Predictive theory for the grain boundary character distribution

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Introduction

Mesoscale experiment and simulation permit harvesting information about both geometric features and texture of microstructure. The grain boundary character distribution (GBCD) is an empirical distribution of the relative length (in 2D) or area (in 3D) of interface with a given lattice misorientation and normal. During the growth process, an initially random texture distribution reaches a steady state that is strongly correlated to the interfacial energy density [5]. In simulation, it is found that if the given energy depends only on lattice misorientation, then the steady state GBCD and the energy are related by a Boltzmann distribution. This is among the simplest non-random distributions, corresponding to independent trials with respect to the energy. Why does such a simple distribution arise from such a complex system?

We outline a new entropy based theory which suggests that the evolution of the GBCD satisfies a Fokker-Planck Equation. Coarsening in polycrystalline systems is a complicated process involving details of material structures, chemistry, arrangement of grains in the configuration, and environment. In this context, we consider just two global features: cell growth according to a local evolution law and space filling constraints. The growth process may a gradient flow or curvature driven growth. We shall impose the Mullins Equation of curvature driven growth. Space filling requirements are managed by critical events, rearrangements of the network involving deletion of small contracting cells and facets. The interaction between the evolution law and the constraints is governed primarily by the Herring Condition, the boundary condition associated to curvature driven growth, and which determines a dissipation relation. To assist in the derivation, a simplified model is introduced which is driven by the boundary conditions and reflects the dissipation relation of the grain growth system. It resembles an ensemble of inertia-free spring-mass-dashpots. For this simpler coarsening network, we are able to see how the implicit scheme which characterizes the Fokker-Planck Equation emerges from the dissipation relation. The theory predicts the results of large scale 2D simulations [1] and is consistent with experiment. We are able to distinguish the scale of coarsening for general geometric features, like average grain area in 2D, from that of texture development. Ongoing work involves analysis of 3D simulation and incorporation of normal dependence.

View of the problem

Reprise of mesoscale theory For our derivation, we confine our attention to a two dimensional structure and interfacial energy densities which depend only on lattice misorientation. We describe the dissipation relation satisfied by this system. Suppose two grains are separated by an arc Γ with misorientation α, normal $n = (\cos\theta, \sin\theta)$, tangent direction b and curvature κ. Let $\psi = \psi(\alpha)$ denote the energy density on Γ, which we take to be a function of α alone. The Mullins Equation of evolution is

$$v_n = \psi\kappa \text{ on } \Gamma. \tag{1}$$

Assume that only triple junctions are stable and that the Herring Condition holds at triple

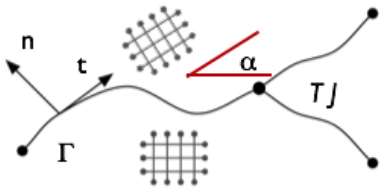

Fig. 1: An arc Γ with normal n, tangent t, and lattice misorientation α, illustrating lattice elements.

junctions. This means that whenever three curves $\{\Gamma^{(1)}, \Gamma^{(2)}, \Gamma^{(3)}\}$, meet at a point p the force balance, (2) below, also known as Young'a Law for this case, holds:

$$\sum_{i=1,..,3} \psi b^{(i)} = 0, \tag{2}$$

Dissipation relation for a network We turn now to a network of grains bounded by $\{\Gamma_i\}$ subject to some condition at the border of the region they occupy, like fixed end points or periodicity. The total energy of the system is given by

$$E(t) = \sum_{\{\Gamma_i\}} \psi|b|ds \tag{3}$$

Owing exactly to the Herring Condition (2), the instantaneous rate of change of the energy

$$\begin{aligned} \frac{d}{dt}E(t) &= -\sum_{\{\Gamma_i\}} \int_{\Gamma_i} v_n^2 ds + \sum_{TJ} v \cdot \sum \psi b \\ &= -\sum_{\{\Gamma_i\}} \int_{\Gamma_i} v_n^2 ds \leqq 0, \end{aligned} \tag{4}$$

rendering the network dissipative for the energy in any instant absent of critical events. Indeed, in an interval $(t_0, t_0 + \tau)$ where there are no critical events, we may integrate (4) to obtain a local dissipation equation

$$\sum_{\{\Gamma_i\}} \int_{t_0}^{t_0+\tau} \int_{\Gamma_i} v_n^2 ds dt + E(t_0 + \tau) = E(t_0) \tag{5}$$

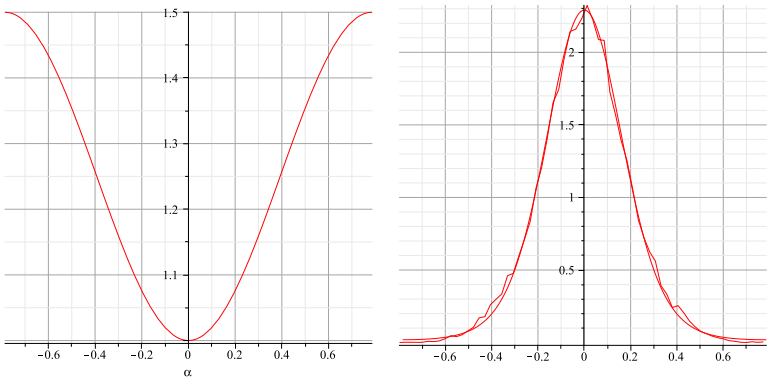

Fig. 2: The energy density $\psi(\alpha) = 1 + \epsilon \sin^2 2\alpha,\ \epsilon = \frac{1}{2}$, used for the examples in this note.

which bears a strong resemblance to the simple dissipation relation for an ensemble of inertia free springs with friction. It is complicated, however, because the first term in (5) is not the sum of velocities of elementary 'elements'.

Entropy and rearrangement events

A role for rearrangement events To begin we define the grain boundary character distribution, GBCD,

$$\begin{aligned} &\rho(\alpha, t) = \text{relative length of arc of misorientation } \ \alpha \ \text{ at time } t, \\ &\text{normalized so that } \int_\Omega \rho d\alpha = 1. \end{aligned} \tag{6}$$

The GBCD is a derived statistic, that is, it is not among the variables being resolved directly in simulation. These are the positions, curvatures, and velocities of the curves which constitute the configuration. The GBCD is harvested from this data. Thus it is a consequence of upscaling a finer level process. In addition to this, the coarsening process itself is irreversible. Once the system has rearranged following the deletion of a cell or a facet, its history is lost and cannot evolve backwards. For these reasons, it is natural to think that entropy may play a role in the description of GBCD evolution. Rearrangement events themselves play an important role in this process. Consider, for example, cells with 5 facets. A given cell with 5 facets has decreasing area according to well known von Neumann-Mullins $n - 6$-rule, [8], [7]. However, there is both experimental and computational evidence, cf. Figure 3, that the relative area of 5-sided cells is increasing. We deduce that the population of 5-sided cells at a given time consists of cells which had $6, 7, 8 \ldots$ facets at earlier times. Thus in the network setting, the topological changes play a major role. Although we may be reasonably confident that small cells with small numbers of facets will be deleted, their effect on the configuration is essentially random. A significant difficulty in developing a theory of the GBCD, and understanding texture development in general, lies in the lack of understanding of the relationship between these stochastic or critical or rearrangement events and the configuration. This leads us to a technically simpler coarsening model.

A simplified model The simplified model is a one dimensional gradient flow with a dissipation inequality amenable to upscaling to the misorientation ensemble α, [3],[2] . In passing to

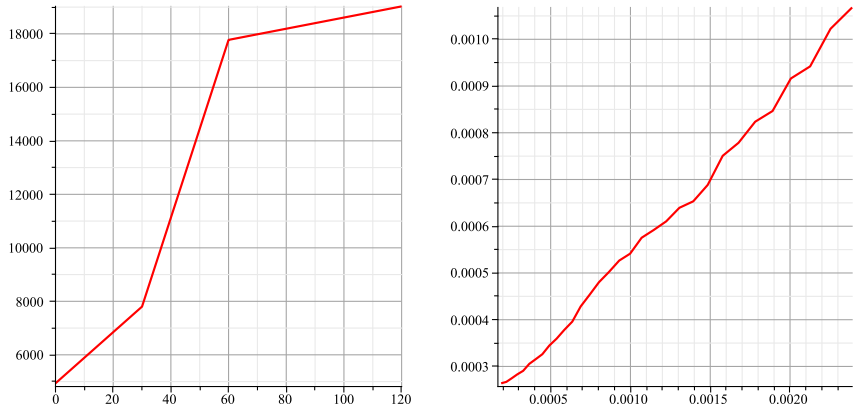

Fig. 3: (a) Simulations tend to exhibit linear average growth in area. (b) Average area in nm^2 of five sided grains in an Al columnar grain structure increases (time in minutes) in distinction to the von Neumann-Mullins rule valid for single cells.

the higher level ensemble, an entropic contribution appears. It is

$$+\int_\Omega \rho \log \rho d\alpha, \tag{7}$$

which is minus the usual physical entropy. Minimizing (7) favors the uniform state, which would be our situation were $\psi(\alpha)$ =constant. Bypassing what might be construed to be mathematical reasoning, the new dissipation relation gives rise to an iterative implicit scheme involving the Monge-Kantorovich-Wasserstein metric. The solution of this scheme has been established, [4], to be the Fokker-Planck Equation

$$\mu \frac{\partial \rho}{\partial t} = \frac{\partial}{\partial \alpha}(\lambda \frac{\partial \rho}{\partial \alpha} + \psi' \rho) \text{ in } \Omega,\ 0 < t < \infty \tag{8}$$

with, in this situation, periodic boundary conditions. There is now an extensive literature about MKW-implicit schemes. We do not know if our statistic $\rho(\alpha, t)$ is a solution of (8) but we may ask if characterizations of solutions may assist in identifying the parameter σ and if solutions have desirable properties which are also shared by ρ.

Relative entropy and validation of the scheme The procedure which leads to the implicit scheme is based on a dissipation inequality, like (5), which holds for the entire configuration but does not identify individual intermediate level 'spring-mass-dashpots'. The consequence of this is that we cannot set the temperature-like parameter σ, but in some way must decide if one exists.

To investigate this, let us introduce the Boltzmann distribution and relative entropy

$$\begin{aligned} &\rho_\lambda(\alpha) = \frac{1}{Z_\lambda} e^{-\frac{\psi(\alpha)}{\lambda}},\ \text{where } Z_\lambda = \int_\Omega e^{-\frac{\psi(\alpha)}{\lambda}} d\alpha,\ \text{and} \\ &\Phi_\lambda = \int_\Omega \rho \log \frac{\rho}{\rho_\lambda} d\alpha \end{aligned} \tag{9}$$

By Jensen's Inequality, $\Phi_\lambda \geqq 0$. If ρ is a solution of (8), then

$$\Phi_\lambda \to 0 \text{ as } t \to \infty,\ \text{exponentially fast.} \tag{10}$$

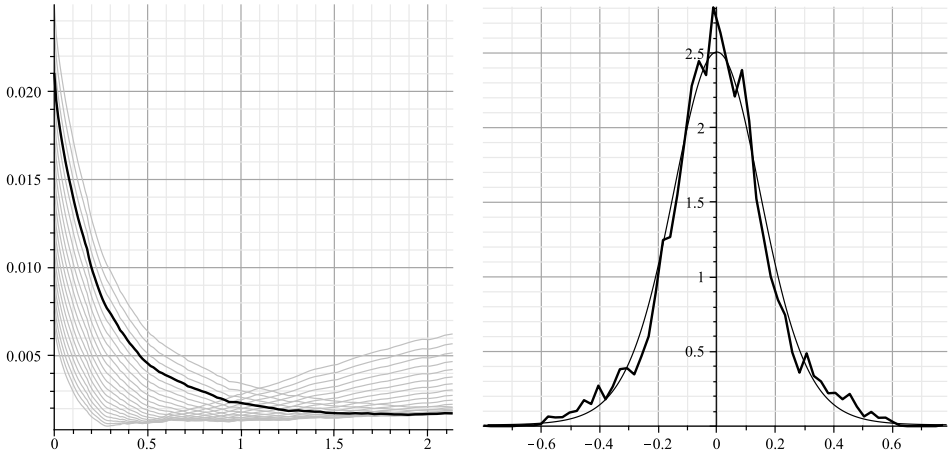

Fig. 4: The relative entropy of the grain growth simulation for a sequence of λ with the optimal choice σ noted in black. (b) Comparison of the empirical distribution at time $t = 2$, when 0.8 of the cells have been deleted, with ρ_σ of (9)

We therefore seek to identify the $\lambda = \sigma$ for which Φ_σ tends to the minimum of all the $\{\Phi_\lambda\}$ as t becomes large, as shown in Figure 4.

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