A stochastic model of grain boundary motion

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Outline of my talk

Y. Epshteyn, C. Liu, M., *Motion of grain boundaries with dynamic lattice misorientations and with triple junctions drag*, SIAM J. Math. Anal. **53** (2021), 3072–3097.

___, *Large time asymptotic behavior of grain boundaries motion with dynamic lattice misorientations and with triple junctions drag*, Commun. Math. Sci. **19** (2021), 1403–1428.

___, *A stochastic model of grain boundary dynamics: A Fokker-Planck perspective*. Math. Models Methods Appl. Sci. **32** (2022), 2189–2236.

1. Fokker-Planck model of grain boundary motion
2. Analysis of the equations
3. Joint distribution

This is a joint work with Yekaterina Epshteyn (The University of Utah), and Chun Liu (Illinois Institute of Technology).

Grain boundaries

Grain boundaries (from Wikipedia)

A grain boundary is the interface between two grains, or crystallites, in a polycrystalline material.

Example (Polycrystalline material)

metal, steel, alloy, ceramic, rock, ice, etc.

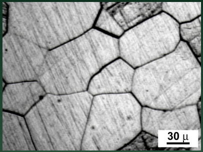


Figure: Micrograph of a polycrystalline metal[1]

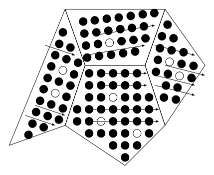


Figure: A schematic diagram for a polycrystalline material

Figure: Multiscale problem?

[1] By Edward Pleshakov - Own work, CC BY 3.0, https://commons.wikimedia.org/w/index.php?curid=3912586

Grain boundary energy

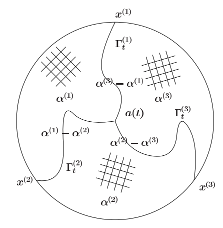
Grain boundaries are related to the properties of materials: Strength, toughness, ductility, electrical and thermal conductivity.

Grain boundary energy

$\Gamma_t^{(j)}$: Grain boundary ($j = 1, 2, 3$)

$$E(t) = \sum_{j=1}^{3} \int_{\Gamma_t^{(j)}} \sigma(\Delta\alpha^{(j)}(t))\, ds$$

isotropic



What is contributed the energy?

shape of the boundaries $\kappa^{(j)} = \kappa^{(j)}(s,t)$: curvature of $\Gamma^{(j)}$

misorientation $\Delta\alpha^{(j)}(t) = \alpha^{(j-1)}(t) - \alpha^{(j)}(t)$: difference in orientation

triple junction $a(t)$: All of $\Gamma^{(j)}$ meets at the point $a(t)$

Governing equations

Governing equations (SIAM MA)

$$v_n^{(j)}(s,t) = \mu\sigma(\Delta\alpha^{(j)}(t))\kappa^{(j)}(s,t), \qquad \text{(M)}$$

$$\alpha_t^{(j)}(t) = -\gamma\left(\sigma_\alpha(\Delta\alpha^{(j+1)}(t))|\Gamma_t^{(j+1)}| - \sigma_\alpha(\Delta\alpha^{(j)}(t))|\Gamma_t^{(j)}|\right), \qquad \text{(O)}$$

$$a_t(t) = \eta\sum_{j=1}^{3}\sigma(\Delta\alpha^{(j)}(t))\frac{\xi_s^{(j)}(0,t)}{|\xi_s^{(j)}(0,t)|}. \qquad \text{(T)}$$

Energy dissipation

$$\frac{d}{dt}E(t) = -\sum_{j=1}^{3}\left(\frac{1}{\gamma}|\alpha_t^{(j)}(t)|^2 + \frac{1}{\mu}\int_{\Gamma_t^{(j)}}|v^{(j)}(s,t)|^2\right) - \frac{1}{\eta}|a_t(t)|^2 \qquad \text{(ED)}$$

Toward singularity, GBCD

Grain boundary character distribution

The grain boundary character distribution is an empirical distribution of the relative length or area of interface with a given lattice misorientation and grain boundary normal (cf. Bardsley-Barmak-Eggeling-Epshteyn-Kinderlehrer-Ta’asan, 2017)

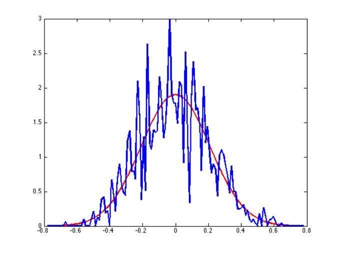


Figure: Steady state GBCD plots versus Boltzmann distribution: 1000 grains

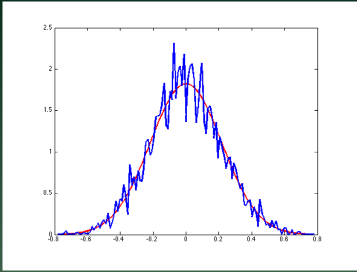


Figure: Steady state GBCD plots versus Boltzmann distribution: 5000 grains

Relaxation of the curvature effect

Take the relaxation limit $\mu \to \infty$: Study interaction $\Delta\alpha$ and a

Governing equations

$$\alpha_t^{(j)}(t) = -\gamma\left(\sigma_\alpha(\Delta\alpha^{(j+1)}(t))|\Gamma_t^{(j+1)}| - \sigma_\alpha(\Delta\alpha^{(j)}(t))|\Gamma_t^{(j)}|\right), \quad \text{(O)}$$

$$a_t(t) = -\eta\sum_{j=1}^{3}\sigma(\Delta\alpha^{(j)}(t))\frac{a(t)-x^{(j)}}{|a(t)-x^{(j)}|}. \quad \text{(T)}$$

Energy dissipation

$$E(\Delta\alpha, a) = \sum_{j=1}^{3}\sigma(\Delta^{(j)}\alpha)|a-x^{(j)}|$$

$$\Longrightarrow \frac{d}{dt}E(t) = -\frac{1}{\gamma}\sum_{j=1}^{3}|\alpha_t^{(j)}(t)|^2 - \frac{1}{\eta}|a_t(t)|^2$$

Relaxation of the curvature effect

Take the relaxation limit $\mu \to \infty$: Study interaction $\Delta\alpha$ and a

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$$\alpha_t^{(j)}(t) = -\gamma\left(\sigma_\alpha(\Delta\alpha^{(j+1)}(t))|\Gamma_t^{(j+1)}| - \sigma_\alpha(\Delta\alpha^{(j)}(t))|\Gamma_t^{(j)}|\right), \quad \text{(O)}$$

$$a_t(t) = -\eta\sum_{j=1}^{3}\sigma(\Delta\alpha^{(j)}(t))\frac{a(t) - x^{(j)}}{|a(t) - x^{(j)}|}. \quad \text{(T)}$$

Problem

How to involve critical events, such as topological change of grain boundaries? How is the relation between the model and GBCD?

- critical events : interaction between $\Delta\alpha$ and a
- GBCD : use $\Delta\alpha$ as a state variable

Change of variables

$$\alpha_t^{(j)}(t) = -\gamma\left(\sigma_\alpha(\Delta\alpha^{(j+1)}(t))|\Gamma_t^{(j+1)}| - \sigma_\alpha(\Delta\alpha^{(j)}(t))|\Gamma_t^{(j)}|\right), \qquad \text{(O)}$$

$$a_t(t) = -\eta\sum_{j=1}^{3}\sigma(\Delta\alpha^{(j)}(t))\frac{a(t)-x^{(j)}}{|a(t)-x^{(j)}|}. \qquad \text{(T)}$$

$$\Leftrightarrow \frac{d(\Delta\alpha)}{dt} = -3\gamma\nabla^{\Omega}_{\Delta\alpha}E =: v_{\Delta\alpha}, \qquad \frac{da}{dt} = -\eta\nabla_a E =: v_a,$$

where $\nabla^{\Omega}_{\Delta\alpha}$ is the gradient of $\Delta\alpha$ with constraint $\Delta^{(1)}\alpha + \Delta^{(2)}\alpha + \Delta^{(3)}\alpha = 0$,

$$\Omega := \left\{\Delta\alpha = (\Delta^{(1)}\alpha, \Delta^{(2)}\alpha, \Delta^{(3)}\alpha) \in \left(-\frac{\pi}{4}, \frac{\pi}{4}\right)^3 : \sum_{j=1}^{3}\Delta^{(j)}\alpha = 0\right\},$$

and $\Omega^{\mathrm{TJ}} = B_R \subset \mathbb{R}^2$ is the state space for triple junction a.

Stochastic model

$$\frac{d(\Delta\alpha)}{dt} = -3\gamma\nabla^{\Omega}_{\Delta\alpha}E =: v_{\Delta\alpha}, \qquad \frac{da}{dt} = -\eta\nabla_a E =: v_a.$$

Consider the interaction as a Brownian motion

$$\frac{d(\Delta\alpha)}{dt} = v_{\Delta\alpha} + \beta_{\Delta\alpha}\frac{dB}{dt}, \qquad \frac{da}{dt} = v_a + \beta_a\frac{dB}{dt}, \qquad \text{(SDE)}$$

where B is a Brownian motion, and constants $\beta_{\Delta\alpha}, \beta_a > 0$ are fluctuation parameters.
Let $f = f(\Delta\alpha, a, t)$ be the probability density function for (SDE). Then f obeys the following Fokker-Planck equation:

$$\frac{\partial f}{\partial t} + \nabla^{\Omega}_{\Delta\alpha}\cdot(v_{\Delta\alpha}f) + \nabla_a\cdot(v_a f) = \frac{\beta^2_{\Delta\alpha}}{2}\Delta^{\Omega}_{\Delta\alpha}f + \frac{\beta^2_a}{2}\Delta_a f, \qquad \text{(FP)}$$

where $\Delta_{\Delta\alpha} = \nabla^{\Omega}_{\Delta\alpha}\cdot\nabla^{\Omega}_{\Delta\alpha}, \quad \Delta_a = \nabla_a\cdot\nabla_a.$

Fluctuation-Dissipation theorem

Recall that $v_{\Delta\alpha} = -3\gamma\nabla^{\Omega}_{\Delta\alpha}E, v_a = -\eta\nabla_a E$ and

$$\frac{\partial f}{\partial t} + \nabla^{\Omega}_{\Delta\alpha}\cdot(v_{\Delta\alpha}f) + \nabla_a\cdot(v_a f) = \frac{\beta^2_{\Delta\alpha}}{2}\Delta^{\Omega}_{\Delta\alpha}f + \frac{\beta^2_a}{2}\Delta_a f, \qquad \text{(FP)}$$

$$\Leftrightarrow \frac{\partial f}{\partial t} = \nabla^{\Omega}_{\Delta\alpha}\cdot\left(f\nabla^{\Omega}_{\Delta\alpha}\left(\frac{\beta^2_{\Delta\alpha}}{2}\log f + 3\gamma E\right)\right) + \nabla_a\cdot\left(f\nabla_a\left(\frac{\beta^2_a}{2}\log f + \eta E\right)\right).$$

We impose the natural boundary condition:

$$f\nabla^{\Omega}_{\Delta\alpha}\left(\frac{\beta^2_{\Delta\alpha}}{2}\log f + 3\gamma E\right)\cdot\nu_{\Delta\alpha}\Big|_{\partial\Omega\times\Omega_{\mathrm{TJ}}} = f\nabla_a\left(\frac{\beta^2_a}{2}\log f + \eta E\right)\cdot\nu_a\Big|_{\Omega\times\partial\Omega_{\mathrm{TJ}}} = 0.$$

Consider the free energy, for a positive constant $D > 0$

$$F[f] := \iint_{\Omega\times\Omega_{\mathrm{TJ}}}(Df\log f + fE)\,d\Delta\alpha\,da. \qquad \text{(FE)}$$

Fluctuation-Dissipation theorem

$$\frac{\partial f}{\partial t} = \nabla^{\Omega}_{\Delta\alpha} \cdot \left(f \nabla^{\Omega}_{\Delta\alpha} \left(\frac{\beta^2_{\Delta\alpha}}{2} \log f + 3\gamma E \right) \right) + \nabla_a \cdot \left(f \nabla_a \left(\frac{\beta^2_a}{2} \log f + \eta E \right) \right) \qquad \text{(FP)}$$

$$\begin{aligned}
\frac{d}{dt} F[f] &= \frac{d}{dt} \iint_{\Omega \times \Omega_{\mathrm{TJ}}} (D f \log f + f E)\, d\Delta\alpha\, da \\
&= \iint_{\Omega \times \Omega_{\mathrm{TJ}}} f_t (D \log f + D + E)\, d\Delta\alpha\, da \\
&= - \iint_{\Omega \times \Omega_{\mathrm{TJ}}} f \nabla^{\Omega}_{\Delta\alpha} \left(\frac{\beta^2_{\Delta\alpha}}{2} \log f + 3\gamma E \right) \cdot \nabla^{\Omega}_{\Delta\alpha} (D \log f + E)\, d\Delta\alpha\, da \\
&\quad - \iint_{\Omega \times \Omega_{\mathrm{TJ}}} f \nabla_a \left(\frac{\beta^2_a}{2} \log f + \eta E \right) \cdot \nabla_a (D \log f + E)\, d\Delta\alpha\, da.
\end{aligned}$$

In order to ensure $\frac{d}{dt} F[f] \leqq 0$,

$$\frac{\beta^2_{\Delta\alpha}}{2} \log f + 3\gamma E \underset{\text{parallel}}{\propto} \frac{\beta^2_a}{2} \log f + \eta E \underset{\text{parallel}}{\propto} D \log f + E$$

Fluctuation-Dissipation theorem

Theorem

f : solution of (FP) subjected to the Natural boundary condition.

$$D = \frac{\beta_{\Delta\alpha}^2}{6\gamma} = \frac{\beta_a^2}{2\eta}, \qquad \text{(FDR)}$$

$$\begin{aligned}
\Longrightarrow \quad & \frac{d}{dt} \iint_{\Omega \times \Omega_{TJ}} (D f \log f + f E) \, d\Delta\alpha \, da \\
&= -\frac{\beta_{\Delta\alpha}^2}{2D} \iint_{\Omega \times \Omega_{TJ}} f \left| \nabla_{\Delta\alpha}^{\Omega} (D \log f + E) \right|^2 d\Delta\alpha \, da \qquad \text{(EnergyLaw)} \\
&\quad - \frac{\beta_a^2}{2D} \iint_{\Omega \times \Omega_{TJ}} f \left| \nabla_a (D \log f + E) \right|^2 d\Delta\alpha \, da.
\end{aligned}$$

- (FDR) is related to the Fluctuation Dissipation Relation
- (EnergyLaw) ensures the existence of the equilibrium state.

Fluctuation-Dissipation theorem

Theorem

f : solution of (FP) subjected to the Natural boundary condition.

$$D = \frac{\beta_{\Delta\alpha}^2}{6\gamma} = \frac{\beta_a^2}{2\eta}, \qquad \text{(FDR)}$$

$$\begin{aligned}
\Longrightarrow \quad & \frac{d}{dt}\iint_{\Omega\times\Omega_{\mathrm{TJ}}} (D f \log f + f E)\, d\Delta\alpha\, da \\
&= -\frac{\beta_{\Delta\alpha}^2}{2D}\iint_{\Omega\times\Omega_{\mathrm{TJ}}} f \left|\nabla_{\Delta\alpha}^{\Omega}(D\log f + E)\right|^2 d\Delta\alpha\, da \qquad \text{(EnergyLaw)} \\
&\quad - \frac{\beta_a^2}{2D}\iint_{\Omega\times\Omega_{\mathrm{TJ}}} f \left|\nabla_a (D\log f + E)\right|^2 d\Delta\alpha\, da.
\end{aligned}$$

Equilibrium f_∞ satisfies $\nabla(D\log f_\infty + E) = 0$

$$f_\infty(\Delta\alpha, a) = C\exp\left(-\frac{E(\Delta\alpha, a)}{D}\right), \qquad \iint_{\Omega\times\Omega_{\mathrm{TJ}}} f_\infty\, d\Delta\alpha\, da = 1.$$

New formula from the asymptotics

Marginal distribution

$$\rho_\infty(\Delta\alpha) := \int_{\Omega_{\mathrm{TJ}}} f_\infty(\Delta\alpha, a)\, da.$$

ρ_∞ is not the Boltzmann distribution in general!!

$$\begin{aligned}\rho_\infty(\Delta\alpha) &= C \int_{\Omega_{\mathrm{TJ}}} \exp\left(-\frac{E(\Delta\alpha, a)}{D}\right) da \\ &= C \int_{\Omega_{\mathrm{TJ}}} \exp\left(-\frac{1}{D}\sum_{j=1}^{3} \sigma(\Delta^{(j)}\alpha)|a - x^{(j)}|\right) da \\ &\neq C \exp\left(-\frac{E_1(\Delta\alpha)}{D}\right).\end{aligned}$$

New formula from the asymptotics

Marginal distribution

$$\rho_\infty(\Delta\alpha) := \int_{\Omega_{\mathrm{TJ}}} f_\infty(\Delta\alpha, a)\, da.$$

ρ_∞ is not the Boltzmann distribution in general!!

$$\begin{aligned}\rho_\infty(\Delta\alpha) &= C\int_{\Omega_{\mathrm{TJ}}} \exp\left(-\frac{E(\Delta\alpha, a)}{D}\right) da \\ &= C\left(\int_{\Omega_{\mathrm{TJ}}} \exp\left(-\frac{E_2(\Delta\alpha, a)}{D}\right) da\right) \exp\left(-\frac{E_1(\Delta\alpha)}{D}\right),\end{aligned}$$

where

$$E(\Delta\alpha, a) = E_1(\Delta\alpha) + E_2(\Delta\alpha, a),$$

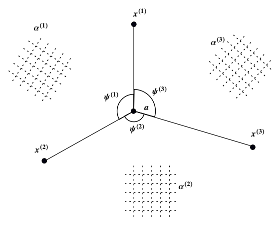
$$E_1(\Delta\alpha) = \exp\left(-\frac{1}{D}\sum_{j=1}^{3} \sigma(\Delta^{(j)}\alpha)|a_* - x^{(j)}|\right), \quad a_* : \text{fixed}$$

How to choose a_*

Weighted Fermat-Torricelli point

$$\sum_{j=1}^{3} \sigma(\Delta^{(j)}\alpha)|a_{\mathrm{wFT}} - x^{(j)}| = \inf_{a \in \Omega_{\mathrm{TJ}}} \sum_{j=1}^{3} \sigma(\Delta^{(j)}\alpha)|a - x^{(j)}| = \inf_{a \in \Omega_{\mathrm{TJ}}} E(\Delta\alpha, a).$$

Let $\psi^{(i)}$ be an angle formed by $a - x^{(i)}$ and $a - x^{(i+1)}$ at the triple junction a.



Proposition

$a = a_{\mathrm{wFT}}$ if and only if,

$$1 - \cos\psi^{(i)} = \frac{(\sigma(\Delta^{(i)}\alpha) + \sigma(\Delta^{(i+1)}\alpha))^2 - \sigma(\Delta^{(i+2)}\alpha)^2}{2\sigma(\Delta^{(i)}\alpha)\sigma(\Delta^{(i+1)}\alpha)}$$

for $i = 1, 2, 3$.

How to choose a_*

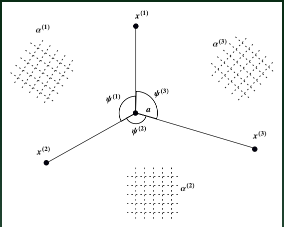
circumcenter

$$|a_{\mathrm{cc}} - x^{(1)}| = |a_{\mathrm{cc}} - x^{(2)}| = |a_{\mathrm{cc}} - x^{(3)}|.$$

If $a_* = a_{\mathrm{cc}}$, then

$$E_1(\Delta\alpha) = \sum_{j=1}^{3} \sigma(\Delta^{(j)}\alpha)|a_* - x^{(j)}|$$

$$= |a_* - x^{(1)}| \sum_{j=1}^{3} \sigma(\Delta^{(j)}\alpha)$$



Proposition

$a = a_{\mathrm{cc}}$, if and only if

$$\frac{1 - \cos\psi^{(1)}}{|x^{(1)} - x^{(2)}|^2} = \frac{1 - \cos\psi^{(2)}}{|x^{(2)} - x^{(3)}|^2} = \frac{1 - \cos\psi^{(3)}}{|x^{(3)} - x^{(1)}|^2}.$$

How to choose a_*

$$a = a_{\mathrm{wFT}} \Longleftrightarrow 1 - \cos\psi^{(i)} = \frac{(\sigma(\Delta^{(i)}\alpha) + \sigma(\Delta^{(i+1)}\alpha))^2 - \sigma(\Delta^{(i+2)}\alpha)^2}{2\sigma(\Delta^{(i)}\alpha)\sigma(\Delta^{(i+1)}\alpha)},$$

$$a = a_{\mathrm{cc}} \Longleftrightarrow \frac{1 - \cos\psi^{(1)}}{|x^{(1)} - x^{(2)}|^2} = \frac{1 - \cos\psi^{(2)}}{|x^{(2)} - x^{(3)}|^2} = \frac{1 - \cos\psi^{(3)}}{|x^{(3)} - x^{(1)}|^2}.$$

Corollary

$a = a_{\mathrm{wFT}} = a_{\mathrm{cc}}$

$$\Longrightarrow \frac{(\sigma(\Delta^{(1)}\alpha) + \sigma(\Delta^{(2)}\alpha))^2 - \sigma(\Delta^{(3)}\alpha)^2}{2\sigma(\Delta^{(1)}\alpha)\sigma(\Delta^{(2)}\alpha)|x^{(1)} - x^{(2)}|^2}$$

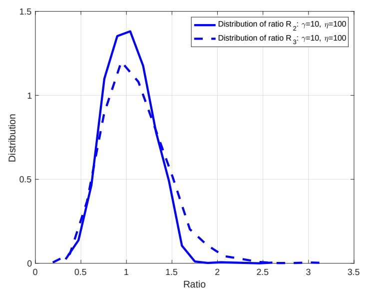
$$= \frac{(\sigma(\Delta^{(2)}\alpha) + \sigma(\Delta^{(3)}\alpha))^2 - \sigma(\Delta^{(1)}\alpha)^2}{2\sigma(\Delta^{(2)}\alpha)\sigma(\Delta^{(3)}\alpha)|x^{(2)} - x^{(3)}|^2}$$

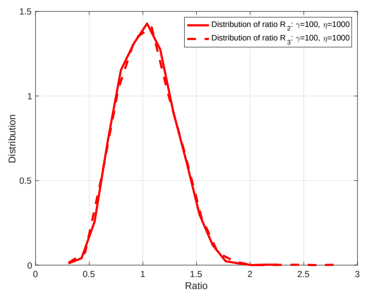
$$= \frac{(\sigma(\Delta^{(3)}\alpha) + \sigma(\Delta^{(1)}\alpha))^2 - \sigma(\Delta^{(2)}\alpha)^2}{2\sigma(\Delta^{(3)}\alpha)\sigma(\Delta^{(1)}\alpha)|x^{(3)} - x^{(1)}|^2}.$$

Numerical experiments

$$\alpha_t^{(j)}(t) = -\gamma\left(\sigma_\alpha(\Delta\alpha^{(j+1)}(t))|\Gamma_t^{(j+1)}| - \sigma_\alpha(\Delta\alpha^{(j)}(t))|\Gamma_t^{(j)}|\right), \qquad \text{(O)}$$

$$a_t(t) = -\eta \sum_{j=1}^{3} \sigma(\Delta\alpha^{(j)}(t)) \frac{a(t) - x^{(j)}}{|a(t) - x^{(j)}|}, \qquad \text{(T)}$$





- $R_2 = 1 \Leftrightarrow$ Triple junction = circumcenter
- $R_3 = 1 \Leftrightarrow$
  Triple junction = circumcenter = weighted Fermat-Torricelli point