Mathematical modeling of interfacial dynamics in polycrystals

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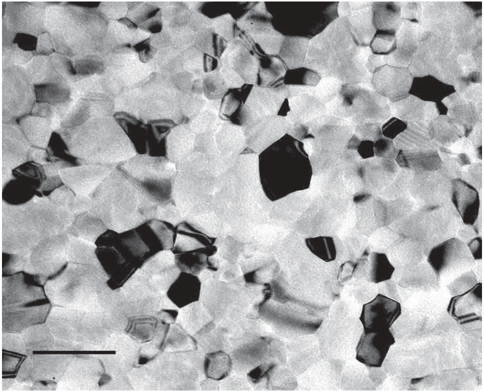
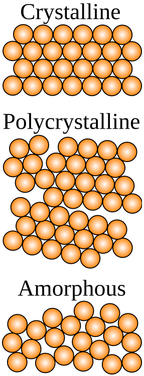
Polycrystals

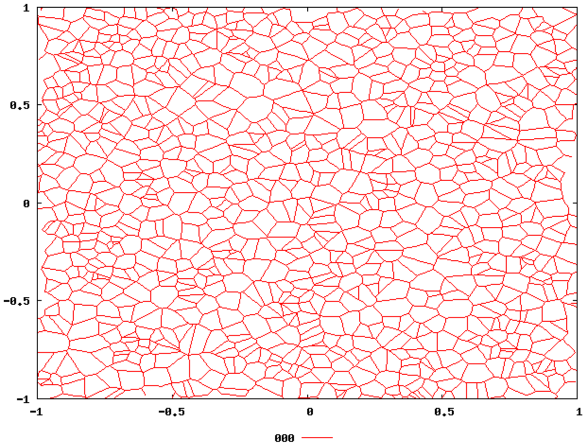
Polycrystalline materials are solids that are composed of many crystallites (grains) of varying size and orientation. The variation in directions is called texture and can be random or directed. Microstructure is the collection of grains with associated orientations.





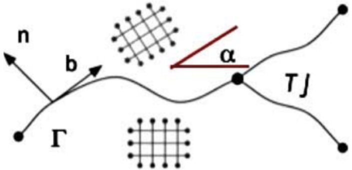
Grain growth

Grain growth is the increase in size of grains (crystallites) in a material at high temperature. This occurs when recovery and recrystallisation are complete and further reduction in the internal energy can only be achieved by reducing the total area of grain boundary.



Animation by Richard Sharp

Mathematical formulation: notations



- GB is a curve $\Gamma : x = \chi(s)$, $0 \leq x \leq L$ with
- $b = \dfrac{d\chi}{ds}$ (tangent) and $n = Rb$(normal), where R =rotation through $\pi/2$.
- α is the lattice misorientation parameter
- $\sigma = \sigma(n, \alpha) > 0$ is the surface tension (surface energy density) of Γ
- the energy of Γ is given by $E = \int_\Gamma \sigma(n, \alpha)|b|\, ds$, the amount of work required to generate an infinitesimal amount of new surface

Mathematical formulation: equilibrium conditions

Start with

$$E = \int_\Gamma \sigma(n, \alpha)|b|\, ds$$

Consider

$$E(\epsilon) = \int_\Gamma \sigma(n_\epsilon, \alpha)|b_\epsilon|\, ds$$

where $n_\epsilon = n + \epsilon R \frac{d\eta}{ds}$ and $b_\epsilon = b + \epsilon \frac{d\eta}{ds}$. This is the work required to deform the arc Γ from χ to $\chi + \epsilon\eta$ with two ends fixed, i.e. $\eta(0) = \eta(L) = 0$.
Then

$$\frac{dE}{d\epsilon}(0) = \int_\Gamma T \cdot \frac{d\eta}{ds}\, ds = -\int_\Gamma \frac{dT}{ds} \cdot \eta\, ds$$

where T is identified with the line stress and $\frac{dT}{ds}$ with the line force per unit length. If the arc is in equilibrium, then

$$\frac{dT}{ds} = 0 \text{ on } \Gamma$$

Mathematical formulation: curvature driven growth

Main assumption

The rate of growth of the area adjacent to Γ is equal to the work done through deformation of the curve, i.e.

$$v_n n = \mu \frac{dT}{ds}$$

where v_n is the normal velocity on Γ and $\mu > 0$ is the GB mobility.

Since

$$\begin{aligned} \frac{dE}{d\epsilon}(0) &= \int_\Gamma \frac{d}{d\epsilon}(\sigma(n_\epsilon, \alpha)|b_\epsilon|)ds \\ &= \int_\Gamma (\nabla_n \sigma \cdot R\frac{d\eta}{ds} + \sigma b \cdot \frac{d\eta}{ds})ds \\ &= \int_\Gamma (R^T \nabla_n \sigma + \sigma b) \cdot \frac{d\eta}{ds} ds \end{aligned}$$

and we know from above that

$$\frac{dE}{d\epsilon}(0) = \int_\Gamma T \cdot \frac{d\eta}{ds}\, ds,$$

we get the exact expression for the line stress as $T = R^T \nabla_n \sigma + \sigma b$

Mathematical formulation: curvature driven growth

So we have

$$T = R^T \nabla_n \sigma + \sigma b$$

If $n = (\cos\theta, \sin\theta)$, we reparameterize the energy as $\hat{\sigma}(\theta, \alpha) = \sigma(n, \alpha)$ and then rewrite the line stress as

$$T = \frac{d\hat{\sigma}}{d\theta} n + \hat{\sigma} b$$

which by Frenet formulas yields $\dfrac{dT}{ds} = (\dfrac{d^2\hat{\sigma}}{d\theta^2} + \hat{\sigma})\kappa n$, where κ is the curvature of Γ.

Hence the equilibrium condition becomes $(\dfrac{d^2\hat{\sigma}}{d\theta^2} + \hat{\sigma})\kappa = 0$ and the evolution equation is

$$v_n = \mu(\frac{d^2\hat{\sigma}}{d\theta^2} + \hat{\sigma})\kappa \text{ on } \Gamma \text{ (Mullins equation)}$$

Thus we have justified that the interfaces move by curvature.

Consequence

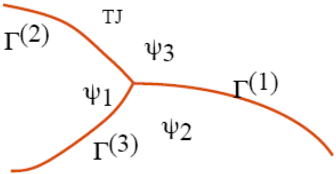
In equilibrium, all GBs are straight lines

Mathematical formulation: from one GB to a network

The energy of the system of GBs is given by

$$E = \Sigma_j \int_{\Gamma^{(j)}} \sigma(n^{(j)}, \alpha^{(j)})|b^{(j)}|\, ds$$

We now consider 3 curves $\Gamma^{(1)}, \Gamma^{(2)}, \Gamma^{(3)}$ forming a triple junction with the endpoints fixed:



Question: when will this TJ be at equilibrium?

Solution:

$$(\sigma''(\theta^{(j)}, \alpha^{(j)}) + \sigma(\theta^{(j)}, \alpha^{(j)}))\kappa^{(j)} = 0 \text{ on } \Gamma^{(j)}$$

subject to boundary conditions

$$\Sigma_j T^{(j)} = 0 \text{ (Herring condition)}$$
$$\chi^{(1)} = \chi^{(2)} = \chi^{(3)} \text{ at } s = 0,$$
$$\chi^{(j)} = x^{(j)} \text{ at } s = L^{(j)}$$

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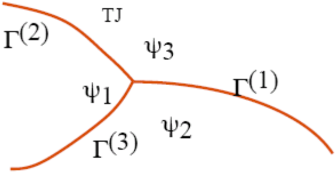

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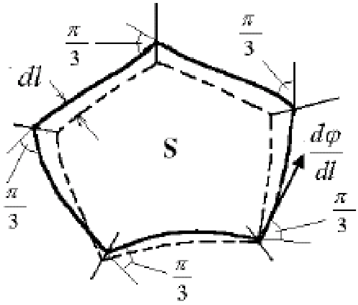
Herring condition

$\Sigma_j T^{(j)} = 0$ implies:

- if $\sigma = const$, $n^{(1)} + n^{(2)} + n^{(3)} = 0$, i.e. surfaces meet at angles of $2\pi/3$.
- If $\sigma = \sigma(\alpha)$ (does not depend on θ), we get

$$\frac{\sigma(\alpha_1)}{\sin(\theta_1)} = \frac{\sigma(\alpha_2)}{\sin(\theta_2)} = \frac{\sigma(\alpha_3)}{\sin(\theta_3)} \text{ (Young's law)}$$



Mathematical formulation: motion of TJs

Assuming the system of GBs evolves according to the curvature driven growth, i.e.

$$v_n^{(j)} n^{(j)} = \mu \frac{d}{ds} T^{(j)} \text{ on each } \Gamma_t^{(j)}$$

we need to find the boundary condition at TJs during evolution.

We can compute the total rate of dissipation of the TJ system as:

$$\frac{dE}{dt}(t) = -\Sigma_j \int_{\Gamma_t^{(j)}} \frac{1}{\mu^{(j)}} |v_n^{(j)}|^2 ds^{(j)} + v(t) \cdot \Sigma_j T^{(j)}(x^{(0)})$$

where $v(t)$ is the velocity of the triple junction.

Hence to ensure dissipation of the energy condition $dE/dt \leq 0$ is met, we have to require

$$\Sigma_j T^{(j)} = -\lambda v, \lambda \geq 0$$

which conforms with the Herring condition $\Sigma_j T^{(j)} = 0$ at equilibrium.

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Simulations

There are a number of numerical simulations that adhere to the curvature-driven growth formalism:

- Monte Carlo Potts models (Srolovitz, Holm, Rollett etc)
- Boundary-tracking PDE models (Kinderlehrer, Ta'asan, Livshitz, Emelianenko, Eggeling, Sharp)
- Vertex model simulations (Kawasaki, Otto, Niethammer)
- Diffusion generated motion simulation(Elsey, Esedoglu, Smereka)
- . . .

A typical vertex simulation

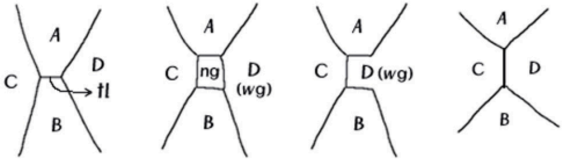
1024 grains, $\gamma(\alpha) = 1 + 0.01(1 - cos(2\pi\alpha)^3)$

(Loading movie)

Reconfiguration events

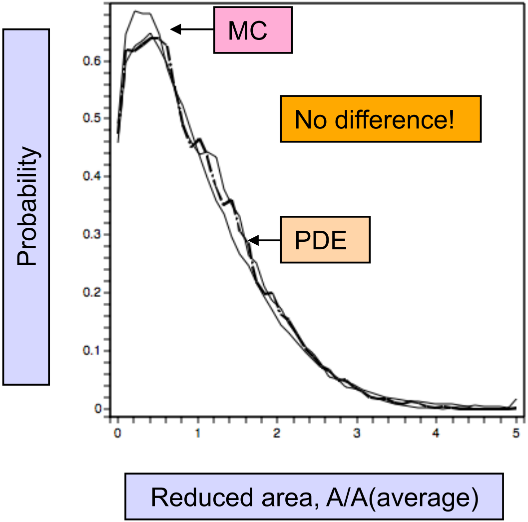
In addition to continuous evolution, grain boundary network experiences the following topological changes during grain growth:

- Loss of a facet (facet flipping)
- Loss of a small grain



Simulations differ in treatment of these events.
Question: how do they compare to each other? to experimental data?

Simulations agree with experiments on some accounts



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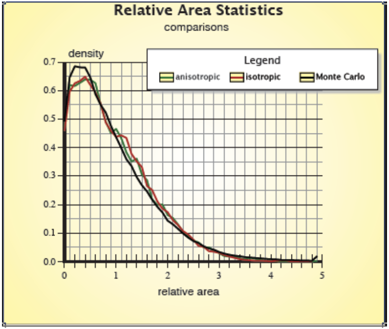
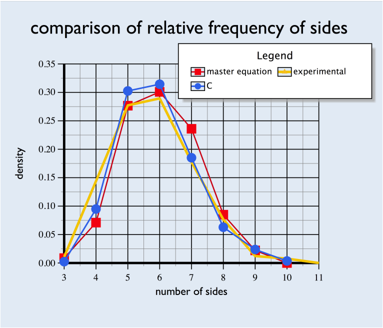
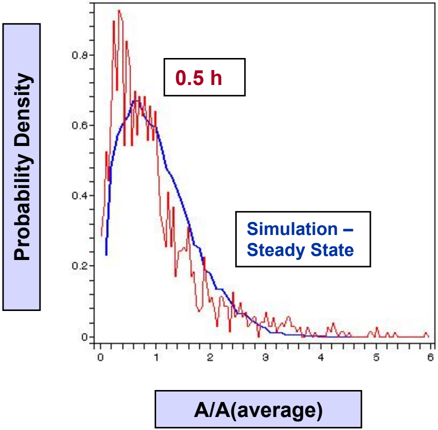
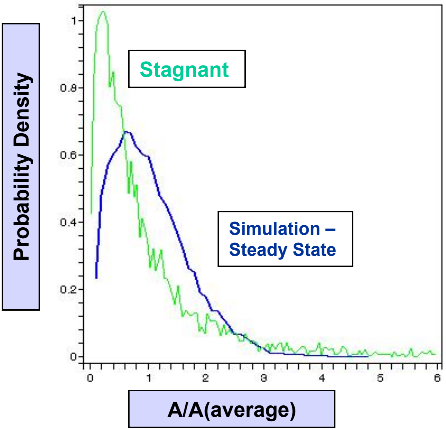




...and disagree on other





But which statistics is more important?

Materials characterization through statistical features

Question: Which statistics

- represents all 5 degrees of freedom of the polycrystalline network and
- is robust and physically meaningful?

Answer:

- One answer is texture, also called grain boundary character distribution (GBCD)
- Other distributions like ODF, MDF can be derived from GBCD
- It characterizes material texture better than the relative area or average number of sides statistics

More questions:

- What are the mechanisms that control the development of these distributions?
- How are these distributions affected by impurities?

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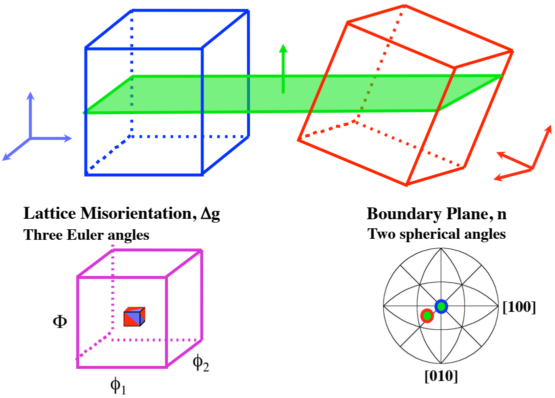
Definitions

GBCD = Grain boundary character distribution: relative area of grain boundaries distinguished on the basis of $\Delta\alpha$ and **n**.



Grain boundaries can be classified by means of 5 angle parameters

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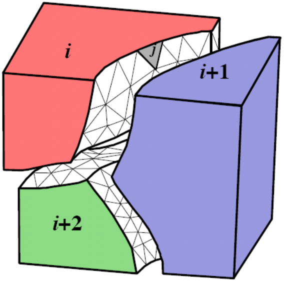
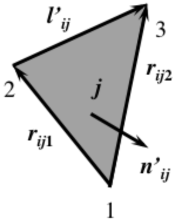
Misorientations $\Delta\alpha_{i,i+1}$
3 parameters



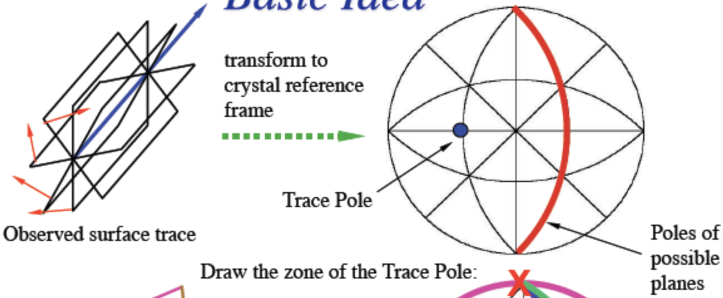
Grain boundary plane orientation $\mathbf{n}_{ij}$
2 parameters

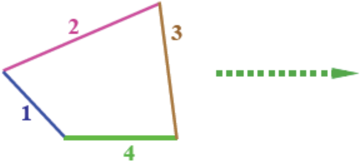


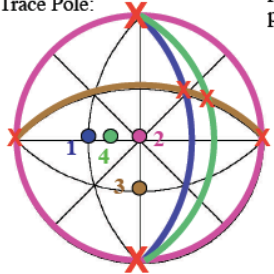
Key point

Measurements of the grain boundary character distribution, $\rho(\Delta\alpha, \mathbf{n})$, yield all of the information needed to specify conventional metrics such as grain size, grain size distribution, ODF, and MDF

Basic Idea







The normal to a given facet type is always perpendicular to its trace:

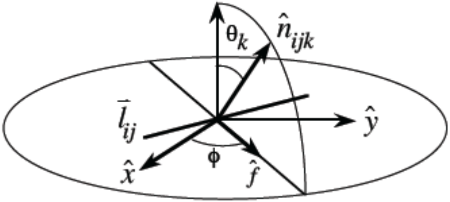
Changsoo Kim, 2004]

Therefore, if we repeat this procedure for many WC grains, high intensities (peaks) will occur at the positions of the habit plane normals

Habit function

$$\vec{p}(\hat{n}') = \frac{\sum_{i,j,k} g_i \hat{n}_{ijk} \, | l_{ij} | \sin\theta_k}{\sum_{i,j,k} | l_{ij} | \sin\theta_k}$$

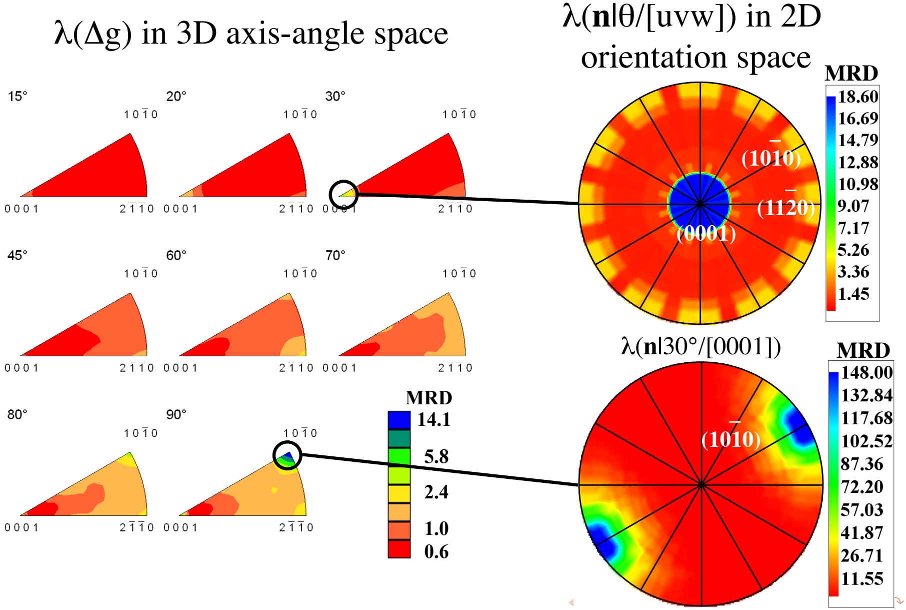
When this probability is plotted as a function of the normal, n', (in the crystal frame) maxima will occur at the habit planes.



The probability that a plane is observed is proportional to $\sin\theta_k$ and to the line length $|l_{ij}|$. Planes parallel to the section plane are not observed whereas planes perpendicular to the section have the maximum probability of being observed.

3D reconstruction : The dot product of any l_{ij} with each habit plane vanishes for the habit plane that created the surface trace. Since the total length of a set of randomly distributed lines intersecting an area is proportional to that area, the ratios of the line lengths associated with each plane is an estimate of the relative surface areas.

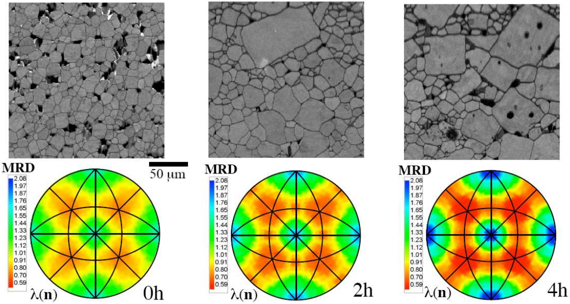
Visual Representation of the 5D GBCD



Why GBCD matters

Experiment: evolution of grain boundary character distribution (GBCD)

GBCD = relative areas of grain boundaries sorted by misorientation angles and normal



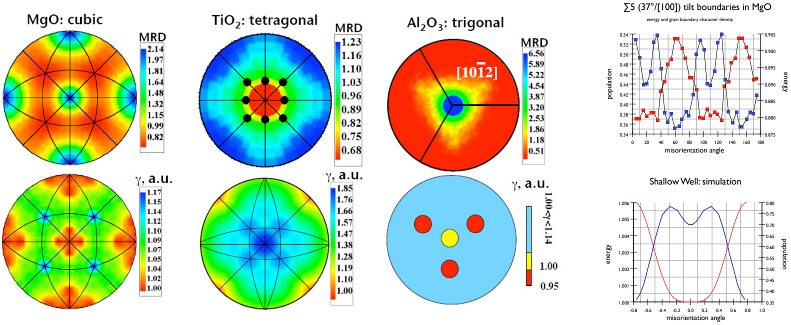
Gorzkowski et al. Zeitschrift fur Metallkunde, 96 (2005) 207.

$Pb(Mg_{1/3}Nb_{2/3})O_3 - 35\ PbTiO_3$

Materials texture characterization

GBCD is a scale invariant steady state characteristic of a material.

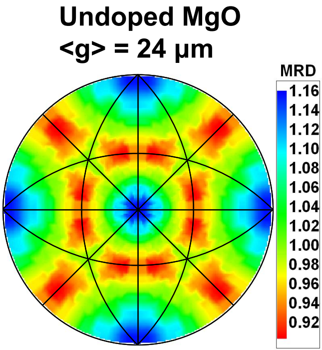
Interfacial energy and GBCD correlation

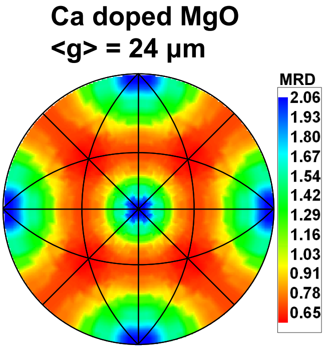


Observation

Grain boundary character distribution is inversely correlated with interfacial energies and is strongly dependent on crystallography.

Effect of impurities on GBCD





Observation

Added solute increases the anisotropy of the distribution.

Back to the main question: can we mathematically model texture development?

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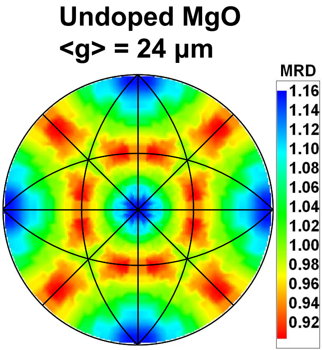

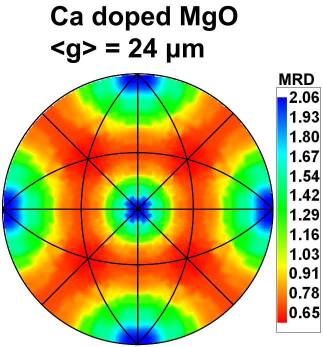

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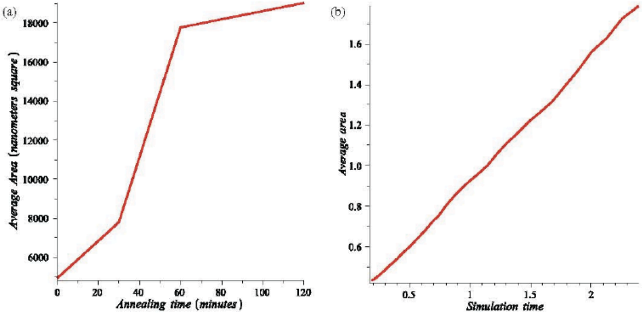
Role of reconfigurations in coarsening

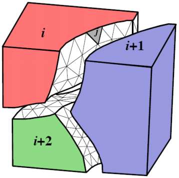
Mullins-von Neumann rule: $\dfrac{dA_n}{dt} = c(n-6)$
Experimental result for 5-sided grains in Al:



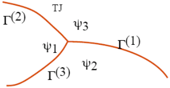
Can study this effect via a simplified model that retains critical events and kinetics but neglects curvature-driven motion of the boundaries. It is an abstraction of the role of triple junctions in the presence of the rearrangement events.

Towards a continuum model: simplified framework

3D

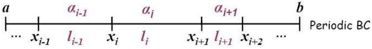


2D



α_i - misorientations
$\gamma(\alpha)$ - interfacial energies

1D



x_j	—	"triple junctions"
(x_j, x_{j+1})	—	"grain boundaries"
$l_j = x_{j+1} - x_j$	—	"GB areas"
$\{\alpha_i\}_{i=1,\ldots,n}$	—	"misorientations"

Given initial orientations α_i and total system energy in the form

$$E_n(t) = \sum \gamma(\alpha_i)(x_{i+1}(t) - x_i(t))$$

define equations of motion through gradient flow dynamics

$$\dot{x}_i = \gamma(\alpha_i) - \gamma(\alpha_{i-1}), \ \ i = 0, \ldots, n.$$
$$v_i = \dot{l}_i = \dot{x}_{i+1} - \dot{x}_i = \gamma(\alpha_{i+1}) - 2\gamma(\alpha_i) + \gamma(\alpha_{i-1})$$

where $\gamma(\alpha)$ plays the role of an interfacial energy.

Energy Dissipation

Reduced gradient flow model is designed to enforce dissipation. In fact, between reconfigurations

$$\frac{dE}{dt} = \sum \gamma(\alpha_i) v_i = -\sum (\gamma(\alpha_{i+1} - \gamma(\alpha_i))^2$$

If a boundary disappears at time $t = t_c$,

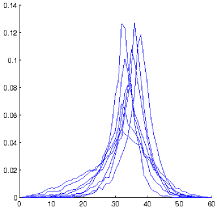
$$E(t_c) = \lim_{t \to t_c} \sum_{i \neq c} f(\alpha_i) l_i \leq \lim_{t \to t_c} E(t)$$

So the energy decreases for any t.

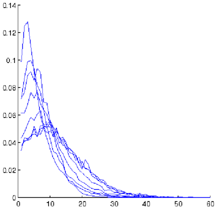
Stable statistics

$\rho_{or}(\alpha, t) = \sum_k \delta(\alpha - \alpha_k)$	pdf of orientations
$\rho_{len}(l, t) = \sum_i \delta(l - l_i)$	pdf of lengths
$\rho_w(\alpha, t) = \sum_k l_k \delta(\alpha - \alpha_k)$	weighted pdf of orientations (GBCD)
$\rho_{vel}(v, t) = \sum_j \delta(v - v_j)$	pdf of velocities

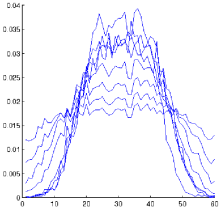
Distributions harvested from simulation stabilize early in the process. Gives evidence for a well-defined dynamic process.



grain boundary velocities



grain boundary lengths



orientations

GBCD for 1d model

Conforming to experimental observations, distribution of orientation parameters α is inversely correlated with interfacial energies $\gamma(\alpha)$.
It matches 2-dimensional simulation results, and has a Boltzmann distribution shape.

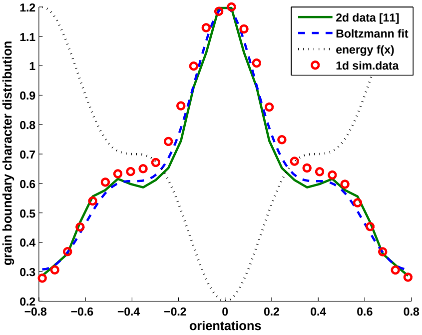


Figure: `GBCD comparison.`

Entropy-based theory of GBCD

The total surface energy of the system: $E[\rho] = \int \gamma(\alpha)\rho(\alpha, t)\, d\alpha$.

Let us add a configurational entropy term to get the free energy:

$$F_\lambda[\rho] = E[\rho] + \lambda \int \rho(\alpha) \log(\rho(\alpha))\, d\alpha$$

where λ is a temperature-like parameter.
Variational principle:

$$\frac{\mu}{2\tau} d(\rho, \rho^*)^2 + F_\lambda(\rho) = \inf_\eta \{ \frac{\mu}{2\tau} d(\eta, \rho^*)^2 + F_\lambda(\eta) \}$$

Shown: GBCD is obtained as a limit of an iterative process $\rho^* = \rho^{k-1}, \rho^k = \rho$ and satisfies Fokker-Planck equation:

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial \alpha}(\lambda \frac{\partial \rho}{\partial \alpha} + \frac{d\gamma}{d\alpha} \rho)$$

Validation

Minimization of F_λ gives a Boltzmann distribution (stationary solution to Fokker-Planck):

$$\rho_\lambda(\alpha) = \frac{e^{-\gamma(\alpha)/\lambda}}{Z_\lambda}$$

where $Z_\lambda = \int_\Omega e^{-\gamma(\alpha)/\lambda}$.
Kullback-Leibler relative entropy for the Fokker-Planck equation:

$$\Phi_\lambda(\eta) = \lambda \int_\Omega \eta log \frac{\eta}{\rho_\lambda} d\alpha$$

It is a nonnegative convex function of η, and

$$\Phi_\lambda(\eta) = F_\lambda(\eta) + \lambda log Z_\lambda$$

For a solution ρ with $\lambda = \sigma$ we have $\lim_{t\to\infty} \Phi_\sigma(\rho) = 0$ exponentially fast.
From Csiszar-Kullback inequality, $\rho(\alpha, t) \to \rho_\sigma(\alpha)$ exponentially fast.

Entropy-based model validation

Minimization of F_λ gives a Boltzmann distribution (stationary solution to Fokker-Planck):

$$\rho_\lambda(\alpha) = e^{-\gamma(\alpha)/\lambda}$$

where $Z_\lambda = \int_\Omega e^{-\gamma(\alpha)/\lambda}$.
Question: how does one pick λ?

Entropy-based model validation

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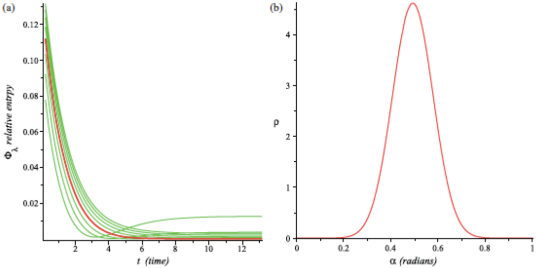
$$\rho_\lambda(\alpha) = e^{-\gamma(\alpha)/\lambda}$$

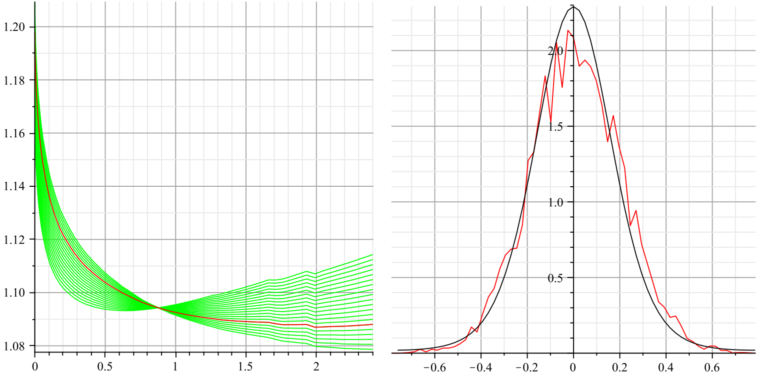
where $Z_\lambda = \int_\Omega e^{-\gamma(\alpha)/\lambda}$.
Question: how does one pick λ?

Relative entropy approach: Seek λ s.t. relative entropy $\Phi_\lambda(\eta) = F_\lambda(\eta) + \lambda \log Z_\lambda$ exhibits an exponential decay. There is a unique such λ.



Does it match the distribution obtained in simulation?

(1) There is a unique such λ
(2) The distribution for this λ precisely matches the simulation result

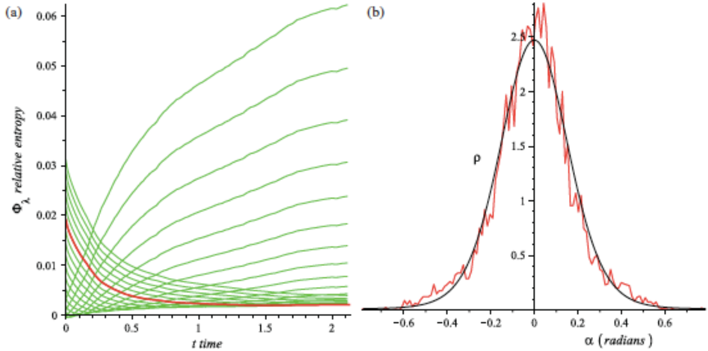


[Barmak, Eggeling, Emelianenko, Epshteyn, Kinderlehrer, Taasan, Sharp, PRB (2011)]

Applying entropy theory to 2d simulation

Given interfacial energy $\gamma(\alpha)$, we compare Boltzmann distribution for the special value of parameter λ with simulation:

- Compute relative entropy - it is exponentially decaying for a unique value of λ
- Compute Boltzmann distribution for the same λ
- Compare with the stationary GBCD



Observations

Compelling evidence: Theory developed on the basis of the 1d model yields a good fit in 2d.

What it does: offers a physically sound way to describe development of the stationary texture distribution

Needed: generalization to the case with normal dependence.

What it does not do:
describe dynamical features of the coarsening process.

Observations

Compelling evidence: Theory developed on the basis of the 1d model yields a good fit in 2d.

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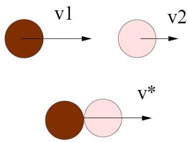
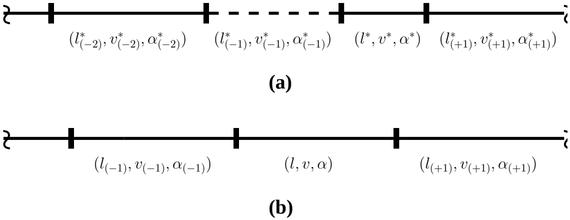
describe dynamical features of the coarsening process.

Modeling critical events via inelastic Boltzmann equation

We can think of a critical event as a collision of inelastic particles: particle $\equiv$ GB.

$$(\alpha_2, v_2) + (\alpha_1, v_1) \Rightarrow (\alpha_1, v^*), \text{ where } v^* = v_1 + v_2 + f(\alpha_2) - f(\alpha_1),$$





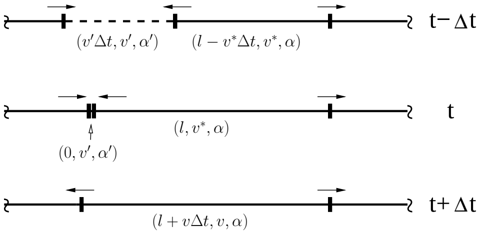
Continuity equation:

$$\frac{\partial \rho(l,v,\alpha,t)}{\partial t} + v\frac{\partial \rho(l,v,\alpha,t)}{\partial l} = \{gain\} - \{loss\}.$$

where the right hand side term can be written as an integral over all possible collisions:

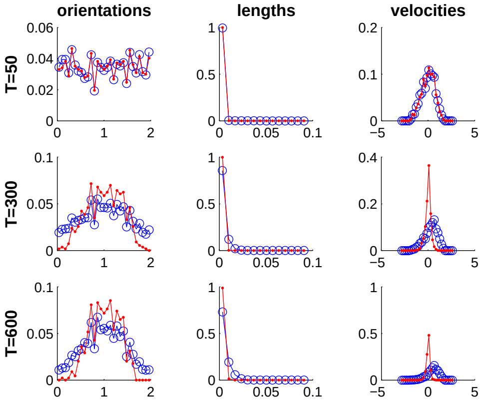
$$-\frac{2}{N(t)}\int_{A_+} v'\rho(0,v',\alpha',t)\rho(l,v-v'+f(\alpha)-f(\alpha'),\alpha,t)\,d\alpha' dv'$$
$$+\frac{2}{N(t)}\int_{A_-} v'\rho(0,v',\alpha',t)\rho(l,v,\alpha,t)\,d\alpha' dv'.$$

subject to restricting conditions:
$A_- := \{f(\alpha) \le v' + 2f(\alpha')\} \cap \{f(\alpha') \le v + 2f(\alpha)\} \cap \{v' < 0\}$,
$A_+ := \{f(\alpha) \le v' + 2f(\alpha') \le v + 3f(\alpha)\} \cap \{v' < 0\}$.



[Barmak, Emelianenko, Golovaty, Kinderlehrer, Ta'asan, Intl. J. Num. Anal. Mod. (2008)]

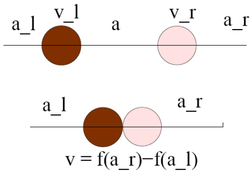
Simple model performance for quadratic potential



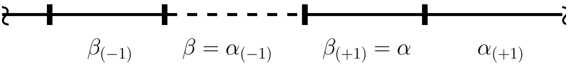
Lengths and orientations fit experimental results well, but velocities start to deviate at later stages. Possible correlations?

Extended space model

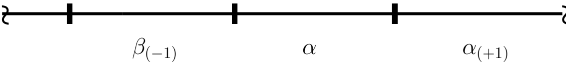
Is there a remedy for complexity and correlation issues?
Then let us expand the state space to include incidence relations: $\rho(l, \alpha_{(-1)}, \alpha, \alpha_{(+1)}, t)$.



Grain boundaries $\equiv$ colliding particles.



(a)



(b)

By following these simple collision rules, we can write a Boltzmann-type collision equation for the density function:

$$\frac{\partial \rho\left(l, \alpha_{(-1)}, \alpha, \alpha_{(+1)}\right)}{\partial t} + \left(f\left(\alpha_{(-1)}\right) + f\left(\alpha_{(+1)}\right) - 2f(\alpha)\right) \frac{\partial \rho\left(l, \alpha_{(-1)}, \alpha, \alpha_{(+1)}\right)}{\partial l} = W,$$

where $W = W_+ - W_-$ with

$$W_+ := \frac{1}{N(t)} \int_{\mathcal{B}} \left(2f(s) - f(\alpha) - f(\alpha_{(-1)})\right) \rho\left(0, \alpha_{(-1)}, s, \alpha\right) \rho\left(l, s, \alpha, \alpha_{(+1)}\right) \, ds$$
$$+ \frac{1}{N(t)} \int_{\mathcal{B}} \left(2f(s) - f(\alpha) - f(\alpha_{(+1)})\right) \rho\left(0, \alpha, s, \alpha_{(+1)}\right) \rho\left(l, \alpha_{(-1)}, \alpha, s\right) \, ds.$$

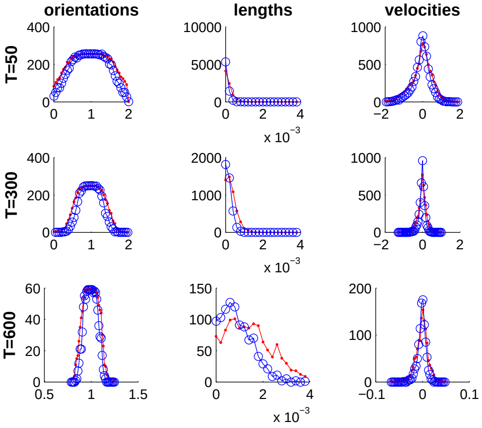
Similarly

$$W_- := \frac{1}{N(t)} \int_{\mathcal{B}} \left(f(\alpha) + f(s) - 2f(\alpha_{(-1)})\right) \rho\left(0, s, \alpha_{(-1)}, \alpha\right) \rho\left(l, \alpha_{(-1)}, \alpha, \alpha_{(+1)}\right) \, ds$$

$$+ \frac{1}{N(t)} \int_{\mathcal{B}} \left(f(\alpha) + f(s) - 2f(\alpha_{(+1)})\right) \rho\left(0, \alpha, \alpha_{(+1)}, s\right) \rho\left(l, \alpha_{(-1)}, \alpha, \alpha_{(+1)}\right) \, ds.$$

where $\mathcal{B} := \mathbf{R}_+ \times \mathbf{R}^3$.

Extended model performance for quadratic potential



Lengths, orientations and velocities are in agreement with experimental results.

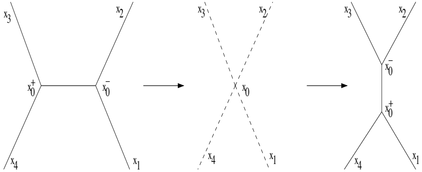
2-dimensional model

- $\Gamma^{(j)}$: $x = \chi_j(s)$ - j-th grain boundary parameterized by $0 \leq s \leq L$
- Three boundaries meet at a triple junction (TJ)
- $b = \dfrac{d\chi}{ds}$ is its tangent
- Curvature driven flow: $v_n = \mu f \kappa$, where κ is the curvature of the boundary
- Total energy can be given by $E = \sum_j \int_{\Gamma^{(j)}} f(\alpha^{(j)})|b^{(j)}|$
- It was shown by Kinderlehrer & Liu (2001) that the system is dissipative under curvature driven flow as long as

$$\sum_j T^{(j)} = -\lambda v, \; \lambda \geq 0$$

  where $T^{(j)} = f(\alpha^{(j)})b^{(j)}$ is the expression for line stress for the case of energy that does not depend on the normal direction.
- Hence $v = -\dfrac{1}{\lambda} \sum_j T^{(j)}$ can be used as a velocity of the TJ, similar to the 1-dimensional case.

Boltzmann mesoscopic description in 2d



The "collision" event involves 5 grain boundaries, with misorientation angles $\alpha_1 = \phi_1 - \phi_2, \alpha_2 = \phi_2 - \phi_3, \alpha_3 = \phi_3 - \phi_4, \alpha_4 = \phi_4 - \phi_1, \alpha_5 = \phi_1 - \phi_3$.
Notice that $\alpha_2 = \alpha_5 - \alpha_1, \alpha_4 = -\alpha_3 - \alpha_5$.

The collision event then can be represented as follows:

$$(\alpha_1, \mathbf{v}_1) + (\alpha_3, \mathbf{v}_3) + (\alpha_5, \mathbf{v}_5) \Rightarrow (\alpha_1, \mathbf{v}_1) + (\alpha_3, \mathbf{v}_3) + (\alpha_5^*, \mathbf{v}_5^*)$$

where $\mathbf{v}_5^* = \mathbf{v}_5 + 2\mathbf{b}(f(\alpha_3) - f(\alpha_1))$ and $\alpha_5^* = \phi_2 - \phi_4$.

Boltzmann equation then can be written by integrating over all possible collisions, similar to 1d.

Features of the Boltzmann approach

The 2d Boltzmann description:

- provides a mechanism for describing dynamical features of grain growth
- can incorporate disappearance of small grains
- can incorporate grain nucleation
- can provide high accuracy results

Drawbacks:

- high dimension of the state space
- numerically challenging

Alternative approaches include:

- Master equation models (Kinderlehrer, Niethammer)
- Read-Shockley models (Rohrer, Rollett)
- Levy process evolution equations, fractional PDE models (Emelianenko, Golovaty)

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Summary and challenges

Summary of results:

- Texture development can be explained via entropy-based theory
- Other statistics evolution can be obtained with Boltzmann-type approach

Active research directions:

- How does microstructure and in particular texture affect materials properties, e.g. mechanical response?
- Can one extend these approaches to 3d and include dependence on the normal direction?
- Is it possible to obtain a first principles justification for these theories?
- Can a comprehensive unbiased comparative analysis of various grain growth simulations based on experimental data for both stationary and dynamic materials characteristics be performed?