Summary. Coarsening in polycrystalline materials is a complex process. These systems are often composed of several thousands of grain cells, giving a high degree of freedom. Describing the behavior of each individual cell is unfeasible, hence continuum models are introduced. Although losing information at microscopic level, this is crucial since continuum models are generally much simpler and very powerful in describing system's behavior at meso/macroscopic level. It is found that during coarsening self-similarity holds, that is the geometric pattern looks the same though at different length scales.

An important problem is to determine quantities with predictable behavior. This leads to the notion of Grain Boundary Characteristic Distribution (GBCD), which is predicted to follow a Fokker-Planck type equation. Such prediction is supported by numerical simulations and experiments on two-dimensional polycrystals. Due to the significant geometric complexity of such systems, the a satisfactory mathematical modeling exists only in one-dimensional setting in literature. My contributions involve developing the mathematical modeling for such predictive theory in two-dimensional and three-dimensional settings, with more general energy densities.

Coarsening in polycrystalline materials

Description of the problem. Coarsening in polycrystalline materials is a complex and widely studied physical phenomenon, both theoretically and experimentally [1, 2, 5, 10, 7, 4, 6, 9, 11, 8, 14, 15, 19, 16, 18, 26, 27, 28, 29]. Most engineered materials are polycrystalline microstructures composed of thousands of small grains separated by grain boundaries. The degree of freedom of such systems easily reaches the order of thousands, thus (even with formally simple law governing the evolution at microscope level) studying its behavior by analyzing the behavior of each single cell is unfeasible. Statistical description (at meso/macroscopic) level is required. Mullins first studied ([21, 22, 23]) the local dynamics of grain boundaries, by developing a "curvature driven system", in which the law governing local evolution has the form

$$v_n = \left(\frac{\partial^2 \psi}{\partial \theta^2} + \psi \right) \kappa.$$

Here v_n denotes the velocity orthogonal to grain boundaries (for the sake of simplicity, regularity issues are neglected), κ denotes the curvature, $\psi = \psi(\theta, \alpha)$ the energy density, θ the normal direction and α the misorientation angle (see Figure 1). A commonly accepted simplification is to impose that the energy density depends only on misorientation angle, and that triple junctions are stable (Herring condition). Barmak, Eggeling, Emelianenko, Epshtein, Kinderlehrer, Golovaty, Sharp and Ta'asan formulate a predictive theory for curvature driven systems, and introduce the concept of Grain Boundary Characteristic Distribution (GBCD). In [5, 10] the GBCD is found to be the distribution $\rho(\alpha, t)$ of misorientation angles (rescaled to a probability measure). The energy has the form

$$\int \psi(\alpha)\rho(\alpha, t) d\alpha,$$

where ψ denotes the energy density, which is assumed bounded away from zero. It is suggested by simulations and experiments in 2D ([7]) that for curvature driven evolutionary systems, the GBCD admits a steady state which is a Boltzmann distribution. The model comprises two key points:

- the surface energy $\int \psi(\alpha)\rho(\alpha, t) d\alpha$ is decreasing in time,
- and an entropy term $\lambda \int \rho \log \rho d\alpha$ is introduced to account for critical events (i.e. grain cells disappearing).

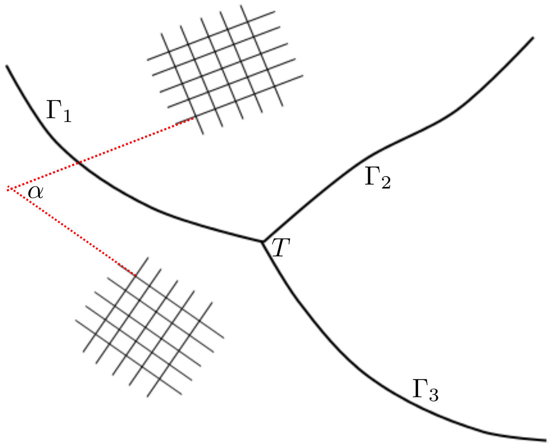

FIGURE 1. A schematic representation of a grain boundary. Here α denotes the misorientation between two grains. Grain boundaries Γ_1, Γ_2, Γ_3 meet at the triple junction T, which is stable due to the Herring condition.

Thus the authors propose in [5, 10, 7] that the GBCD evolves as steepest descent in the 2-Wasserstein space of the "free energy"

$$\int \psi \rho d\alpha + \lambda \int \rho \log \rho d\alpha, \tag{1}$$

where λ is a temperature-like value to be determined experimentally. In the 2-Wasserstein space, the dissipation along steepest descent path is formally similar to the physical dissipation due to frictional and viscous forces in fluid dynamics (as highlighted by Benamou and Brenier [12], Landau and Lifschiz [20]). The theory of gradient flows in metric spaces is quite rich (the main reference being the monograph [3] by Ambrosio, Gigli and Savaré), with several applications in differential equations (cf. [13, 24, 25], also [30] and references therein). In particular a central result (proven by Jordan, Kinderlehrer and Otto [13]) is that steepest descent paths of (1) are solutions of Fokker-Planck type equations. Thus the GBCD satisfies a Fokker-Planck type equation

$$C\frac{\partial \rho}{\partial t} = \lambda \frac{\partial^2 \rho}{\partial \alpha^2} + \frac{\partial}{\partial \alpha}\left(\rho \frac{\partial \psi}{\partial \alpha}\right)$$

for some constant $C > 0$. This is supported by both simulations and experiments in 2D. Figure 2 (from [5]) is from a simulation with energy density

$$\psi(\alpha) := 1 + 0.5 \sin^2 2\alpha, \qquad \alpha \in (-\pi/4, \pi/4),$$

starting with $2^{15} + 1$ cells, showing the distribution of misorientation angles at time T at which 80% of cells have disappeared. The distribution of misorientation angles is compared against the Boltzmann distribution

$$\eta_\sigma := \frac{e^{-\psi(\alpha)/\sigma}}{Z_\sigma}, \qquad Z_\sigma := \int_{-\pi/4}^{\pi/4} e^{-\psi(\alpha)/\sigma} d\alpha, \qquad \sigma := 0.0296915.$$

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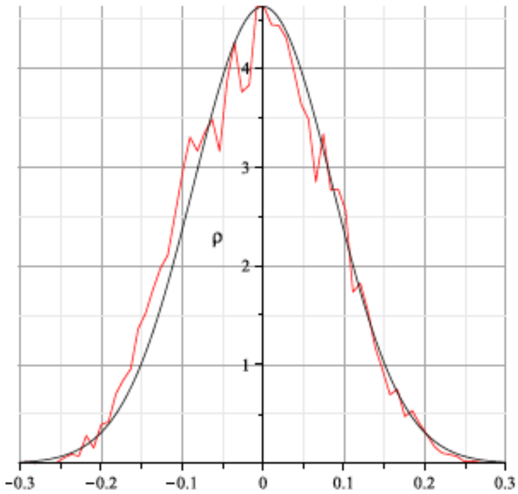

FIGURE 2. The distribution of misorientation angles at T (red), compared against the Boltzmann distribution η_σ (black).

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