dislocation density evolution and nucleation was published elsewhere [6, 7]. It was found that the simulated dependences of stress and mean grain size on CA-steps correlate with the experimental observations [5] and with CA-simulations of other authors [8].

Fifty percent probability of recrystallization event acceptance and point (iii) in the above list are simplifications of the used model. Can we remove those rather artificial simplifications from DRX-model? Nature is more sophisticated than this simple model. It has a simple and effective tool that protects appearance of re-entrant bulges and ”wrong” shapes; it simply

checks the local GB energy within used neighbourhood. It has to be stressed out here that CA simulations have no access to global variables from definition. All variables are changed only locally! The trend is to decrease GB energy but with help of fluctuations a small local increase of GB energy can occur as well. It naturally leads to a CA-model of GBM that is just a part of DRX-model. Such GBM is a modified pure GBM because of simultaneous presence of different driving forces – as, for example, difference of stored energy – beside the curvature driven force.

It was found in this model [6, 7] that single peak or multiple peak stress curve occurs for low or high GB velocity, respectively, see Fig. 1a. It is accompanied by single or multiple peak on evolution curves of mean grain size (MGS), see Fig. 1b. Simulated evolution of stress [6, 7] correlates with simulations [8] and with the experiment [5] but the predicted presence of oscillations in evolution of MGS [6, 7] is still experimentally unclear to the best knowledge of the authors. A strong sensitivity of the flow stress curves to the initial grain size (in accordance with experiment, see Fig. 1) and to nucleation rate is observed [6, 7]. Sensitivity of the flow stress curves to nucleation rate should be experimentally confirmed. Different thermomechanical histories of a given sample can lead to different numbers of nuclei and hence to different nucleation rates.

Strain rate jump test for two different initial grain sizes $D_0 = 2.9$ and 7.0 – carried out under the same deformation conditions as in Fig. 1 – is depicted in Fig. 2a. It is confirmed in accordance with the experiment [5] that an abrupt increase of strain rate, i.e. energy deposition into the sample, can switch multiple peak behaviour into single peak one. The dependence of corresponding MGS curves on CA–steps is shown in Fig. 2b.
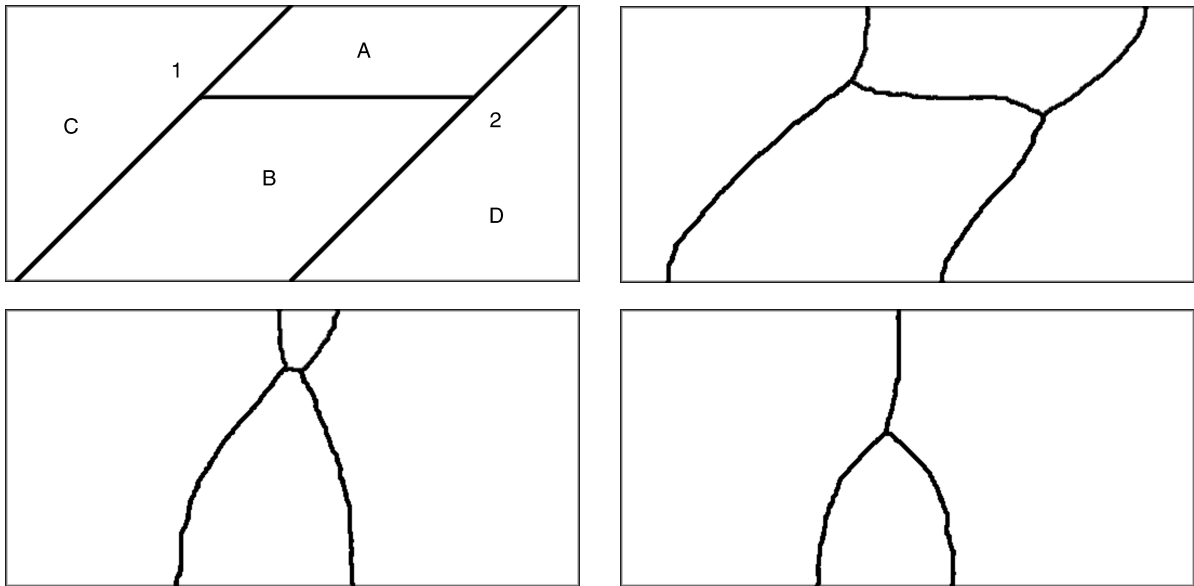

Fig. 3. Development of microstructure is shown here for time 0, 2k, 32k, and 40k. Triple junctions and grains in the initial configuration are marked by numbers, and by letters, respectively. The origin is in the left-lower corner with x and y coordinate in horizontal and vertical directions, respectively.

4 Grain Boundary Migration

Simulation of GBM was done by a CA-model using minimization of the local GB surface line within given neighbourhood as the only driving force. Minimization of the total surface line results from a large number of such local minimization events. A local minimization event works with a CA-rule that is equivalent to minimization of local surface, see the following definition

of CA-rule used to model GBM. Despite simplicity of this model where other driving forces are omitted – such as triple junction drag, grain orientation and inclination of GB – migration of the points of intersections of the grain boundaries with the free surfaces obeys a parabolic kinetics, $x = t^{1/2}$, that correlates with experimental observations [9].

Essential characteristics of the used cellular automaton [10, 11] are the following: (i) the sample is divided into cells where orientation variable of each cell is assigned to one of 4 differently oriented grains, (ii) the Moore neighbourhood of a cell is composed of 8 first and second nearest neighbouring cells, (iii) the transition rule of a cell - its reorientation into the neighbouring crystal - requires: (iii_a) the cell is situated at grain boundary, and (iii_b) the number of contiguous cells (going one after the other without interrupts in the Moore neighbourhood) belonging to the same grain is equal to four or higher, or in the Moore neighbourhood restricted by the free surface, this number is equal to two or higher (the latter applies only to the cells lying on the outer surfaces). The reorientation is occurring with the probability of 50% in order to prevent non-physical anisotropic growth reflecting the symmetry of the square grid.
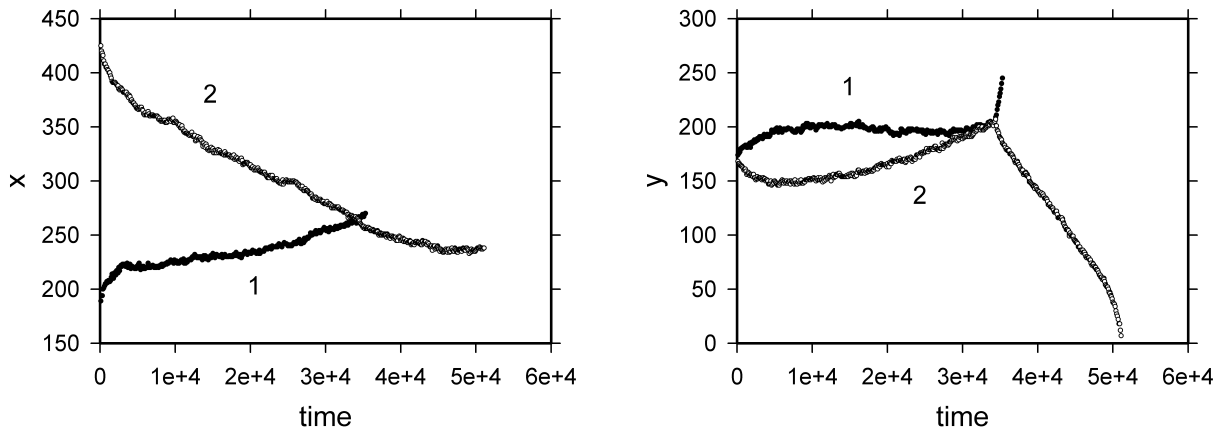

Fig. 4. Migration of two triple junctions for the topology defined in Fig. 3: (a) x coordinates, (b) y coordinates. See Fig. 3 where one triple junction disappears between CA-steps of 32k and 40k.

Development of microstructure is shown in Fig. 3 for times 0, 2k, 32k, and 40k where gradual shrinkage and finally disappearance of grain A, and subsequently of grain B occurs. The grain boundary segment between the lower A and upper B grains vanishes and a new boundary between the left- and right-hand grains is formed. Two new triple junctions at the ends of vertical segment start to move from this point in the opposite directions. When the y-coordinate reaches upper free surface the upper grain disappears at time slightly greater than 32k; when the other branch reaches the lower free surface the lower grain disappears and the transformation of the quadricrystal into bicrystal is accomplished.

The motion of x and y coordinates of both triple junctions that are present in this microstructure are recorded in Fig. 4 where the left and/or upper triple junction is marked by number 1 and the right and/or lower one by number 2.

It is surprising that in spite of very simple CA-model which is defined locally, the following experimentally observed features of GBM are observed during simulations. All GBs start to be perpendicular to the side surfaces from the very beginning of the simulation. If this is not true then GB can shorten its surface near the free surface until it becomes perpendicular. Velocity of GB decreases with increasing distance from the surface. GB migrates towards the center of curvature that leads to shrinkage of the total grain line. The equilibrium values of dihedral angles between the grain boundaries of 120° are changed by the influence of triple junctions

that is caused by lower mobility of triple junctions [11]. Triple junction drag is not explicitly defined in the model. Further information about this model could be found in [10, 11].

5 Conclusions

Usefulness of the theory of complex systems has been demonstrated on two processes modelled by CA, namely, DRX and GBM. Despite the fact that physically simplified definitions of those models were used, global responses correlate with experiments. Detailed evolution of microstructure can be involved in simulation as well. There is a plenty of space to make models more complicated and physically relevant because we know what we omitted but it is necessary to keep in mind that refinement of those models is not straightforward. It has been demonstrated mainly in the part dealing with DRX that CA-models can answer questions given by experimental measurements on one hand and rise new questions to be answered by experiments on the other hand.

Acknowledgements

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