Microstructure by Design: Integrating Grain Growth Experiments, Data Analytics, Simulation and Theory

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Project Scope

The principal objective of this project is to quantify statistical measures of grain growth obtained from experimental data garnered from metallic films and to employ these measures to inform mesoscale models of grain growth. This link forged between experiment and theory via analysis and simulations will result in improved models of grain coarsening that properly reflect the underlying physics. Data analytics will be employed to study the evolution of experimental and computational microstructures, regarded here as a collection of interacting grain triple junctions, to validate and refine the models and guide future experiments.

Relevance to MGI

The MGI goal of rapid discovery and deployment of advanced materials requires, in the case of polycrystalline materials, an enhanced understanding of microstructural development to guide subsequent materials design. Thus, this project integrates experiment, theory and simulation to obtain a better, quantitative understanding of grain growth that properly reflect the underlying physics. Data analytics will be employed to study the evolution of experimental and computational microstructures, regarded here as a collection of interacting grain triple junctions, to validate and refine the models and guide future experiments.

Technical Progress

- Established thermodynamically consistent models for deterministic evolution, as well as stochastic dynamics of grain boundaries. The new models incorporate and explore the specific dynamics of misorientations and the triple junctions, in contrast to the conventional approaches with equilibrium Herring conditions.
- Systematically studied the mathematical structures of the derived systems. Designed corresponding structure-preserving numerical algorithms to validate the analytical results, as well as to validate against current and future experimental data.

Automated Boundary Detection

Different Time Scales of 2D Coarsening Networks: Curvature, Mobility of Triple Junctions and Misorientations Dynamics

Total grain boundary energy:

\[ \alpha(t) = \sum_{\Delta \alpha} \alpha(\Delta \alpha) \delta(\Delta \alpha) \]

Grain boundary energy density:

\[ \psi(\Delta \alpha) = 1 + 0.25 \sin^2(2\Delta \alpha) \]

Motion of interfaces:

\[ \nu_{\Delta \alpha} = \mu \psi(\Delta \alpha) \text{ on } \Gamma \]

Dynamics of misorientations:

\[ \frac{\Delta (\Delta \alpha)}{\Delta t} = -\gamma \int_{\Gamma} \Delta \alpha \cdot \frac{\partial \alpha}{\partial \nu} d\Gamma \]

Motion of triple junctions:

\[ \nu_{\Delta \alpha} = \frac{1}{2\eta} \int_{\Gamma} \Delta \alpha \cdot \frac{\partial \alpha}{\partial \nu} d\Gamma \]

The associated probability density function \( f(\Delta \alpha, \nu, t) \) obeys the Fokker-Planck equation:

\[ \frac{\partial f}{\partial t} = \frac{1}{2} \int_{\Gamma} \Delta \alpha \cdot \frac{\partial^2 f}{\partial \nu^2} d\Gamma + \frac{1}{2} \int_{\Gamma} \Delta \alpha \cdot \frac{\partial^2 f}{\partial \Delta \alpha^2} d\Gamma \]

Effect of dynamic misorientations relaxation time scale on Grain Boundary Character Distribution (GBCD)

Marginal probability density:

\[ \psi(\Delta \alpha, \nu, t) = \int f(\Delta \alpha, \nu, t) d\nu \]

- Consistent with the dissipation-fluctuation principle.
- Established and verified in grain growth simulations sufficient condition (which connects triple junctions geometry with grain boundary energies) to observe Boltzmann distribution for the grain boundary energy density as a steady-state distribution for the GBCD.

Distribution of Triple Junctions in a Tungsten Film

References