Acta Materialia 107 (2016) 366–376

Contents lists available at ScienceDirect

Acta Materialia

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

Full length article

A statistical ensemble cellular automaton microstructure model for primary recrystallization

M. Kühbach*, G. Gottstein, L.A. Barrales-Mora

Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Kopernikusstraße 14, D-52074 Aachen, Germany

ARTICLE INFO

Article history:
Received 27 December 2015
Received in revised form
26 January 2016
Accepted 26 January 2016
Available online 12 February 2016

Keywords:
Recrystallization
3D Cellular Automaton
Grain Size Distribution
Heterogeneity
Parallelization
Spatial Statistics

ABSTRACT

A new model for the simulation of primary recrystallization is presented. The model is based on the cellular automaton method but departs from the classical 'representative volume element' (RVE) approach by considering a microstructure as a statistical ensemble of numerous solitary units. Individually these are significantly smaller than an RVE and can be simulated independently on a parallel computer. The model showed excellent accuracy compared to RVE simulations. The substantial reduction of the time-to-solution achieved by the model makes parametric studies practical and close to real-time recrystallization simulations in industrial processing lines possible.

1. Introduction

Tailoring microstructures in cold-rolled sheet metal with economical annealing concepts requires a sound physical understanding of the underlying grain boundary migration processes. These are of particular interest during primary recrystallization, which is a microstructure restoration process during which strain-free crystals nucleate, their mobile grain boundaries migrate into the deformed microstructure, and finally they impinge on one another [1–4]. Thereafter, curvature-driven migration (grain growth) controls the evolution of the interface network further. An analytical description of primary recrystallization processes is complicated owing to the concomitant temporal activation of the nucleation sites, the spatial heterogeneous consumption of the deformation structure, and the three-dimensional impingement problem. It is appropriate to consider the grain boundary migration speed v as a continuum-scale quantity $v = mp$ which is proportional to the local driving pressure p and the grain boundary mobility m. However, additional intrinsic effects of a microstructure, such as the heterogeneity of the dislocation density, texture, solute elements and second-phase particles [4–15] modify v locally, and hence only for several idealized cases analytical solutions were found [16–20].

To mitigate this complexity, modeling and simulation can be utilized to predict microstructure and texture evolution during recrystallization under heterogeneous conditions and to better understand this phenomenon. Most models used for recrystallization are based on representative volume element (RVE) approaches where an arbitrary section of a bulk specimen is sampled, large enough to be a statistical representative of some microstructure state variables [21–35].

However, in order to comprehensively represent a microstructure in an RVE, two conditions have to be met: (i) a large number of sampled grains and (ii) a fine discretization of each grain [36,37]. This is to reduce the bias in the volume of each grain and the representation of the grain boundary curvature [38]. In fact, the more heterogeneous the structure is, the finer it has to be resolved [38–40] and often the larger the domain has to be chosen to be representative [41]. In effect, these requirements render most simulation models very memory-consumptive. Hence, in most cases, the size of the RVE is restricted and limited by the available physical memory of the computer [21,24,26,42] which is not necessarily a sufficiently large size for a statistical representation of the system.

For this reason, the applicability of RVE-based recrystallization microstructure modeling appears questionable for heterogeneous and large grain populations or for substantially refined physical descriptions that require improved resolution. Different solutions for this problem have been proposed, for instance, extensions of the

* Corresponding author.
E-mail address: kuehbach@imm.rwth-aachen.de (M. Kühbach).

http://dx.doi.org/10.1016/j.actamat.2016.01.068
1359-6454/

JMAK approach [20,43], statistical modeling [44,45], enlargement of the RVE by utilizing distributed memory parallel computing [46] and averaging over multiple simulations of small systems, i.e. solitary modeling [21,24,42,47]. In solitary models multiple copies of a microstructure are instantiated and separately simulated to finally compile the global results by various averaging schemes. Since the simulation domains are small and independent (i.e. solitary), they allow rapid memory access, and parallel computer architectures can thus be utilized much more efficiently [48]. However, a common problem of solitary modeling is that the size reduction of the simulation domains causes finite size effects, whose significance and potential detrimental effect on the model predictions is difficult to quantify.

The present contribution is also motivated by the requirement to adjust recrystallization modeling paradigms to modern parallel computer architectures, for which solitary modeling is expected to yield access to statistics over larger populations at finer discretization. Hence, a solitary model for the simulation of recrystallization is introduced. Our approach is based on a random sampling of many observation domains from a large bulk specimen into so-called solitary units, each of which specifies a deformation microstructure that can be locally heterogeneous and is solved concurrently in parallel with others. The domains, which are defined as a solitary cellular automaton grid, remain without mutual communication during the whole simulation. Different simulation cases were devised to cover an ample range of nucleation and growth parameters affecting primary recrystallization. The results of the simulations with the solitary model were compared to those of finely-discretized RVE simulations under conditions which were exactly the same. With this strategy we aim at understanding in detail the cause and evolution of potential finite size effects and to formulate quantitative guidelines on how to devise optimal scaling setups for the utilization of the model.

2. Simulation model

Cellular automata (CA) simulations of recrystallization are the method of choice when the capillary driving force ($p_c \approx 0.01 - 0.1\ MPa$) is negligible compared to the contribution from the stored elastic energy ($p_d \approx 1 - 10\ MPa$) [4], which corresponds to most of the relevant cases of primary recrystallization [2]. For this reason, the proposed solitary model was based on a 3D cellular automaton (CORe) model that uses the partial RX step method [27] to infect the cubic cells into which the microstructure is discretized in a 3D Moore neighborhood [46]. The reader is referred to [28,46] for details of the model as it is used in RVE simulations.

A peculiarity of the present implementation is that it allows the simultaneous initialization and distribution of independent real time- and space-scaled 3D CA domains (solitary unit domains) on the computing nodes of a distributed computer. Additionally, it includes analysis routines that pool the individual results into ensemble statistics. The basic computational scheme of this Statistical Cellular Operator Recrystallization Ensemble (SCORE) model is presented in Fig. 1.

The basic idea of the SCORE model is to separate pieces of information into independent and many as small as possible solitary units, also referred to as spatial domains or just domains in the following, in order to minimize the time-to-solution and, in general, to increase the statistical significance of the simulation setup. The solitary units sample randomly from a large reference volume into an ensemble that adequately represents the essential properties of the desired physical system. For recrystallization, this physical system reflects basically the impact of the prior processing history of the material and is synthesized in the same way as in the CORe model [27,28]. It comprises the deformed microstructure in the form of grains and their dislocation densities and a separate nucleation model, e.g. Refs. [49,50] or others. During the simulation, the computing domains develop independently and concurrently, and finally the results are compiled and evaluated. It is evident that the representation of the recrystallization behavior of a large contiguous grain assembly by a statistical average of the behavior of independent solitary units will depend on the size and the number of solitary units. In order to assess the predictive quality of a model based on such solitary units we conducted a study where the behavior of a contiguous large grain assembly (RVE) was compared with the statistically averaged behavior of independent spatial domains, which were cut out of the RVE (Fig. 1).

2.1. Deformation microstructure and nucleation model

Recrystallization proceeds in a deformed crystalline structure. Therefore, each simulation requires the definition of an initial structure. Two cases were considered, namely a deformed single crystal and a deformed polycrystal. The single crystal consisted of only one grain with a given orientation and a specific and uniform dislocation density. By contrast, the polycrystal was composed as an assembly of cubic grains of only three different components, A, B, and C, each of which had a specific orientation and a specific dislocation density (Table 1). The assembly was constructed by randomly picking grains from components A, B or C such that their spatial arrangement was random. The dimensions of the grains were chosen to be 1200 μm for the single crystal and 80 μm for the polycrystal. In both cases a total volume of $(1200\ \mu m)^3$ was simulated with each solitary unit ensemble by discretizing the grains into cubic cells with a resolution of $(1\ \mu m)^3$ each.

Two nucleation site densities were studied which we refer to as simulations with a high and a low nucleation site density, respectively. Specifically, a simulation with a high nucleation site density contained a total of 125000 nuclei, whereas 15625 nuclei in total (i.e. an eighth) were seeded in simulations referred to be of a low site density, respectively. In all cases, the reference volume was $(1200\ \mu m)^3$ for each setup. These settings assured a fine spatial discretization with an equivalent discrete spherical radius of 15 cells on average even for the setup with a high nucleation site density. Nucleation was assumed to occur instantaneously, i.e. all nuclei started growing at the beginning of the simulation without retardation. A nucleus was assigned randomly one of two orientations (Table 2), which were chosen in such a way as to assure that the nuclei had a high angle boundary in a particular disorientation angle relationship to each of the 3 components A, B, or C.

We implemented the mobility model suggested by Sebald and Gottstein [44], which distinguishes particularly mobile high-angle grain boundaries from the general high-angle and the practically immobile low-angle grain boundaries based on the disorientation angle [44]. In effect, the nuclei shared one of two possible disorientation angles with the deformed matrix grains which made them either “fast” nuclei, as their boundaries migrated fast, or slow nuclei, respectively (Table 2). Specifically, the ratios of the mobility of fast and slow grains were set to 1, 2, 4, and 8, respectively. In addition, the fraction of fast nuclei in the population was varied between 20%, 40%, 60%, and 80% of the total population, respectively. The spatial arrangement of the fast nuclei was uncorrelated, as it was the case for the slow nuclei. To allow for a successful comparison in this parametric study, nucleation was deterministic in terms of position and orientation. All internal disorientation calculations were performed for computational efficiency in quaternion representation based on the methods suggested by Ref. [51] in Bunge Euler notation [52,53].