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

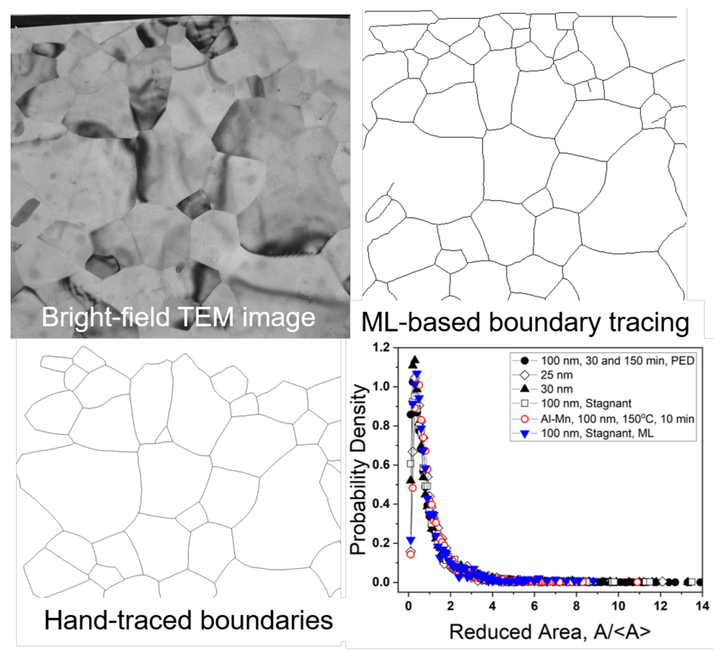
Relevance to MGI

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 mechanisms, using thin metallic films as the experimental testbed.

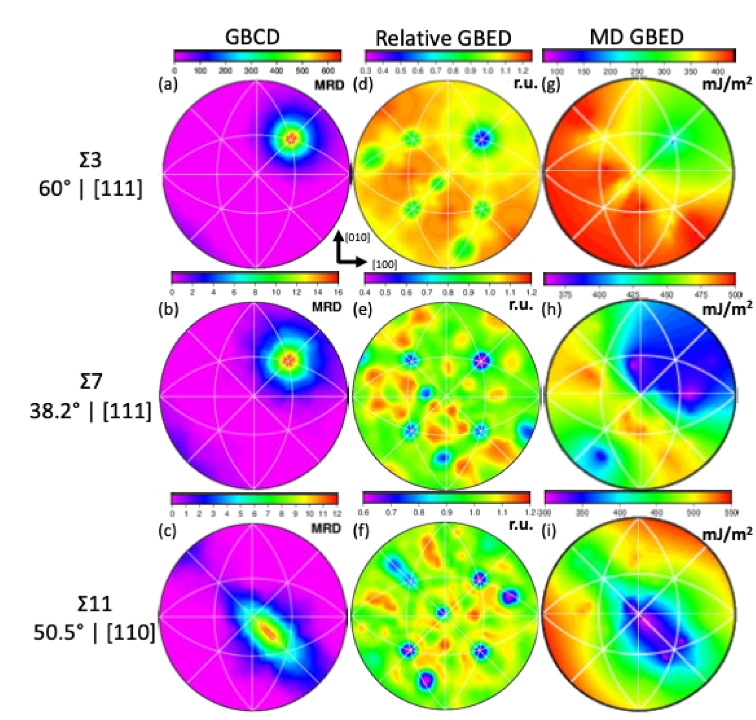
Technical Progress

- Achieved automated grain boundary detection in bright-field TEM images using a modified U-Net convolutional neural network.
- Experimentally obtained correlations between grain boundary character distribution (GBCD) and grain boundary energy distribution (GBED) imply that the force balance at the triple junction (Herring condition) does not fully specify triple junction geometry.
- Developed statistical tools to characterize distribution of triple junctions in experimental crystal orientation maps.
- 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.

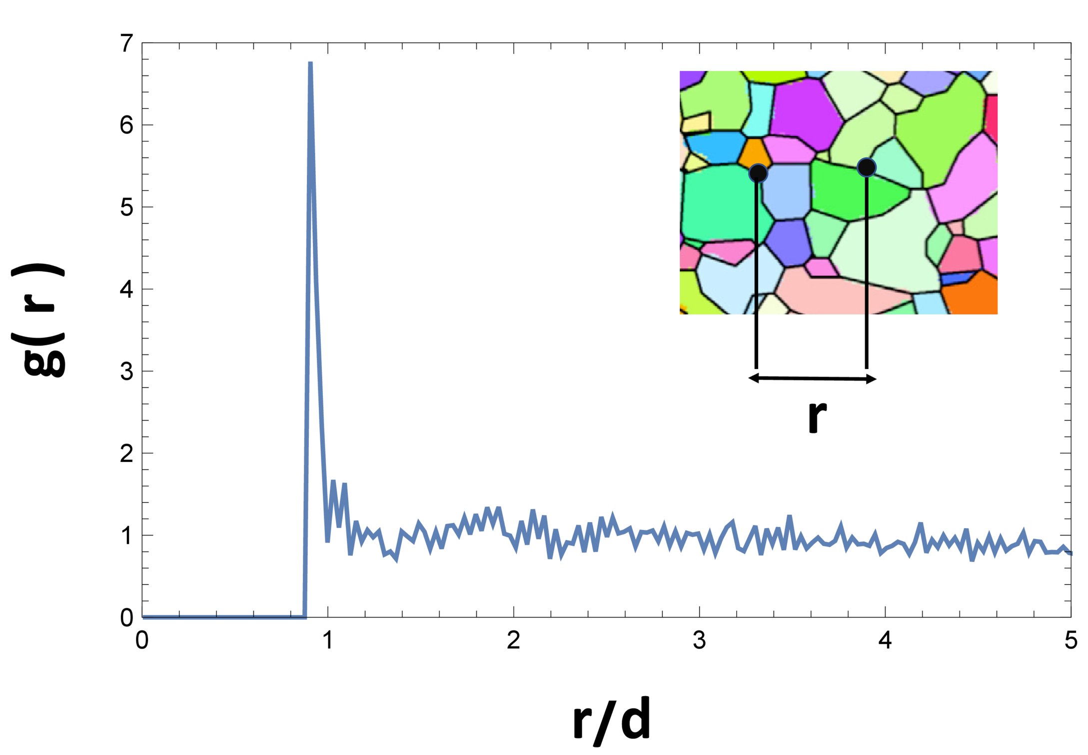
Automated Boundary Detection



Aluminum Film GBCD-GBED



Distribution of Triple Junctions in a Tungsten Film



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

Total grain boundary energy: $E(t)=\sum_{\Gamma^k}\int_{\Gamma^k}\psi^k\left(\Delta\alpha^k\right)d\mathcal{H}^1$

$$\frac{\mathrm{d}E(t)}{\mathrm{d}t}=-\sum_k\int_{\Gamma^k}\frac{1}{\mu^k}\left|v_n^k\right|^2\mathrm{d}\mathscr{H}^1-\sum_m\frac{1}{\eta^m}\left|v^m\right|^2-\sum_l\frac{1}{\gamma^k}\left|\frac{\mathrm{d}\alpha^k}{\mathrm{d}t}\right|^2$$

Grain boundary energy density:

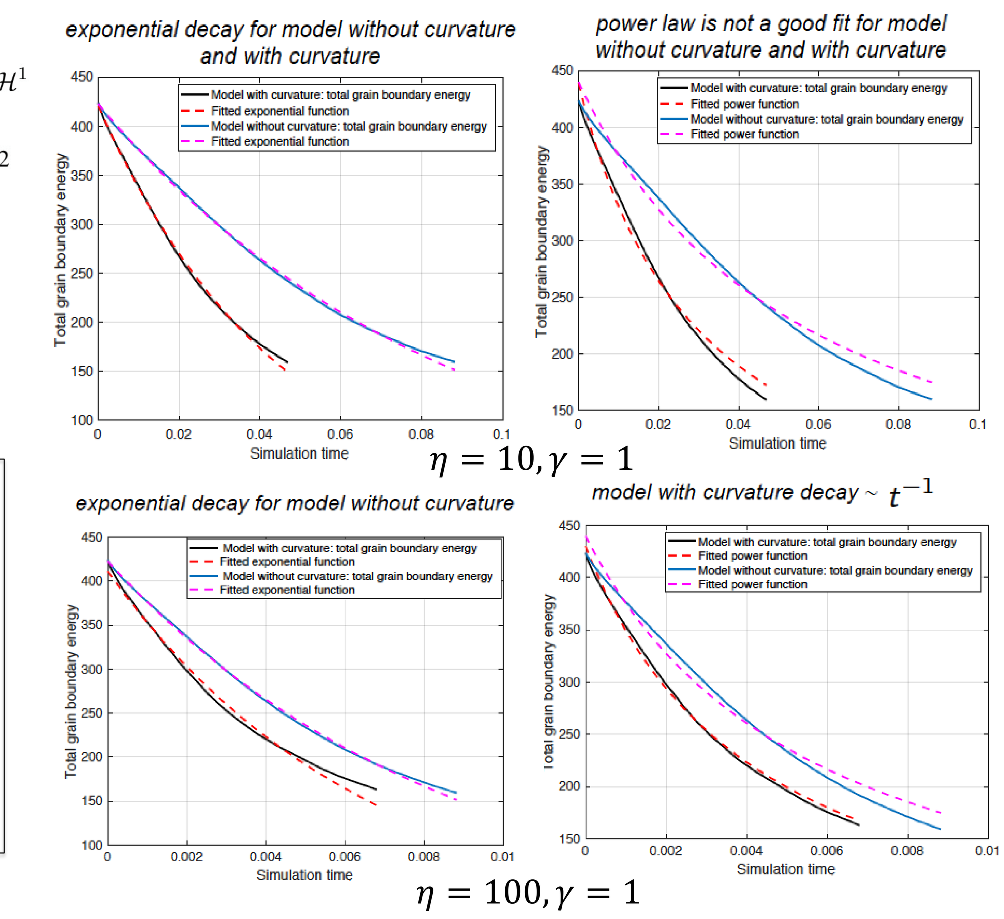
$$\psi(\Delta\alpha)=1+0.25\sin^2(2\Delta\alpha)$$

Motion of interfaces: $v_n=\mu\psi\kappa \quad \text{on } \Gamma$

Dynamics of misorientations:

$$\frac{d(\Delta\alpha)}{dt}=-\gamma\int_\Gamma\frac{\partial\psi}{\partial(\Delta\,\alpha)}\,d\mathcal{H}^1$$

Motion of triple junctions: $v^m=-\eta^m\sum T^{m,\ell}$

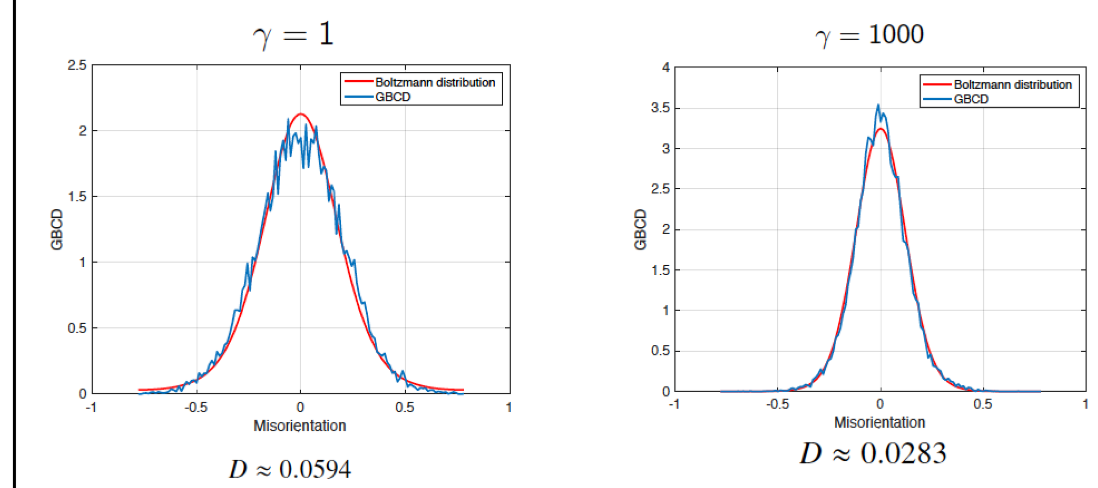


The associated probability density function $f(\Delta\alpha,a,t)$ obeys the Fokker-Planck equation $\frac{\partial f}{\partial t}+\nabla_{\Delta\alpha}^{\Omega}\cdot(v_{\Delta\alpha}f)+\nabla_a\cdot(v_af)=\frac{\beta_{\Delta\alpha}^2}{2}\Delta_{\Delta\alpha}^{\Omega}f+\frac{\beta_a^2}{2}\Delta_a f$ subject to the natural boundary condition. If the relaxation time scales and the fluctuation parameters satisfy $\frac{6\gamma}{\beta_{\Delta\alpha}^2}=\frac{2\eta}{\beta_a^2}$, the Fokker-Planck equation has the energy law ($D:=\frac{\beta_{\Delta\alpha}^2}{6\gamma}$):

$$\frac{\mathrm{d}}{\mathrm{d}t}\iint_{\Omega\times\Omega_{\mathrm{TJ}}}(Df\log f+fE)\mathrm{d}\Delta\alpha\mathrm{d}a=-\frac{\beta_{\Delta\alpha}^2}{2D}\iint_{\Omega\times\Omega_{\mathrm{TJ}}}f\left|\nabla_{\Delta\alpha}^{\Omega}(D\log f+E)\right|^2\mathrm{d}\Delta\alpha\mathrm{d}a-\frac{\beta_a^2}{2D}\iint_{\Omega\times\Omega_{\mathrm{TJ}}}f\left|\nabla_a(D\log f+E)\right|^2\mathrm{d}\Delta\alpha\mathrm{d}a$$

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

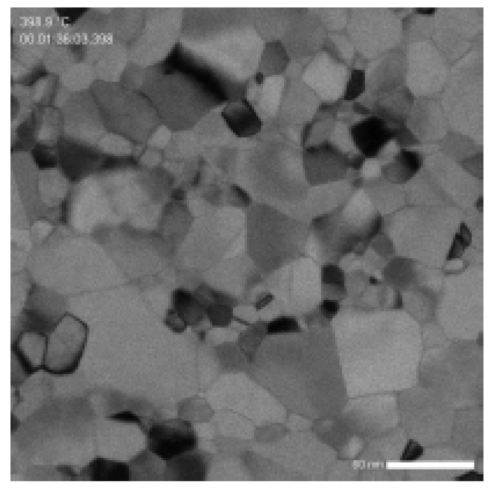
Marginal probability density: $\rho_1(\Delta\alpha,t)=\int_{\Omega_{TJ}}f(\Delta\alpha,a,t)\,da$; the Herring angle condition ($\eta\to\infty$)



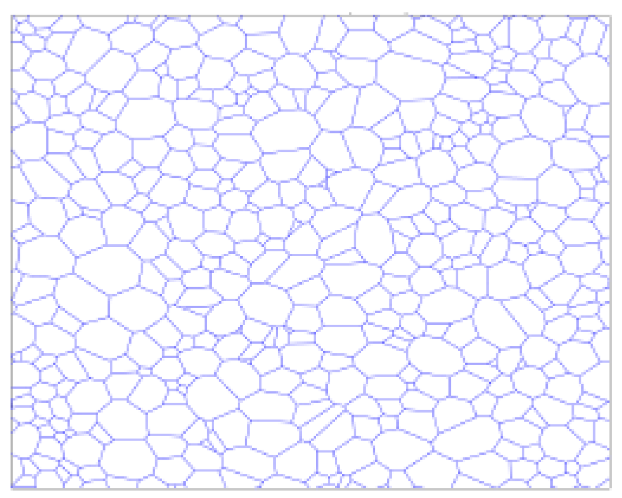
- Consistent with the dissipation-fluctuation principle.

- 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.

Platinum film from instance of an in-situ grain growth experiment



Instance of the simulation: No-curvature



References (1) Y. Epshteyn, C. Liu, M. Mizuno, SIMA, 53(3), 3072-3097, 2021. (2) K. Barmak, A. Dunca, Y. Epshteyn, C. Liu, M. Mizuno, AWM-Springer Volume, In Press, arXiv:2105.07255, 2022. (3) Y. Epshteyn, C. Liu, M. Mizuno, Submitted, arXiv:2106.14249, 2021.