Simulation of Grain Growth Under the Effect of Stress

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Abstract. During anisotropic curvature driven grain growth, high-energy grain boundaries are preferentially eliminated, thus leading to interface texture development and a higher population of low energy grain boundaries. However, when stress is introduced as an additional driving force, the dynamics of grain growth change. To model these effects, a three dimensional anisotropic multi-level set model was modified in order to account for the effect of stress field on grain growth. For this mesoscale study, grain boundaries were treated as dislocation structures and their associated net Burgers vectors were calculated using the misorientation information and boundary inclinations. Using these net Burgers vectors and their associated densities, additional forces due to stress field were calculated via the Peach-Koehler equation. Qualitative comparisons of 5 parameter grain boundary character distribution will be carried out in order to analyze the differences in texture evolution during grain growth.

Introduction

Materials properties and performance of polycrystalline solids are linked to the distribution of grain boundaries. Through grain boundary engineering [1], certain populations of grain boundaries are enhanced thus a grain boundary character distribution is favored [2]. Recent developments in three dimensional imaging techniques and simulations have extended the five dimensional grain boundary character distribution analysis [3]. In this analysis, grain boundary populations are specified by the grain boundary character distribution, $\lambda\left(\Delta g, \hat{\mathbf{n}}\right)$, which is the distribution of relative areas of distinguishable grain boundaries parameterized by their lattice misorientation $\left(\Delta g\right)$ and boundary plane orientation $(\hat{\mathbf{n}})$ [4]. Previous experimental work has demonstrated that significant texture can appear in grain boundary character distributions and that low energy boundaries occur in these distributions with greater frequency than higher energy boundaries [4] and [5]. Recent three dimensional grain growth simulation with anisotropic grain boundary energy was successful in replicating the experimental observations of grain boundary character distribution [6].

Stress induced grain boundary (GB) migration has been shown in small angle bicrystals [7, 8] and also for high angle grain boundaries [9, 10]. Atomistic simulations using Molecular dynamics have demonstrated very clearly that even high angle boundaries can move under stress driving forces, just as if they possessed dislocation-like structures. The possibility to affect microstructural evolution with stress opens up new engineering opportunities [11]. In view of the renewed interest in using

stress as an additional field in grain growth, it is important to be able to predict the influence of stress on the evolution of grain boundary character distribution. This then motivates the current work, which computes the dislocation character of each boundary by net burgers vector analysis and uses a multi-field level set algorithm to simulate grain coarsening with both curvature and stress driving forces.

Dislocation Content Analysis

We follow the standard Frank-Bilby approach to calculate the dislocation structure of a general grain boundary [12]. We assume that boundaries adopt the minimum energy configuration in well annealed materials. Thus the configuration is sought that minimizes the total dislocation density of the boundary. The standard set of six independent Burgers vectors in fcc metals are considered, i.e. $\mathbf{b} = \{a/\sqrt{2} < 110 >\}$. Each set of three independent Burgers vectors is considered in turn. The reciprocal Burgers vectors, $\mathbf{b}^*$, are calculated as in the following example.

$$\mathbf{b_1^*} = \frac{\mathbf{b_2} \times \mathbf{b_3}}{\mathbf{b_1} \cdot \mathbf{b_2} \times \mathbf{b_3}} \tag{1}$$

Other coefficients are obtained by permutation of the suffices. For each Burgers vector, a vector, $\mathbf{N}$, can be defined whose length is equal to the reciprocal of the dislocation spacing, d_l, and that is perpendicular to the line sense of the dislocations. The magnitude of each $\mathbf{N}$ represents the dislocation density associated with that particular Burgers vector.

$$\mathbf{N}_i = 2\ sin(\theta/2)\left\{\hat{\rho} \times \mathbf{b}_i^* - \hat{\mathbf{n}}(\hat{\mathbf{n}} \cdot \hat{\rho} \times \mathbf{b}_i^*)\right\}, \tag{2}$$

where the suffix on $\mathbf{N}$ and $\mathbf{b}^*$ denotes the Burgers vector index, $\hat{\rho}$ is the misorientation axis and $\hat{\mathbf{n}}$ is the boundary normal (both unit vectors). The appropriate configuration is then that which minimizes $\Sigma|\mathbf{N}|$, i.e. the total dislocation density required to satisfy the geometry of the interface. To compute the dislocation structure of each location on a given boundary, the normal and the misorientation are provided to the procedure and the energy of all possible combinations of Burgers vectors are calculated, which, in effect, considers all the symmetrically equivalent positions of the crystal lattices. This calculation is repeated for each of the two lattices and the minimum energy configuration is selected for computation of the force on the boundary.

Anisotropic Multi-Level Set Method

The level set method can be used to accurately simulate the evolution of the sharp interface between two domains when a theoretical expression for the local velocity of this interface is known and computable. The level set method was first popularized by Osher et al. [13] and is used extensively in the fields of fluid dynamics and image analysis. Numerous books [14, 15] have been written about the level set method. For a brief introduction to the level set method, the reader is referred to [16].
Work with the level set method is not widespread within the materials science community, although application to second-phase particle dissolution has received some attention [17]. The lack of interest is perhaps due to the fact that the level set method is a velocity-based formalism, and not an energy-based approach. However, if we are to develop computational models that simulate microstructure evolution on a truly mesoscopic scale, at lengths such that gradients in the free energy and diffuse boundary widths are not available at runtime, sharp-interface velocity-based models would seem to be an inevitable next step.

Given a theoretical expression for the local boundary velocity v, the level set method advects a scalar function $\phi(x)$ in such a way so that the contour $\phi(x) = 0$ (which represents the boundary) moves appropriately, via the simple PDE given by Eq. 3.

This may be implemented by a finite difference scheme on a regular grid. The mathematics community has provided a rigorous foundation for working with this equation even when $\phi(x)$ develops discontinuities or undergoes topological transformations (see e.g. [15]).

One of the difficulties with the level set method is the need to extract explicit mesoscopic boundary velocity laws as functions of mesoscopic quantities from microscopic considerations. Because boundary normals n are obtained by simply taking gradients of the level set function $\phi(x)$, i.e. $\mathbf{n} = \text{grad}(\phi) / |\text{grad}(\phi)|$, the Peach-Koehler force and its associated boundary velocity may be explicitly computed as long as the misorientation is known. Therefore the level set method provides an ideal computational model to investigate boundary motion coupled to a strain field.

We seek to model not only single boundary evolution, but also the resulting microstructural evolution in a polycrystalline material. The level set method was originally developed for modeling the motion of a single interface that decomposes space into only two separate domains namely, the region where $\phi(x) > 0$; and the region where $\phi(x) < 0$. Although a few authors [13, 18] have presented multi-level set methods for modeling the evolution of grain boundaries in polycrystalline materials, this paper is based upon a novel approach that we refer to as the interface level set method. The principal subject of this work is the application of the interface level set method to study the affect of microstructure evolution when boundary motion is coupled to the local strain. Therefore a much more detailed exposition of the interface level set method will be presented in a later work. For completeness, however, we provide here a brief description of the interface level set method.

To every grain associate the level set function $\phi_i(x)$. The interior of grain i will be defined as the set of all points x such that $\phi_i(x) > \phi_j(x)$, for all other grains j. In contrast to the level set method, which defines boundaries as the set of points x such that $\phi(x) = 0$, we will define the grain boundary between grains i and j as the set of points x such that $\phi_i(x) = \phi_j(x)$. To evolve the boundary ij with a known local velocity $\mathbf{v}_{ij}(x)$, we define the interface function $\phi_{ij}(x) = \phi_i(x) - \phi_j(x)$, with $\phi_i(x) > \phi_j(x)$. We then advect the contour $\phi_{ij}(x) = 0$ according to the traditional level set equation:

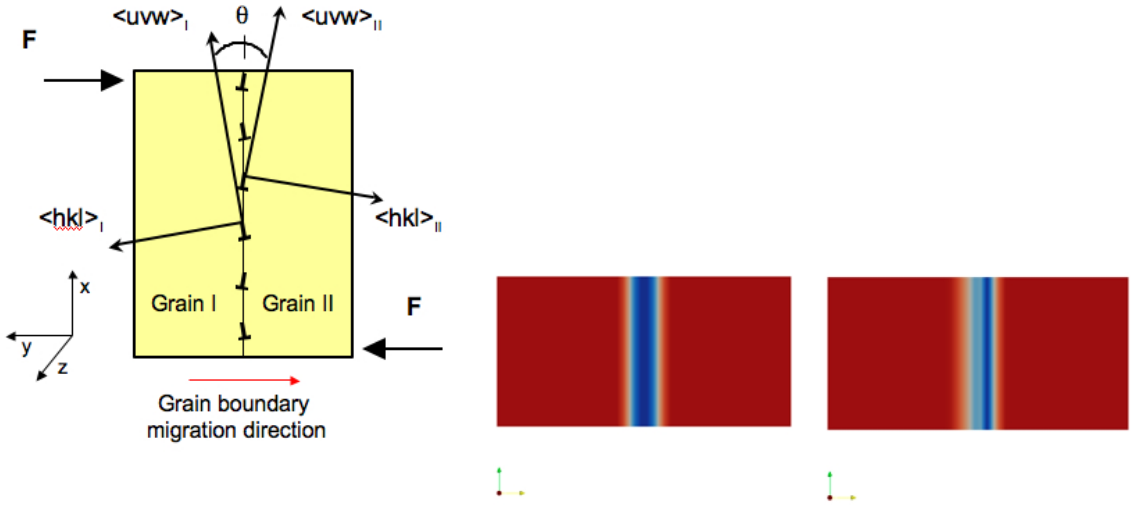
$$\frac{\partial \phi_{ij}}{\partial t} = -\mathbf{v}_{ij} \cdot \nabla \phi_{ij} \tag{3}$$

We note that Steinbach et al. [19] originally proposed such functions in the context of a multiphase field model. As Steinbach points out, there are $N(N-1)$ such functions $\phi_{ij}(x)$ at any point where there are N relevant level set functions. It is thus necessary to select a subset of the functions $\{\phi_{ij}\}$ in order to obtain evolution equations for the $\{\phi_i\}$. We therefore consider only the evolution equations for the interface functions $\phi_{mj}(x)$, with m defined locally by $\phi_m(x) > \phi_j(x)$ for all j. There are $(N-1)$ such fields and so there are $(N-1)$ associated evolution equations, given by 3 with $i = m$ and $1 \leq j \leq N$ and $j \neq m$. One more equation is needed to determine evolution equations for ϕ_i. We choose to impose the constraint

$$\sum_i \phi_i = M \tag{4}$$

The constant M serves as an adjustable parameter in this model and does not have any physical significance.

We note that in regions corresponding to more than two grains, multijunctions are very well-defined, and correspond to points at which all level set functions $\phi_i(x)$ are equal. It follows that triple junctions and quad nodes are represented unambiguously in the interface level set method. We mention in passing that equations 3 must be modified near multijunctions in order to couple boundaries together and enforce any relevant multijunction force balance (such as Young's law).



(a) Diagram of a bi-crystal with a symmetric tilt boundary, showing the expected migration direction for the boundary based on the applied shear stress indicated

(b) Initial bi-crystal state. Red indicates a grain interior and blue a boundary.

(c) Bi-crystal with boundary moving to the right under the stress shown in (a).

Figure 1: Bi-crystal geometry used to verify the calculation of grain boundary motion under the action of an applied shear stress.

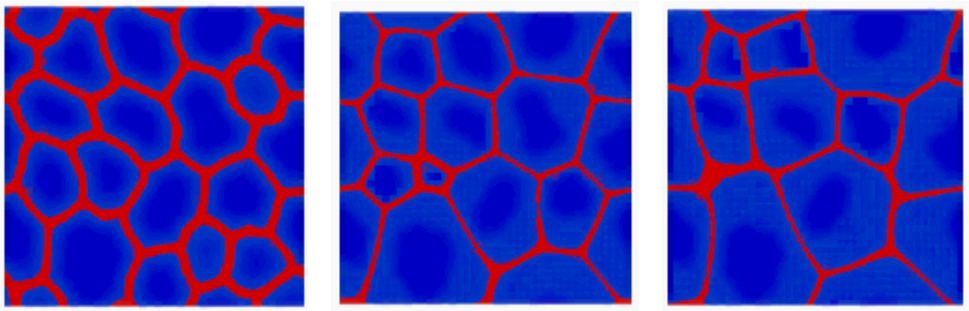
All other issues relevant to level set models (such as initialization, reinitialization, and velocity extension) can be extended to the interface level set framework. These topics will be discussed in greater detail in future publications. In all simulations conducted for this work, a thin-interface convective reinitialization method was used to localize computation to a small region around the grain boundaries, and so boundaries appear to be diffuse. Images represent the scalar function $\left(\phi_m(x) - \phi_j(x)\right)^2$.

Results & Discussion

Figure 1 shows a diagram of a symmetric bi-crystal with a particular applied shear stress and the direction in which the boundary should move in response to this shear stress. This arrangement is used to verify that the level set code with stress driving force correctly calculates the boundary migration.

The first the three panels, Fig. 1(a), is the initial bi-crystal configuration; red indicates a grain interior and blue indicates a boundary, where the color is related to the maximum value of any of the fields. The second panel, Fig. 1(b), shows the initial state of the fields where red signifies the bulk of a grain and blue (low) the boundary. The third panel, Fig. 1(c) shows the boundary moving to the right. The orientations used here (Bunge Euler angles, in degrees) were (176.6 90 90) for Grain1(left) and (93.2 90 90) for Grain2 (right).

Figure 2 shows results from simulation of grain growth in a two-dimensional polycrystal, such as might be expected in a thin film. The simulation is, in fact, three dimensional, but the grid is 128 x 128 x 10 voxels such that the grain structure is columnar and the images are shown in the x-y plane. The first panel 2(a) shows the initial microstructure. The second panel, Fig. 2(b), illustrates the result of grain growth with only curvature as a driving force. The third panel, Fig. 2(c) , shows the microstructure with stress applied in addition to curvature. The magnitude of the applied stress was chosen so as to compete with the curvature driving forces at approximately the same level. The



(a) Initial microstructure. Blue indicates a grain interior and red a boundary.

(b) Curvature driven

(c) Curvature and Stress driven

Figure 2: Comparison of curvature-only and curvature-with-stress driven grain growth in 2D

microstructures are visibly different as a consequence of adding the stress driving force.

These preliminary results demonstrate that stress as a driving force has been successfully incorporated into a mesoscale algorithm for simulating grain growth, in addition to the curvature driving force. It is clear that stress changes the evolution of the grain boundary network during grain growth. Future work will examine the effect of adding stress as a driving force on the Grain Boundary Character Distribution to find out which boundary types are favored under these circumstances.

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