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Grain size distribution under simultaneous grain boundary migration and grain rotation in two dimensions

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ABSTRACT

We explore the effects on grain size distribution of incorporating grain rotation into the curvature driven grain boundary migration model of Mullins. A new, extremely streamlined and efficient algorithm allows simulations with large numbers of grains. Some of these simulations yield size distributions and microstructures close to those from recent, atomistic simulations of microstructural evolution using the phase field crystal method that was shown to reproduce experimental size distributions observed in fiber textured, nanocrystalline, thin metallic films.

1. Introduction

Polycrystalline materials, such as most metals and ceramics, are composed of many single crystal pieces of differing orientation that are known as grains. The shapes and sizes of the grains are well-known to have significant implications for the physical properties of a polycrystalline material, such as its yield strength and conductivity. It is therefore of great practical interest to understand how the sizes and shapes of grains change under common manufacturing processes such as annealing. A well known model for how the grains evolve during annealing was given by Mullins [21]. It is a continuum description of the grain boundaries as a network of surfaces that move via gradient flow to decrease a weighted surface energy. Different versions of this model, often with additional simplifying assumptions, have been studied numerically using a variety of algorithms, such as kinetic Monte Carlo, front tracking, phase field, level sets, and threshold dynamics. Various statistics of grains, such as grain size distribution, grain boundary character distribution, and distribution of the number of neighbors are typically reported in these numerical studies.

In [2,3], an important discrepancy between the grain size distribution (GSD) obtained from numerical simulations of Mullins' continuum model in 2D and that from experiments with fiber textured nanocrystalline thin films is reported. In this setting, the crystallographic orientation of each grain is described by a single parameter: the angle of rotation about the axis normal to the film. In the reported experiments, grains range in size from 10 to 100 nm. The eventual GSD observed differs considerably from that of numerical simulations in having far more very small as well as very large grains compared to the median.

Backofen et al. [1] carried out simulations of grain growth in two dimensions using the phase field crystal (PFC) model [6]. This is an atomistic model that appears to allow for simulations on time scales beyond what is possible with other atomic scale strategies such as molecular dynamics. As such, it is a promising new tool for very detailed simulations of mesoscale features such as grain boundaries. In [1], the authors report that the resulting GSD resembles the experimentally observed one in [2,3] far more than the distribution obtained from Mullins' model. They suggest a number of different mechanisms not captured by Mullins' continuum model that may be responsible for the more faithful reproduction of experimental results by the PFC simulations. One of these mechanisms is grain rotation [10]. More recently, incorporating triple junction drag into Mullins' model has been shown in [23] to yield GSDs resembling the experimental results of [2,3]. Despite being overruled in [3], it thus appears that triple junction drag may be at least partially responsible for the discrepancy in size distribution.

A prominent feature of the results of [1] is that the shapes of the grains in the PFC simulation appear to be quite different from the very regular, almost polygonal grains seen in essentially all two dimensional simulations of Mullins' model (especially with equal surface tensions), computed whether by phase field (e.g. [18]), front tracking (e.g. [15]), or threshold dynamics (e.g. [7]) techniques. In the images and videos of the PFC simulation provided in [1], it is abundantly clear that grain rotation and other fine scale dynamics such as the motion of dislocations frequently lead to

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elimination of certain grain boundaries resulting in coalescence events that yield many grains with very eccentric, meandering shapes. A natural question is whether elimination of some of the very low energy grain boundaries through such processes may be at least partially responsible in deforming the GSD towards the one reported in [1]. In particular, our goal in this paper is to explore whether grain rotation and coalescences, when incorporated into Mullins' continuum model, may explain the GSDs and unusual microstructures seen in PFC simulations of [1].

To investigate these questions, we propose a new, very simple model of grain rotation that is inspired by [20,26] and which turns out to be quite similar to a model considered in [11,12,19]. Our model can be seen as the natural multiphase version of the one introduced in [26], which uses an additional phase field variable to describe the orientations of grains in the network. This variable, which is observed to be approximately piecewise constant, is part of the gradient descent dynamics and leads to gradual variations in the orientations of the grains as an additional dissipation mechanism besides the geometric (curvature) flow of the grain boundaries. The numerical treatment of this very interesting model appears to be quite challenging. Here, for our much simpler, multiphase version, we are able to give an extremely streamlined algorithm by leveraging some of the recent advances in numerical treatment of curvature motion in networks [9]. In fact, the basic version of the algorithm can be implemented in literally a few lines of Matlab code; a slightly more sophisticated version allows us to carry out large scale simulations that probe the effects of grain rotation and coalescence on the GSD in Mullins' model.

2. Our model and algorithm

Let $\Sigma_j \subset \mathbb{R}^d$ denote the space occupied by the j-th grain in the microstructure. Although the algorithms discussed below work in any dimension and for more general energies, in this study we focus on the two dimensional version of Mullins' model for which the energy of the grain network is given by

$$\sum_{i<j} \sigma(\theta_i, \theta_j) \text{Length}(\Gamma_{i,j}) \tag{1}$$

where $\Gamma_{i,j} = \partial\Sigma_i \cap \partial\Sigma_j$ denotes the boundary between the i-th and j-th grains. In particular, we will neglect normal dependence of the energy density. The surface tension factor σ is chosen in accordance with the Read–Shockley model [22] along with a Brandon angle [4] that will be denoted θ_*, often taken to be between 15° and 30°:

$$\sigma(\xi, \eta) = \min_{k=1,2,3,\ldots} f\left(\left|\xi - \eta + \frac{k\pi}{4}\right|\right) \tag{2}$$

where

$$f(\theta) = \begin{cases} \frac{\theta}{\theta_*}\left(1 - \log\left(\frac{\theta}{\theta_*}\right)\right) & \text{if } \theta \in [0, \theta_*] \\ 1 & \text{if } \theta > \theta_*. \end{cases} \tag{3}$$

According to Mullins, the dynamics associated with energy (1) is given by L^2 gradient descent for the interfaces, leading to the normal speed

$$v_{i,j} = \mu_{i,j}\sigma(\theta_i, \theta_j)\kappa_{i,j} \tag{4}$$

for interface $\Gamma_{i,j}$. Here $\kappa_{i,j}$ denotes the mean curvature of $\Gamma_{i,j}$, and $\mu_{i,j} > 0$ is a mobility factor. Along triple junctions formed by the meeting of three distinct grains Σ_i, Σ_j, and Σ_k, Herring angle conditions [13] hold:

$$\sigma(\theta_i, \theta_j)n_{i,j} + \sigma(\theta_j, \theta_k)n_{j,k} + \sigma(\theta_k, \theta_i)n_{k,i} = 0 \tag{5}$$

so that angles formed by normals $n_{i,j}$, $n_{j,k}$, and $n_{k,i}$ to the three interfaces $\Gamma_{i,j}$, $\Gamma_{j,k}$, and $\Gamma_{k,i}$ along the triple junction are determined by their associated surface tensions. As we have ignored normal dependence of surface tensions in (1), torque terms to not appear in (5); in this simpler form, the angle conditions are also known as Young's law.

The algorithms used in this study are obtained from a non-local approximation to energy (1): These approximate energies are given by

$$\frac{1}{\sqrt{\delta t}} \sum_{i<j} \sigma(\theta_i, \theta_j) \int_{\Sigma_i} G_{\delta t} * \mathbf{1}_{\Sigma_j}\, dx \tag{6}$$

where G_t denotes the Gaussian kernel in two dimensions

$$G_t(x) = \frac{1}{4\pi t} \exp\left(-\frac{|x|^2}{4t}\right) \tag{7}$$

and $\mathbf{1}_\Sigma(x)$ for a set Σ denotes its characteristic function:

$$\mathbf{1}_\Sigma(x) = \begin{cases} 1 & \text{if } x \in \Sigma, \\ 0 & \text{otherwise.} \end{cases}$$

The width δt of the Gaussian kernel appearing in (6) ends up playing the role of the time step size for our scheme, described below, that approximates gradient descent of (1) in L^2 sense, as prescribed by [21]. Energy (6) has been proposed in [9] and has been shown to converge in a very precise sense (namely, that of Gamma convergence) to energy (1) in the limit $\delta t \to 0^+$. Intuitively, we have

$$\frac{1}{\sqrt{\delta t}} \int_{\Sigma_i} G_{\delta t} * \mathbf{1}_{\Sigma_j}\, dx \approx \text{Length}(\Gamma_{i,j})$$

since the function $\frac{1}{\sqrt{\delta t}} \mathbf{1}_{\Sigma_i} G_{\delta t} * \mathbf{1}_{\Sigma_j}$ approximates a delta function concentrating near $\Gamma_{i,j}$ as $\delta \to 0$. The reason for our interest in this specific – perhaps unusual – approximation of Mullins' energy is that it generates exceptionally simple and efficient algorithms for simulating the gradient descent dynamics associated with (1). Indeed, it has been shown in [9] to lead in a systematic way to the correct multiphase, arbitrary surface tension analogue of a very fast algorithm known as *threshold dynamics* that was originally proposed in [16,17] for networks with all equal surface tensions (i.e. $\sigma(\theta_i, \theta_j) = 1$ for all i and j). Let us recall the simplest version of the generalization of threshold dynamics to arbitrary surface tensions given in [9]:

Given the initial grain shapes Σ_i^0 and orientations θ_i and a time step size δt, obtain the grain shapes Σ_i^{n+1} at the $(n+1)$-th time step from the grain shapes Σ_i^n at the end of the n-th time step as follows:

1. Compute the convolutions:
$$\phi_i^n = G_{\delta t} * \mathbf{1}_{\Sigma_i^n}. \tag{8}$$
2. Form the comparison functions:
$$\psi_i^n = \sum_{j \neq i} \sigma(\theta_i, \theta_j)\phi_j^n. \tag{9}$$
3. Update the grain shapes:
$$\Sigma_i^{n+1} = \left\{x : \psi_i^n(x) < \min_{j \neq i} \psi_j^n(x)\right\}. \tag{10}$$

Benefits of Algorithm (8)–(10) include its unconditional stability (time step size δt can be chosen arbitrarily large, constrained only by accuracy considerations), seamless handling of topological changes in any dimension (the algorithm is the *very same* three