Simulating Polycrystalline Grain Growth Accurately and Efficiently via Distance Function-Based Diffusion-Generated Motion

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Mullins Model for Grain Growth

Assumptions:
- Interfacial energy ψ associated with interfaces Γ between grains.
- $\psi = \psi(\mathbf{n}, \phi)$ depends on the normal $\mathbf{n}$ and misorientation ϕ.

Mullins model

The energy $\mathcal{E}$ of a collection of grains in $\mathbb{R}^d$ is given by:

$$\mathcal{E} = \sum_{k<\ell} \int_{\Gamma_{k\ell}} \psi(\mathbf{n}_{k\ell}, \phi_{k\ell}) d\mathbf{s}.$$

The L^2 gradient flow on $\mathcal{E}$ is:

$$v_{\mathbf{n}(\Gamma_{k\ell})} = \mu_{k\ell} \sum_{i=1}^{d-1} \left(\frac{\partial^2 \psi(\mathbf{n}_{k\ell}, \phi_{k\ell})}{\partial (\mathbf{p}_{k\ell}^{(i)})^2} \kappa_{k\ell}^{(i)} \right),$$

with interfacial mobility $\mu_{k\ell}$, principal curvatures $\kappa^{(i)}$ in the tangent directions $\mathbf{p}^{(i)}$, and ψ extended to a one-homogenous function on $\mathbb{R}^d$.

A natural (Herring) boundary condition along triple lines is enforced. Under the assumption that the mobility of triple lines is infinite, this boundary condition corresponds to the vanishing of forces along the triple line.

Unequal Interface Energy Model

Simplifications:
- $\mu_{k\ell} \equiv 1$.
- Surface energy independent of normal: $\psi(\mathbf{n}_{k\ell}, \phi_{k\ell}) = \psi(\phi_{k\ell}) \equiv \psi_{k\ell}$.

Simplified model

Energy:

$$\mathcal{E} = \sum_{k<\ell} \int_{\Gamma_{k\ell}} \psi_{k\ell} d\mathbf{s}.$$

Dynamics:

$$v_{\mathbf{n}}(\Gamma_{k\ell}) = \psi_{k\ell} \kappa_{k\ell},$$

with

$$\sum_{\Gamma_{k\ell} \in \mathrm{TL}} \psi_{k\ell} \mathbf{b}_{k\ell} = \mathbf{0},$$

where $\mathbf{b}_{k\ell}$ is orthogonal to $\mathbf{n}_{k\ell}$ and the tangent to the triple line.

Numerical Schemes

DFDGM algorithm for additive surface energy

Assume: $\psi_{k\ell} = \frac{1}{2}(\gamma_k + \gamma_\ell)$.
Update each collection of grains Ξ_k for a discrete time step δt by:
1. Update: Compute $A_k = d_k^n * G_{\gamma_k \delta t}$.
2. Redistribute: Set $B_k = A_k - \sum_{\ell \neq k} A_\ell$.
3. Redistance: Compute $d_k^{n+1} = \mathrm{Redist}(B_k)$.

- Redistancing is a standard level set technique which computes signed distance to 0-level set of input.
- Unconditionally stable, with $O(N \log N)$ complexity.

Observation: Arbitrary surface tensions ψ_{12}, ψ_{13}, and ψ_{23} can be mapped to $\gamma_{1;23}$, $\gamma_{2;13}$, $\gamma_{3;12}$ so that $\psi_{12} = \frac{1}{2}(\gamma_{1;23} + \gamma_{2;13})$, etc., by:

$$\begin{pmatrix} \gamma_{1;23} \\ \gamma_{2;13} \\ \gamma_{3;12} \end{pmatrix} = \begin{pmatrix} 1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \psi_{12} \\ \psi_{13} \\ \psi_{23} \end{pmatrix}.$$

This suggests an algorithm for full unequal interface energy model:

Unequal interface energy algorithm

Fix ε and $K > 0$.
Replace Update step above by:

1. Update: For each grid location x, define $R(x) = \{k : d_k^n(x) > -\varepsilon\}$, and let $r(x) = \#R(x)$.
   (a) If $R(x) = \{j\}$, set $A_j(x) = d_j^n(x)$.
   (b) If $R(x) = \{j, k\}$, set $A_j(x) = d_j^n(x) * G_{(\psi_{jk}\, \delta t)}$.
   (c) If $R(x) = \{j, k, \ell\}$, set $A_j(x) = d_j^n(x) * G_{(\gamma_{j;k\ell}\, \delta t)}$.
   (d) If $r(x) > 3$,
   - For each $j \in R$, compute

$$T_j(x) = \frac{1}{\binom{r(x)-1}{2}} \sum_{k,\ell \in R} d_j^n(x) * G_{(\gamma_{j;k\ell}\, \delta t)}.$$

   - Compute

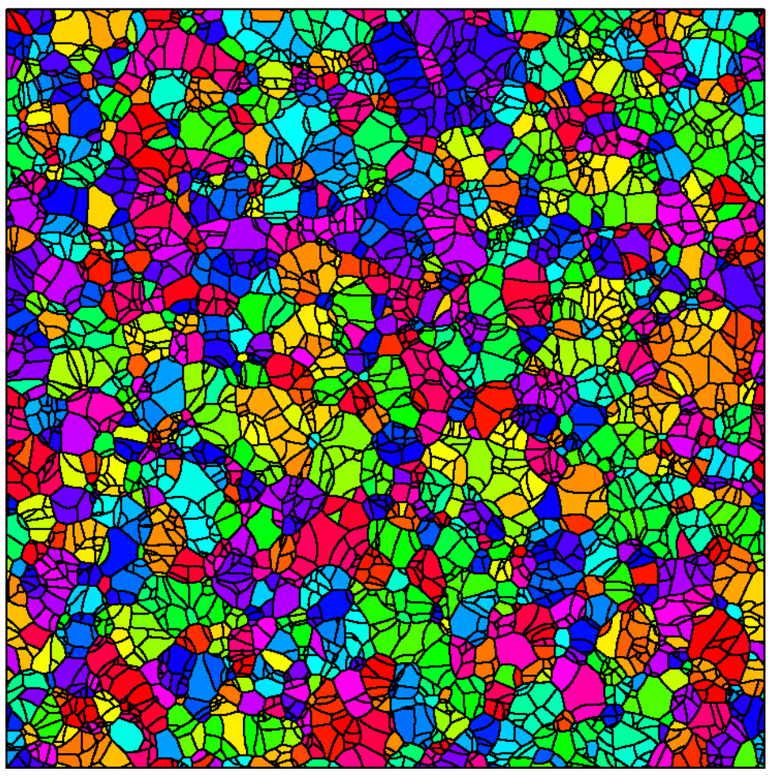
$$w_j(x) = \begin{cases} \varepsilon, & T_j(x) < -K \\ \varepsilon + (1-\varepsilon)\left(\frac{1}{2} + \frac{T_j(x)}{2K}\right), & |T_j(x)| < K \\ 1, & T_j(x) > K. \end{cases}$$

   - Set

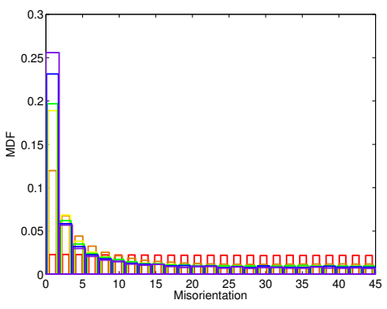
$$A_j(x) = \frac{\sum_{k,\ell \in R} w_j w_k w_\ell\, d_j^n(x) * G_{(\gamma_{j;k\ell}\, \delta t)}}{\sum_{k,\ell \in R} w_j w_k w_\ell}.$$

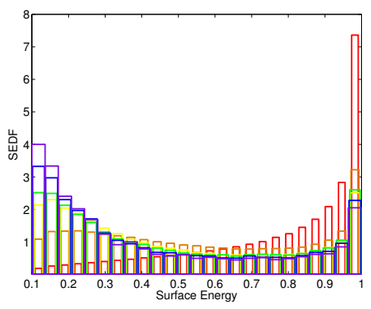
Numerical Results (Fiber Texture)

- Grains with similar orientations tend to form clusters.



- Significant fraction of low-energy boundaries initially.
- MDF coarsens strongly around 0°.

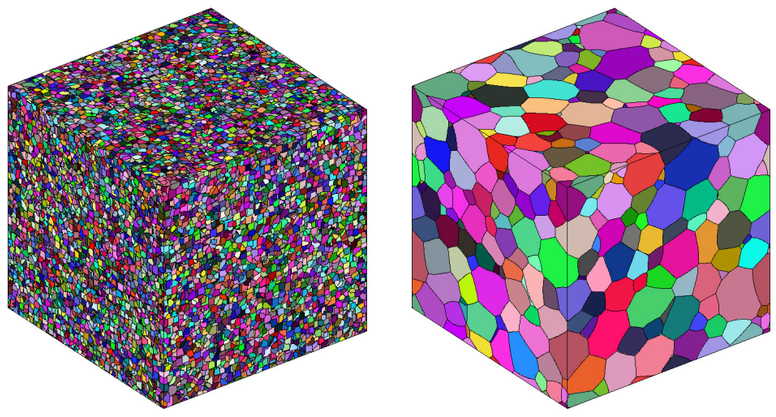




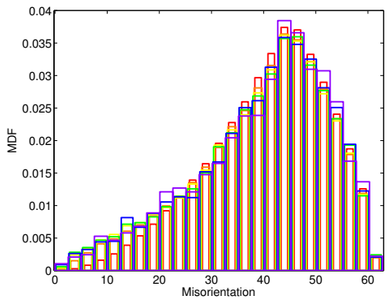
- Difference between fiber and random texture evolutions attributed to "almost-ideal" nature of random texture (very few interfaces feel energy different that $\gamma_{\max}$).
- Assertion supported by numerical tests with different surface energy functions $\gamma(\phi)$.

Numerical Results (3D Random Texture)

- Results qualitatively similar to 2D random texture simulation.
- Only 616 grains remain at end of simulation.



- Little evolution of the MDF.



Additional Notes

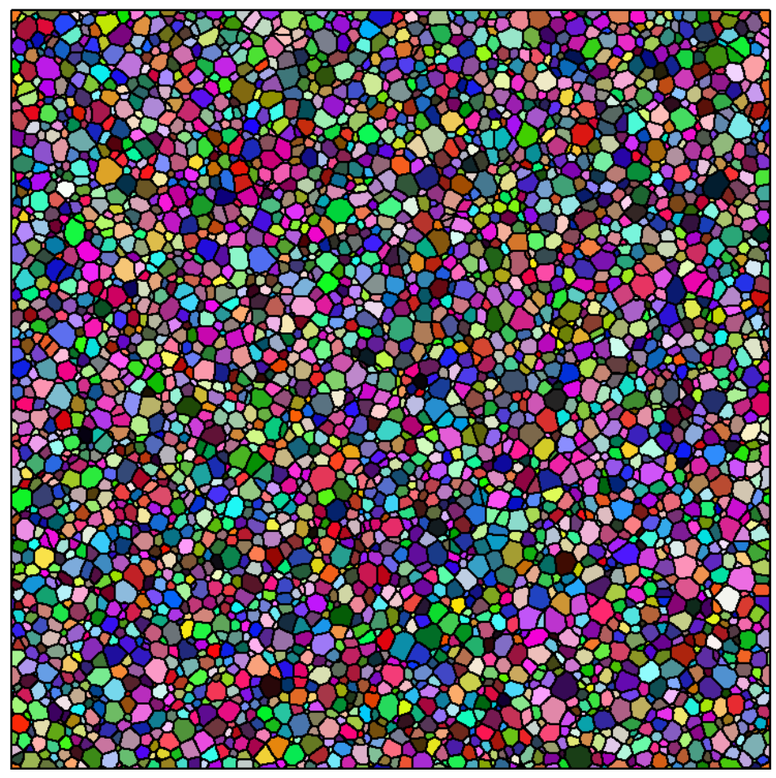
- Simulations begin with over 600,000 grains in 2D and 64,000 grains in 3D.
- Algorithm is expected to be unconditionally stable.
- Methods which implicity represent interfaces *naturally* allow topological changes to occur without additional user input (in contrast to explicit methods).
- Computational efficiency attained by maintaining a collection of spatially-separated grains in each signed distance function. Only one convolution is performed per collection of grains via the replacement of $d_k^n * G_{(\gamma_k \delta t)}$ by

$$\frac{\gamma_k(x)}{\gamma^*} \left(G_{\gamma^* \delta t} * d_k^n\right) + \left(1 - \frac{\gamma_k(x)}{\gamma^*}\right) d_k^n = d_k^n * G_{(\gamma_k\, \delta t)} + O(t),$$

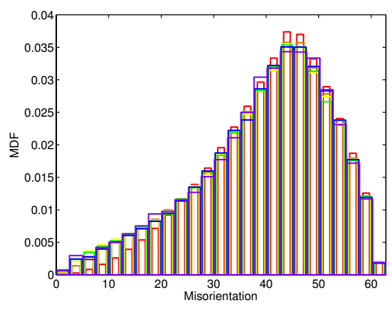
where $\gamma^* = \max_j \gamma_j$ and the γ_k are the weights required by the unequal interface energy algorithm.

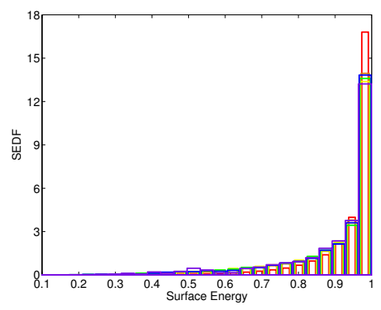
Numerical Results (Random Texture)

- Clustering is not apparent.



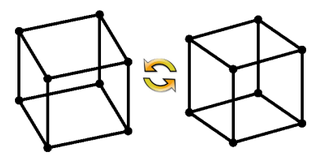
- Very few low-energy boundaries initially.
- Little evolution of the MDF.



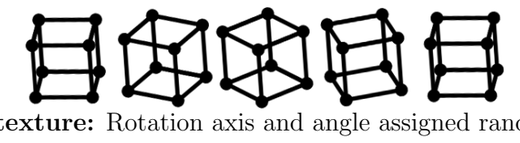


Basic Crystallography

Misorientation: ϕ_{ij}: Magnitude of the smallest rotation bringing the crystal lattice of Σ_i into alignment with that of Σ_j.



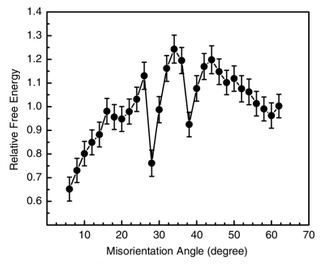
Fiber texture: All grain orientations share common rotation axis.

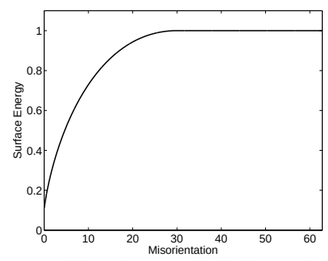


Random texture: Rotation axis and angle assigned randomly.

Surface Energy and Misorientation

Surface energies commonly modeled by Read–Shockley relation:





(left) K. Barmak, et al., "Grain Boundary Energy and Grain Growth in Highly-Textured Al Films and Foils: Experiment and Simulation," Mater. Sci. Forums (2005), 1255.

$$\gamma(\phi) = \begin{cases} \gamma_{\min} + (1 - \gamma_{\min}) \frac{\phi}{\phi_{\max}} \left[1 - \log\left(\frac{\phi}{\phi_{\max}}\right)\right], & \phi \leq \phi_{\max} \\ 1, & \text{otherwise} \end{cases}$$

MDF and SEDF

- The *misorientation distribution function* (MDF) measures the (area-weighted) proportion of grain boundaries with given misorientation.
- The *surface energy distribution function* (SEDF) is the analogous quantity for surface energies.

References

- M. Elsey, S. Esedoḡlu, and P. Smereka. Diffusion generated motion for grain growth in two and three dimensions. *J. Comput. Phys.* **228** (2009), 8015–8033.
- M. Elsey, S. Esedoḡlu, and P. Smereka. Large scale simulation of normal grain growth via diffusion generated motion. *Proc. Royal Soc. A* **467** (2011), 381–401.
- M. Elsey, S. Esedoḡlu, and P. Smereka. Simulations of anisotropic grain growth: Efficient algorithms and misorientation distributions. *Acta Mater.* **61** (2013), 2033–2043.

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