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Full field modeling of recrystallization: Effect of intragranular strain gradients on grain boundary shape and kinetics

D.N. Ilin, N. Bozzolo, T. Toulorge, M. Bernacki*

Mines-ParisTech, PSL-Research University, CEMEF Centre de mise en forme des matériaux, CNRS UMR 7635, CS 10207 rue Claude Daunesse, 06904 Sophia Antipolis Cedex, France

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ABSTRACT

The effect of stored energy field heterogeneity on the microstructure evolution during static recrystallization (SRX) was assessed by performing three dimensional (3D) full field simulations. These simulations were performed by using the Level set (LS) method in a finite element (FE) framework with unstructured tetrahedral FE mesh. An extension of classical LS-FE for SRX was developed to account for average stored energies in zones adjacent to grain boundaries (GBs) in each grain. Annihilation of dislocations by a passing GB was taken into account. The results of 3D simulations were analyzed to compare the "per interface" LS model to the usual "per grain" LS method (with averaging stored energy per grain). Recrystallization is faster at the beginning of the heat treatment when using the "per interface" model. The analysis of the evolution of grain volume and grain surface scattering reveals that the "per interface" approach results in complex shapes of grains which are closer to those observed in experiments. Local simulations for few grains with refined FE mesh were also performed to study the effect of stored energy heterogeneity along interfaces, and even higher complexity of grain topology was observed compared to the results of "per interface" computations.

1. Introduction

Understanding of microstructure evolution during thermo-mechanical processing is crucial for the prediction and optimization of mechanical properties of metals and alloys. Numerical simulations can contribute to the better description of static, dynamic and postdynamic recrystallization, grain growth and Smith-Zener pinning phenomenon [1]. In a full field context, they can be performed using probabilistic Monte Carlo Potts [2–6], Celullar Automata [7–9], deterministic phase field [10–12], vertex [13,14] or level set (LS) [15–26] models. These numerical methods are currently used and developed by numerous researchers [27] and regularly compared for particular metallurgical mechanisms [13,19].

Of course, all the mentioned models have their own strengths and weaknesses. The LS method, with recent developments of optimization techniques, namely, a direct and parallel reinitialization algorithm [28] and a recoloring scheme [29] coupled with a meshing/remeshing strategy in context of unstructured FE mesh can be considered as an efficient and accurate way to model large systems evolution for static [20] or dynamic recrystallization [21]. However, many challenges remain for modeling microstructure evolution with adequate description of all physical aspects at the microscopic scale and in 3D. Influences of stored energy heterogeneities at the grain scale and anisotropy of mobility and interface energy (by taken into account the entire five dimensional domain of GB existence in the description of the GB energy) need to be further investigated. To take into account these effects in the FE-LS approach, a careful analysis of the solution behavior is required since instabilities can raise from heterogeneous velocity field [17].

In previous works using the LS method for modeling the Smith-Zener pinning phenomenon or recrystallization, the effect of dislocation density heterogeneities on the GBs motion was taken into account at the mesoscopic scale by averaging the stored energy per grain (and computing the corresponding energy gradient across GBs). To the authors knowledge, this approximation is systematic for the deterministic methods except in the full field formulation of [30] where, however, the heterogeneous intragranular stored energy field and its evolution are not taken into account directly. The "per grain" approach provides quite good agreement of computed recrystallization kinetics with experimental ones but GBs keep regular shapes without remarkable development of curvatures [20,22–24]. Similar grain topology can be found in a recent paper reporting the results of the vertex method coupled with a crystal plasticity model [31]. Results of simulations without averaging procedure using the Monte Carlo Potts model [3–6] or Celullar Automata [7–9] reported in the literature do not put in

* Corresponding author.
E-mail address: marc.bernacki@mines-paristech.fr (M. Bernacki).

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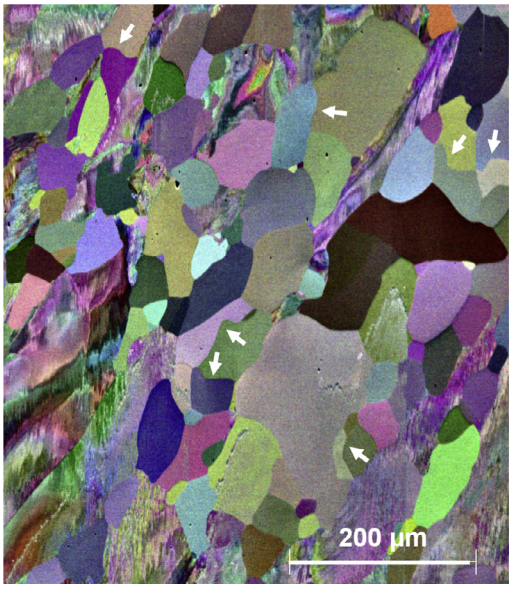

Fig. 1. Experimental micrograph obtained with the FSE detector of a SEM on a partially recrystallized tantalum sample. The color contrast is orientation dependent. Recrystallized grains appears with an homogeneous color contrary to the unrecrystallized ones exhibiting substructures. White arrows indicate few examples of grain boundaries between recrystallized grains with a complex shape. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

evidence either the development of irregular shapes of GBs at the transient states of recrystallized microstructures. The experimental measurements, however, often reveal the appearance of distorted GBs during recrystallization as illustrated by the white arrows in Fig. 1 for an experimental micrograph obtained with the Forward Scattered Electrons (FSE) detector of a Scanning Electron Microscope (SEM) on a partially recrystallized tantalum sample.

In the present work, the effect of stored energy heterogeneity was assessed at the intragranular scale by considering the stored energy per each interface (GB) of a given grain. The energies on one side of each GBs and on its other side can differ due to the heterogeneity of the original stored energy field, as provided by crystal plasticity FE computations [26,32], thereby establishing an energy gradient which contributes to the GBs motion. This approach still provides an approximate estimation of recrystallization kinetics but more accurately from the physical point of view than "per grain" method [20,21], notably at the multiple junctions. In addition, in the developed "per interface" approach, a minimal e_0 value (material dependant) for the stored energy is imposed, as in [21] for "per grain method", in recrystallized zones to account for the annihilation of dislocations by a passing GB. The stored energies near interfaces are updated at each time step. The GB energy and mobility were assumed to be isotropic in the following.

The proposed method was first validated considering simple configurations. Namely, the simulations of 2D and 3D three grain junction motion with constant velocities were performed, and the results were compared with analytical solution discussed in the literature [33]. Then, 3D simulations of static recrystallization were carried out and compared with ones obtained in [20] for 304L stainless steel. Finally, the numerical study was conducted on few grains with refined mesh without averaging to analyze the effect of stored energy heterogeneities along GB. The results were compared with ones obtained using the "per interface" approach.

2. Numerical model

2.1. Level set description of the polycrystals

In this work, the full field modeling was performed by using the LS method in a P1 FE framework. In the LS approach, each sub-domain G (grain) in a given domain Ω (polycrystal) is classically described implicitly by computing the signed distance function $\phi(x,t)$ representing the distance to the sub-domain boundaries $\Gamma = \partial G$ (grain boundaries). In the used P1 formulation, the function $\phi(x,t)$ is calculated at each node on the FE mesh and is chosen, by convention, positive inside of the grain and negative outside:

$$\begin{cases} \phi(x,t) = \pm d(x,\Gamma(t)), x \in \Omega, \\ \Gamma(t) = \{x \in \Omega : \phi(x,t) = 0\}, \end{cases} \tag{1}$$

where $d(x,\Gamma(t))$ means the Euclidean distance from the point $x \in \Omega$ to the boundary $\Gamma(t)$. In the LS method, the evolution of $\phi(x,t)$ is given by the following transport equation [15]:

$$\begin{cases} \frac{\partial \phi(x,t)}{\partial t} + \vec{v}(x,t)\cdot\nabla\phi(x,t) = 0, \\ \phi(x,t=0) = \phi^0(x), \end{cases} \tag{2}$$

where $\vec{v}(x,t)$ is the velocity field. It is generally assumed for metals that the kinetic law for grain boundary motion can be defined as [34]:

$$\vec{v} = MP\vec{n}, \tag{3}$$

where M is the grain boundary mobility, P is the net pressure i.e. the net driving force per unit area, and $\vec{n}$ is the outward unit normal to the GB. In context of deterministic full field approaches, the net pressure is classically defined as:

$$P = \tau[\![\rho]\!] - \gamma\kappa, \tag{4}$$

where τ is the dislocation line energy, $[\![\rho]\!]$ is the dislocation density jump across interfaces, γ is the GB energy and κ is the mean GB curvature (i.e. the curvature in 2D and the sum of main curvatures in 3D). That is the GB motion is governed by the stored energy gradient across the GBs and capillarity. The isotropy hypothesis remains here to consider M as only dependant of the temperature and γ as constant. Let's consider a polycrystal consisting of N_g grains and N_p LS functions are used to represent the polycrystalline aggregate. Assuming that $\|\nabla\phi_i(x,t)\| = 1$, $\forall\, i \in [\![1,N_p]\!]$, i.e. ϕ_i remain distance functions all along the simulation, after substituting Eq. (4) into Eq. (3) and Eq. (3) into Eq. (2), and by considering the following properties of distance functions with the chosen sign convention,

$$\vec{n}_i = -\nabla\phi_i/\|\nabla\phi_i\| = -\nabla\phi_i, \quad \kappa_i = \nabla\cdot\vec{n}_i = -\Delta\phi_i, \tag{5}$$

one can solve a set of N_p convective-diffusive equations to take into account Eq. (3) for all the grains of the considered polycrystal [18]:

$$\begin{cases} \frac{\partial \phi_i(x,t)}{\partial t} - M\gamma\Delta\phi_i(x,t) + \vec{v}_i^{[\![\rho]\!]}\cdot\nabla\phi_i(x,t) = 0, \\ \vec{v}_i^{[\![\rho]\!]} = M\tau[\![\rho]\!]_i\vec{n}_i, \\ \phi_i(x,t=0) = \phi_i^0(x). \end{cases} \tag{6}$$

Details concerning how $\vec{v}_i^{[\![\rho]\!]}$ is finally decomposed by considering a "per grain" or a "per interface" approach are described in the following sections. In the case where $N_p = N_g$, the number of equations is equal to the number of grains. In the present work, we use the coloring scheme [29] which allows to limit the number of needed LS functions. The polycrystal is decomposed into families of distinct grains (not neighboring), and each family is represented by a single Global Level set (GLS) function $\phi_i(x,t)$ verifying Eq. (6). The recoloring scheme introduced in [29] and improved in [20] is used: each family contains only the grains which are separated by a critical distance. To avoid the numerical coalescence of grains represented by the same GLS function, a dynamic swapping procedure (recoloring) is performed at each time