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17 Gauss Way Berkeley, CA 94720-5070 p: 510.642.0143 f: 510.642.8609 www.msri.org

NOTETAKER CHECKLIST FORM

(Complete one for each talk.)

Name: Malgorzata Marciniak **Email/Phone:** mmarciniak@lagcc.cuny.edu 5734620411

Speaker's Name: Jeremy Mason

Talk Title: Predictive simulation of grain structure evolution

Date: 10 /05 /2018 **Time:** 11 : 00 ~~am~~ / pm (circle one)

Please summarize the lecture in 5 or fewer sentences:
Expansion the sets of grain boundary topologies and topological transitions to formulate a physical criterion for the selection of a topological transition. Development of equations of motion suitable for arbitrary grain boundary energies and mobilities. Preparation of a front-tracking code able to perform predictive simulations of grain structure evolution.

CHECK LIST

(This is **NOT** optional, we will **not pay** for **incomplete** forms)

- ☑ Introduce yourself to the speaker prior to the talk. Tell them that you will be the note taker, and that you will need to make copies of their notes and materials, if any.
- ☑ Obtain ALL presentation materials from speaker. This can be done before the talk is to begin or after the talk; please make arrangements with the speaker as to when you can do this. You may scan and send materials as a .pdf to yourself using the scanner on the 3rd floor.
  - **Computer Presentations**: Obtain a copy of their presentation
  - **Overhead**: Obtain a copy or use the originals and scan them
  - **Blackboard**: Take blackboard notes in black or blue **PEN**. We will **NOT** accept notes in pencil or in colored ink other than black or blue.
  - **Handouts**: Obtain copies of and scan all handouts
- ☑ For each talk, all materials must be saved in a single .pdf and named according to the naming convention on the "Materials Received" check list. To do this, compile all materials for a specific talk into one stack with this completed sheet on top and insert face up into the tray on the top of the scanner. Proceed to scan and email the file to yourself. Do this for the materials from each talk.
- ☑ When you have emailed all files to yourself, please save and re-name each file according to the naming convention listed below the talk title on the "Materials Received" check list. (*YYYY.MM.DD.TIME.SpeakerLastName*)
- ☑ Email the re-named files to notes@msri.org with the workshop name and your name in the subject line.

MSRI Hot Topics: Shape and Structure of Materials

Predictive simulations of grain structure evolution

5 October 2018

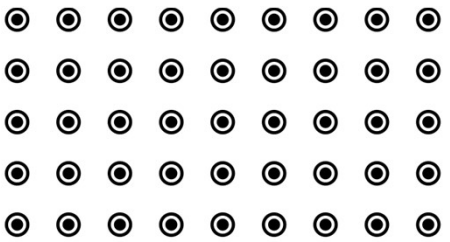
Jeremy Mason
Erdem Eren

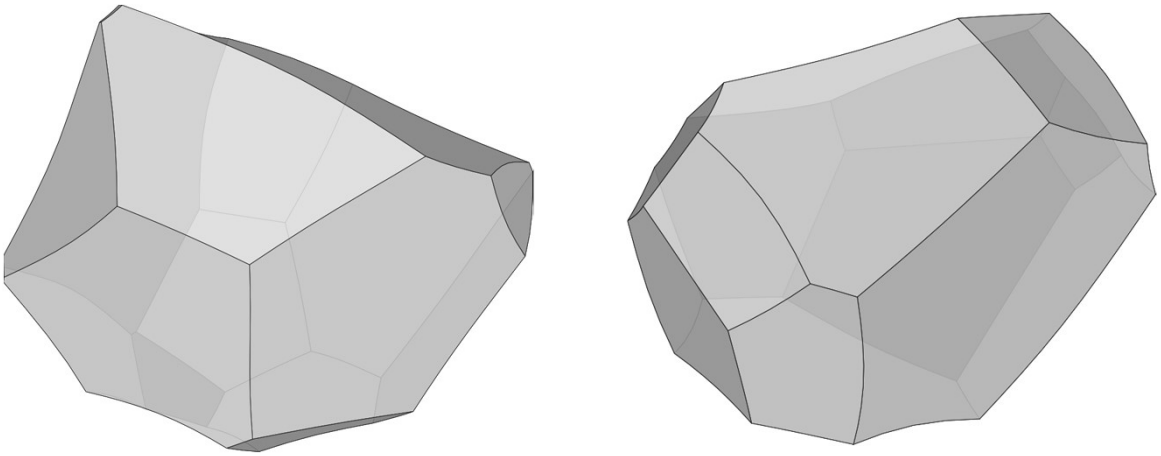
UCDAVIS

Grains and Boundaries

A grain is a domain with long range atomic translational symmetry

The symmetry is broken on a grain boundary





Turnbull Eq: $v_n = m_0 \exp\left(-\frac{Q_{gb}}{k_B T}\right) p$

Young–Laplace Eq: $p = \gamma\kappa$

Governing Eq: $v_n = m\gamma\kappa$

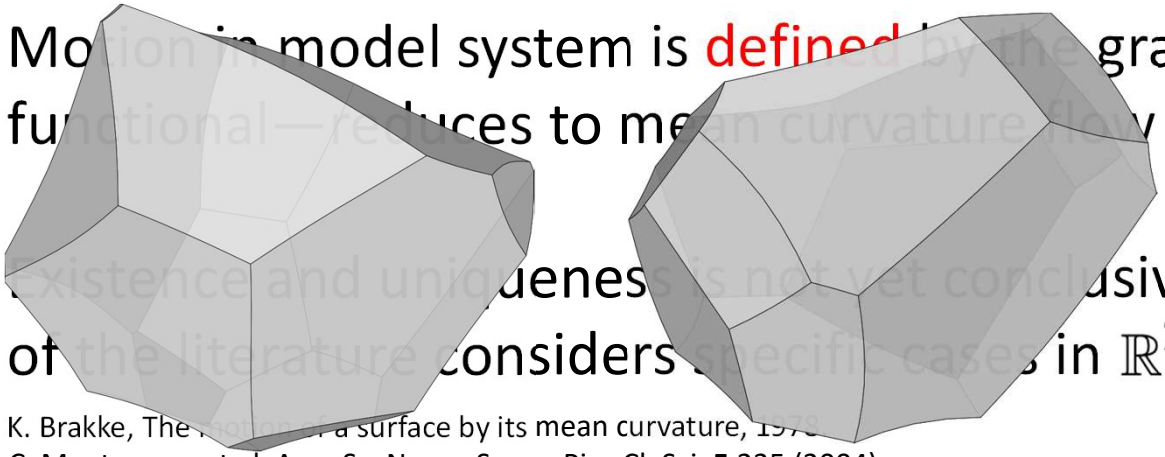
An Idealized Model

Studies of this system usually use the following assumptions:

- Boundary mobility and energy are constants
- Boundaries are smooth surfaces
- System energy is proportional to overall boundary area
- Boundary junction lines and vertices do not have any properties except as specified by adjoining boundaries

Motion in model system is defined by the gradient flow of the area functional—reduces to mean curvature flow away from singularities

Existence and uniqueness is not yet conclusively established, much of the literature considers specific cases in $\mathbb{R}^2$

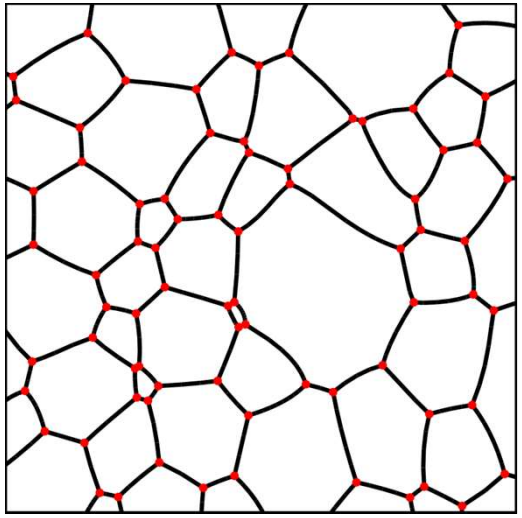


K. Brakke, The motion of a surface by its mean curvature, 1978

C. Mantegazza et al. Ann. Sc. Norm. Super. Pisa Cl. Sci. **5** 235 (2004).
A. Magni et al. Ann. Sc. Norm. Super. Pisa Cl. Sci. **5** 117 (2016).

T. Ilmanen et al. arXiv:1407.4756 (2014).
L. Kim et al. Ann. I. Fourier, **66** 43 (2017).

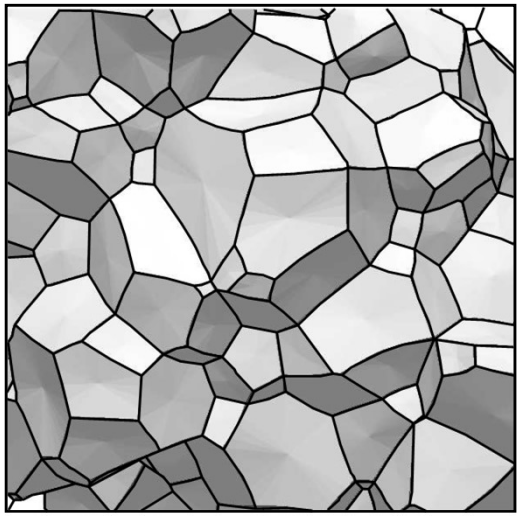
Grain Growth Structures



Topological properties:
- Two grains at an edge
- Three edges at a vertex

Geometric properties:
- Vertex angles go to $2\pi/3$

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\pi}{3} m\gamma(n-6)$$



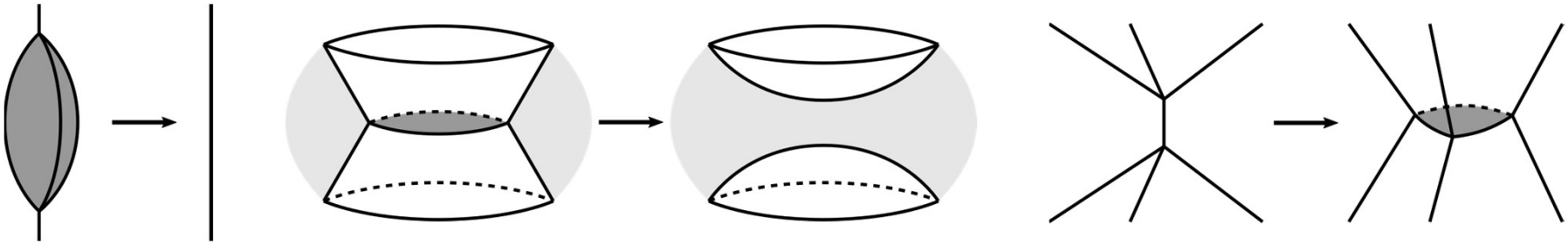
Topological properties:
- Two grains at a face
- Three faces at an edge
- Four edges at a vertex

Geometric properties:
- Edge angles go to $2\pi/3$
- Vertex angles go to $\mathrm{acos}(-1/3)$

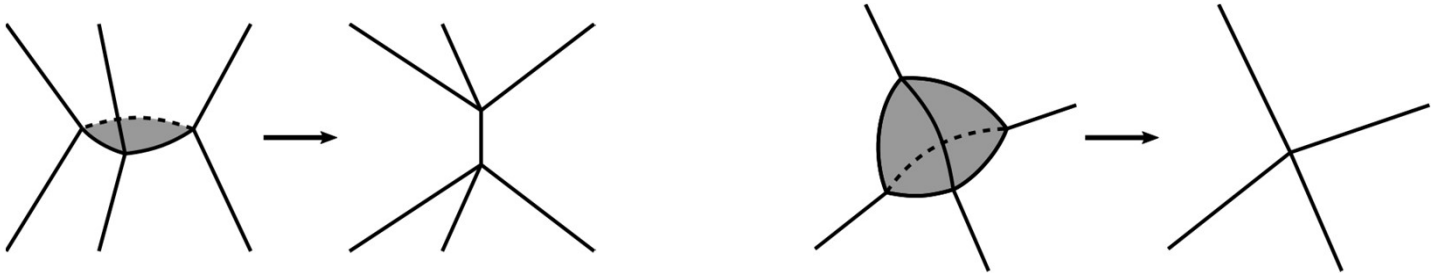
$$\frac{\mathrm{d}V}{\mathrm{d}t} = \frac{\pi}{3} m\gamma(\mathcal{M}-6\mathcal{L})$$

Singularities

Simulations suggest that all singular events (topological transitions) are composed of three fundamental operations*:



Numerically convenient to supplement with two other operations:

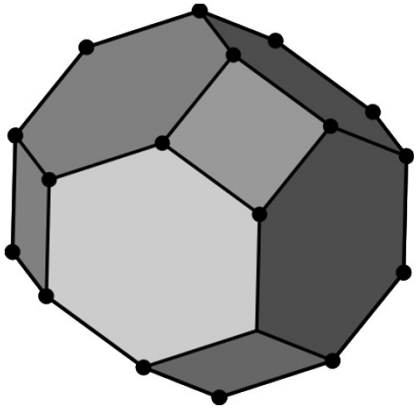


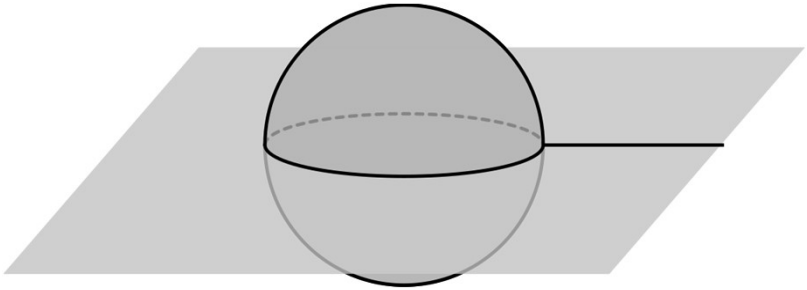
*requires stability of trajectory around the singularity

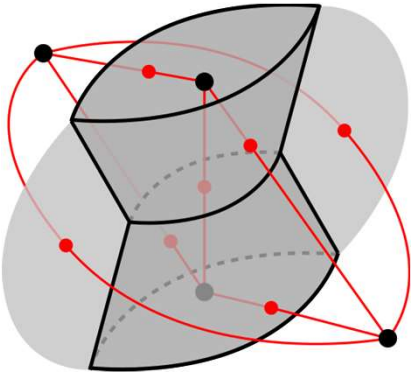
Topology of the Structure

Seems to generically converge to a regular pure CW-complex

- CW-complex is a union of i-dimensional cells with disjoint interiors for $1 \leq i \leq n$
- Regular requires that the attaching maps be homeomorphisms
- Pure requires that every cell is in the closure of some n-cell







Excludes cells without lower adjacencies

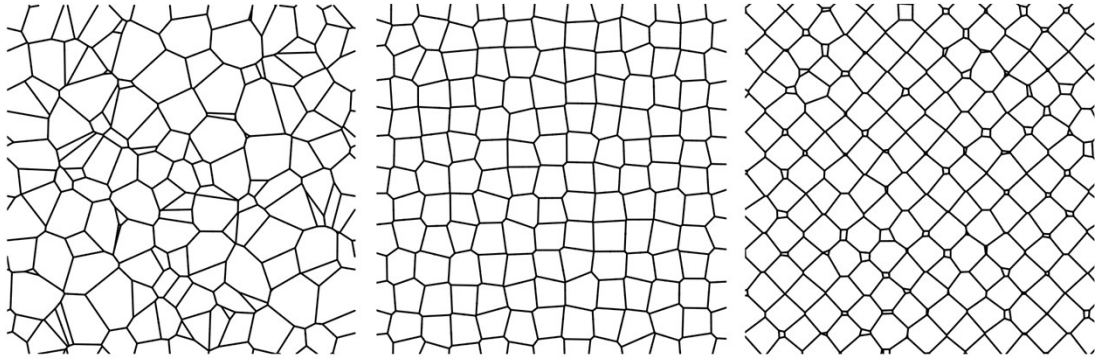
Valence conditions exclude arbitrary subdivisions

Dual object is not a triangulation despite four-valent vertices

Self Similar Structure

Conjecture I: For almost all initial conditions, mean curvature flow eventually results in a self-similar structure

Conjecture II: For almost all initial conditions with a self-similar structure, the self-similar structures are the same.



Self Similar Structure

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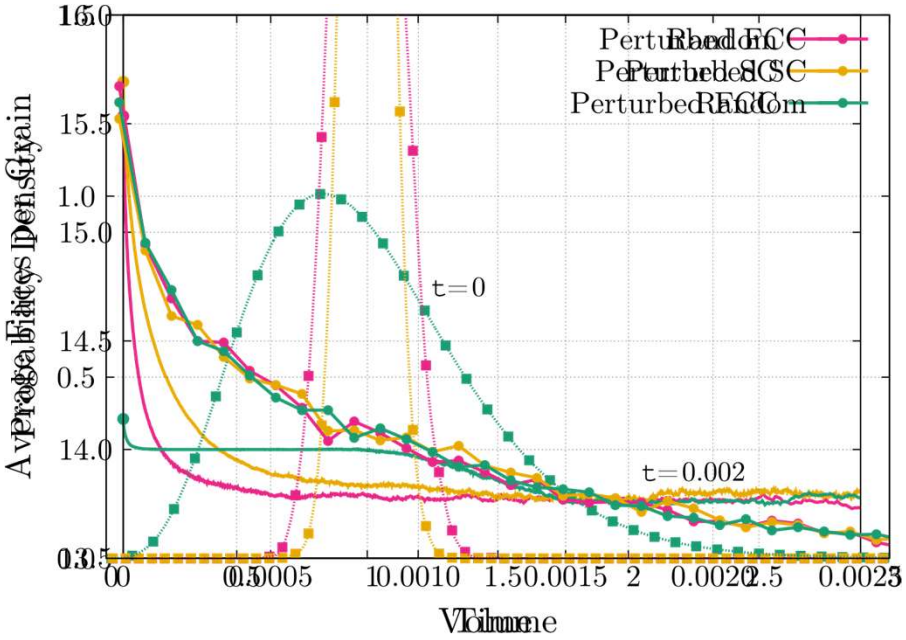
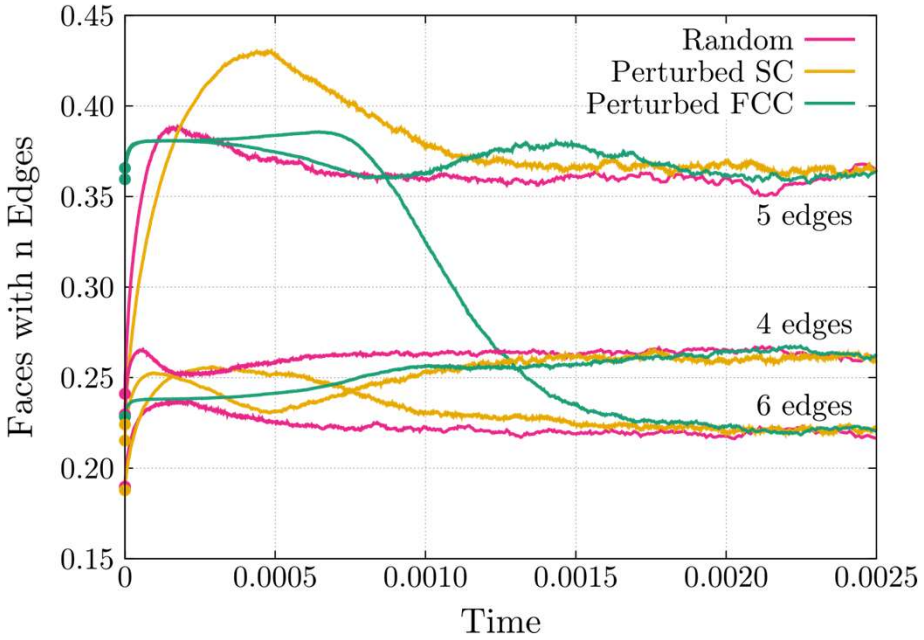


J. K. Mason et al. Phys Rev E **92** 063308 (2015).

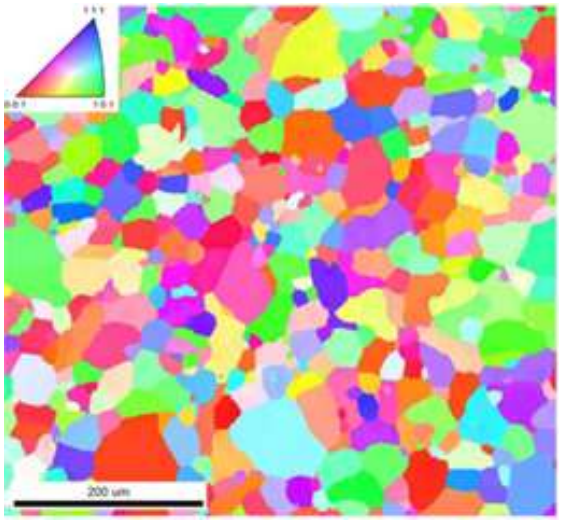


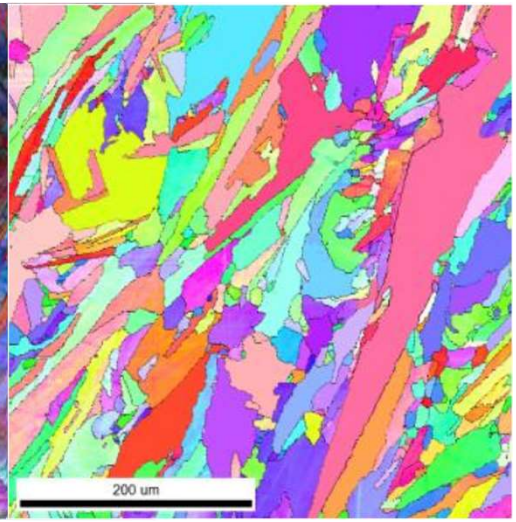
B. Schweinhart et al. Phys Rev E **93** 062111 (2016).

The Reality of the Situation: Part I

The idealized grain structure is not often observed in practice

- Grain boundary properties are neither uniform nor isotropic
- Surfaces are not even once differentiable
- Cell valence conditions are not satisfied
- Cannot assume well-behaved initial conditions





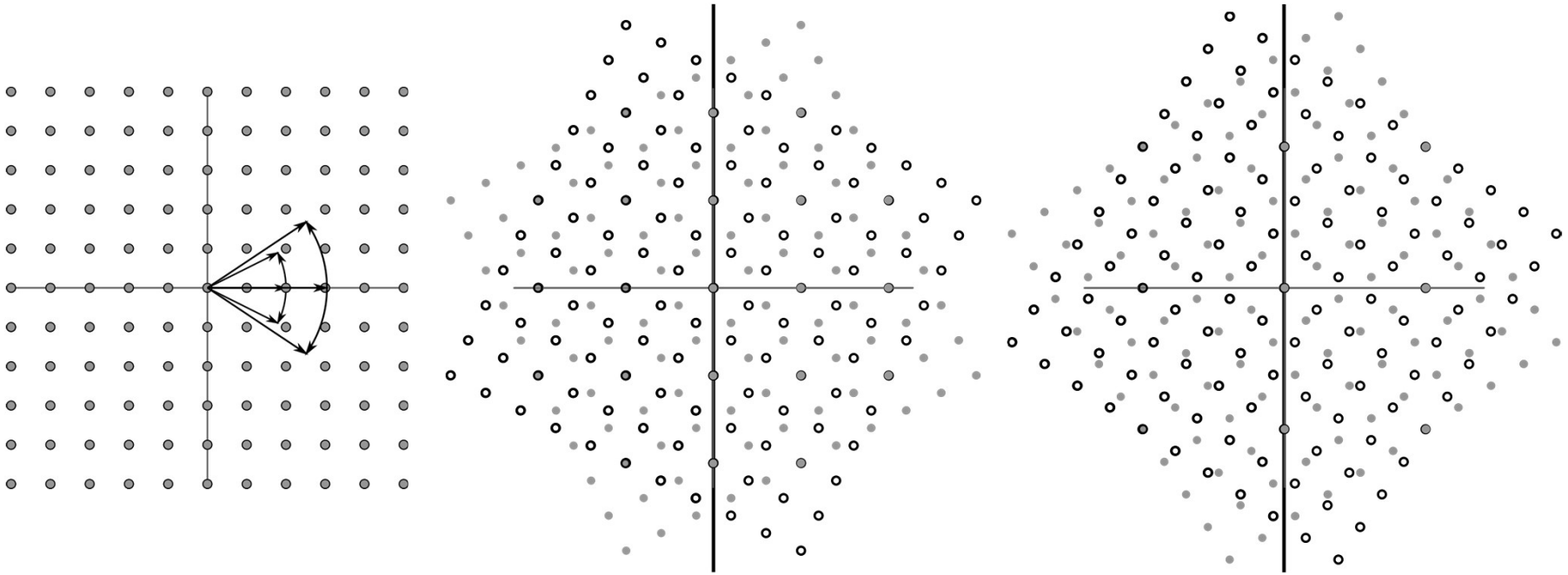
J. Min et al. J Manuf Sci E-T ASME **138** 054501-1 (2016).
S. B. Lee Mater Metall Trans A **31A** 985 (2000).

J. Min et al. J Manuf Sci E-T ASME **138** 054501-1 (2016).
S. B. Lee Mater Metall Trans A **31A** 985 (2000).

Grain Boundary Misorientation

Grain boundary energy and mobility actually functions on a five-dimensional grain boundary space

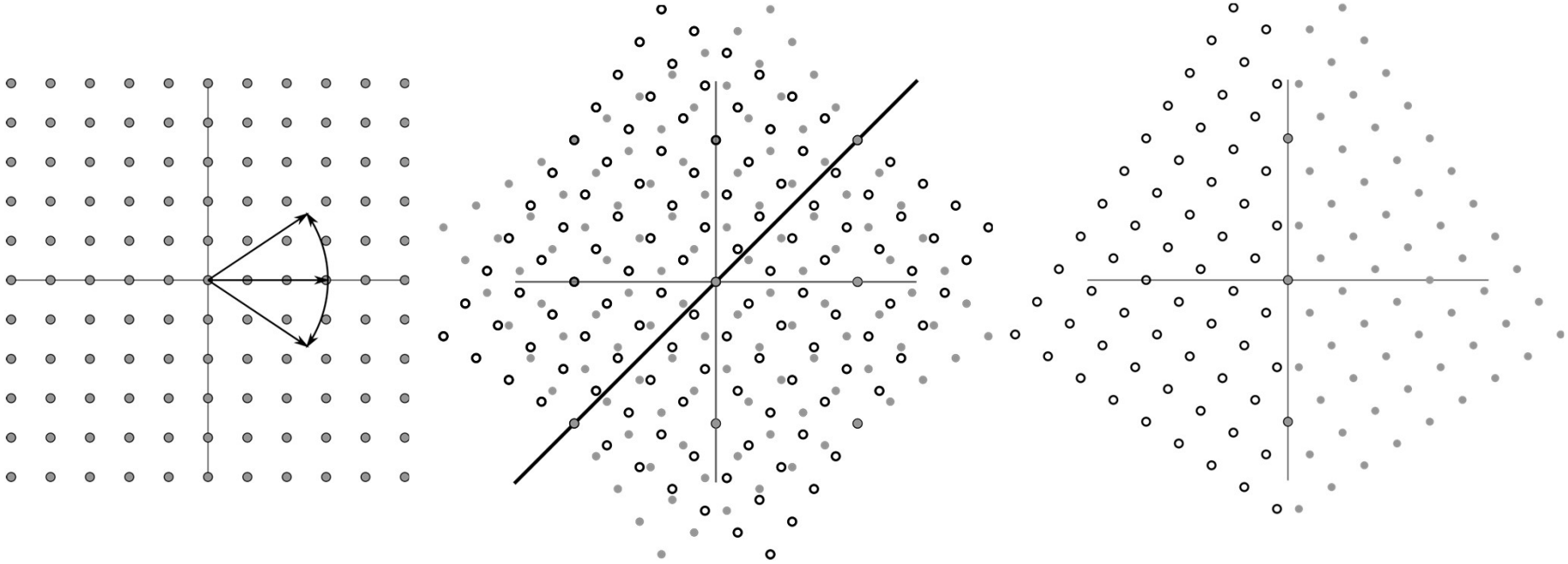
Three dimensions relate to the relative orientation of crystal lattices, or $\mathrm{SO}(3)$ is a 3-manifold



Grain Boundary Inclination

Grain boundary energy and mobility actually functions on a five-dimensional grain boundary space

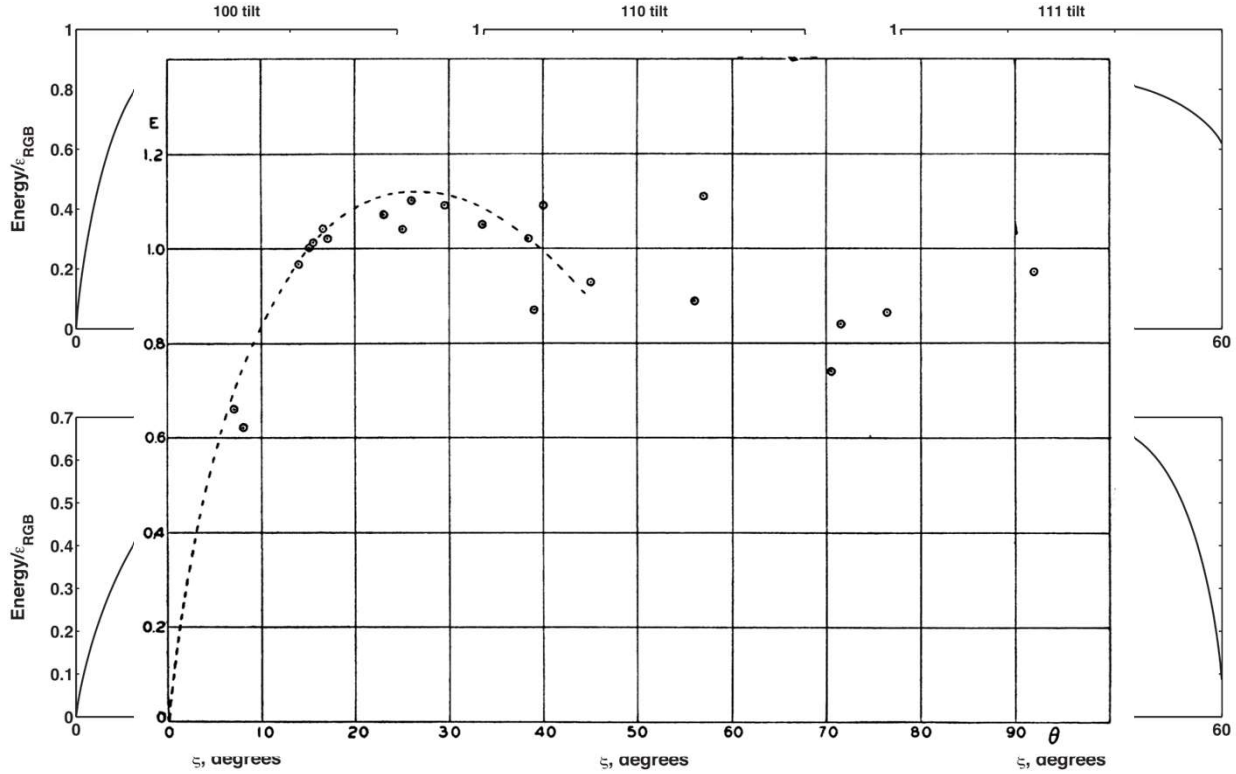
Two dimensions relate to the orientation of the boundary plane, or S^2 is a 2-manifold



Grain Boundary Energy

Early theoretical analysis suggests that function contains logarithmic singularities of the form $E = E_0\theta[A - \log\theta]$

Most recent analysis is not substantially more complete



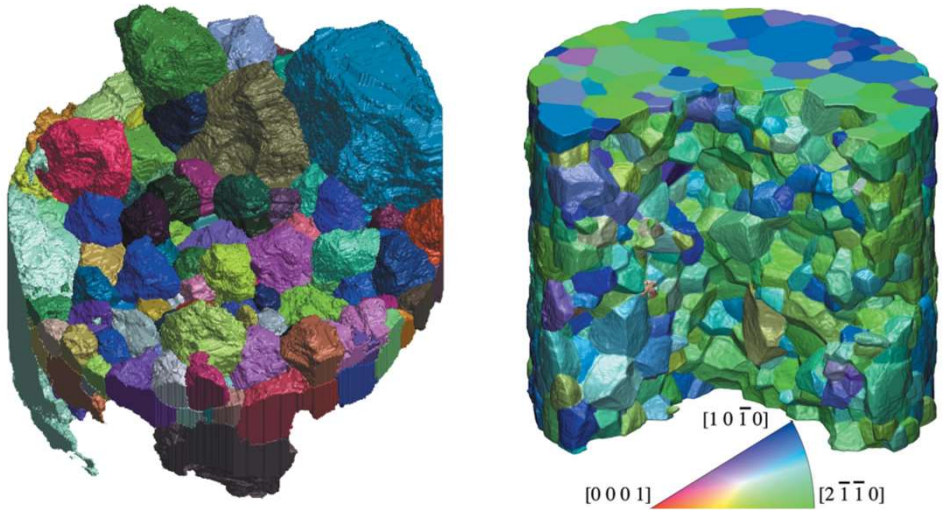
W. T. Read et al. Phys Rev **78** 275 (1950).

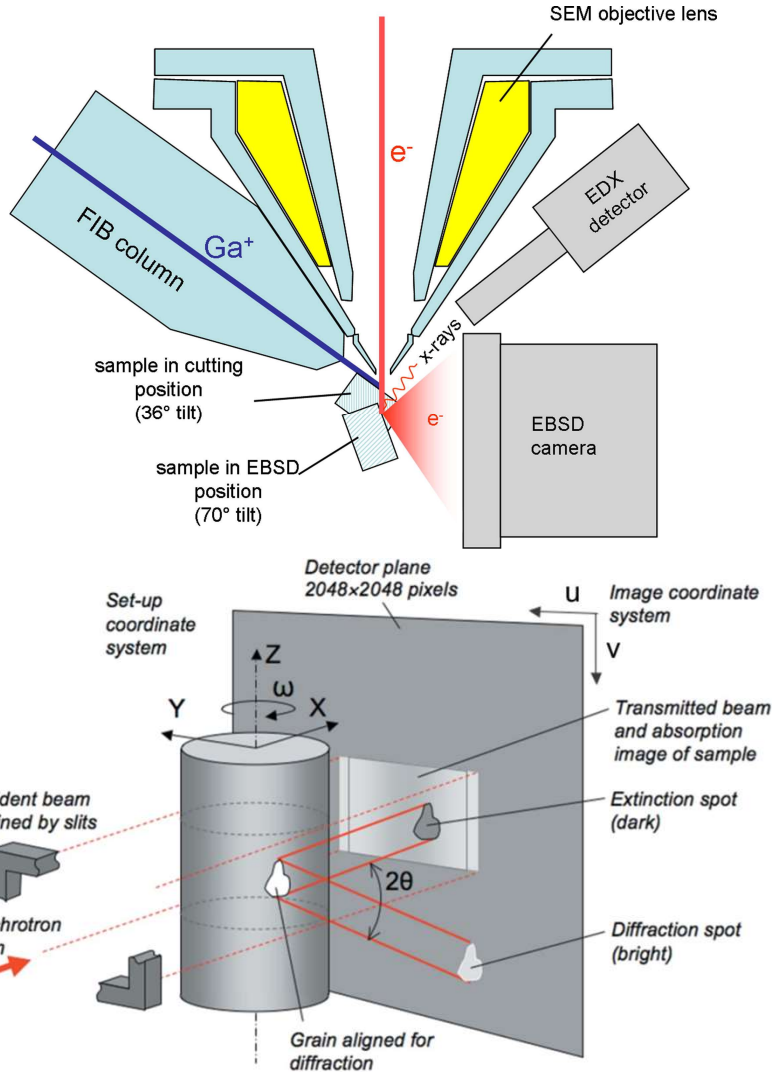
V. V. Bulatov et al. Acta Mater **65** 161 (2014).

3D Microstructures

EBSD-FIB destructively images serial sections to make a reconstruction

3DXRD nondestructively uses synchrotron x-rays (available at ALS) to make a reconstruction





J. Konrad et al. Acta Mater 54 1369 (2006).
G. Johnson et al., J Appl Crystalogr **41**, 310 (2008).
P. Reischig et al., J Appl Crystalogr **46**, 297 (2013).

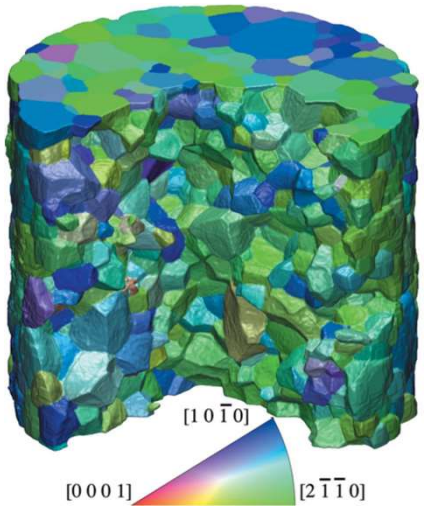
Regression of the Energy Function

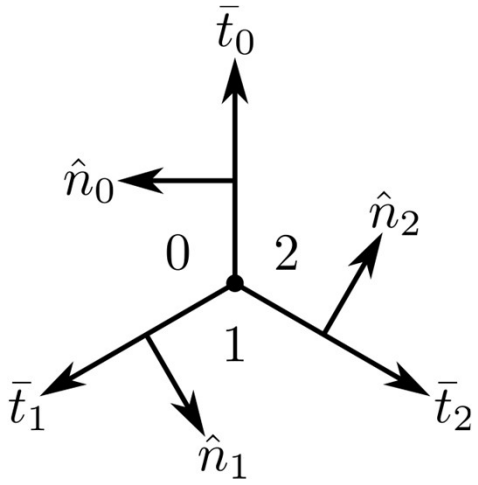
Can use 3D microstructures to reconstruct grain boundary energy

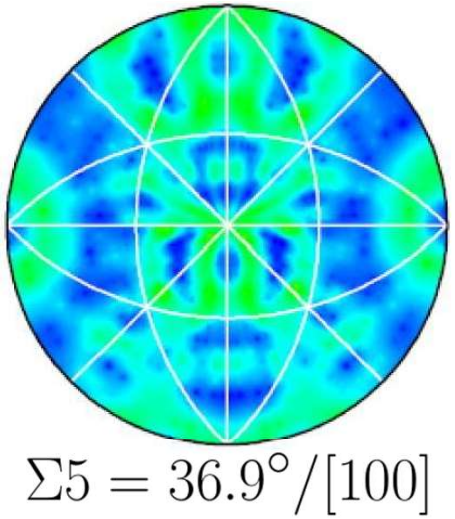
- Junction lines in equilibrium satisfy the Herring equation

$$\sum_i \hat{t}_i \gamma(\hat{n}_i) + \hat{n}_i \frac{\partial \gamma}{\partial \phi}\bigg|_{\hat{n}_i} = 0$$

- Provides a system of equations for expansion coefficients
- Reduce measurement errors and improve basis functions







P. Reischig et al. J Appl Crystallogr **46** 297 (2013).
A. Morawiec, Acta Mater 48 3525 (2000).

H. Beladi et al. Acta Mater **70** 281 (2014).

Aside on Weighted Mean Curvature

The Young–Laplace equation states that the driving pressure is proportional to the surface energy and the mean curvature

Implies a force exerted on an infinitesimal surface element

$$H = \kappa_1 + \kappa_2 \qquad p = \gamma H \qquad \mathrm{d}\bar{F} = \hat{n} p \mathrm{d}A$$

The mean curvature is the negative of the rate of change of area with respect to the volume swept out

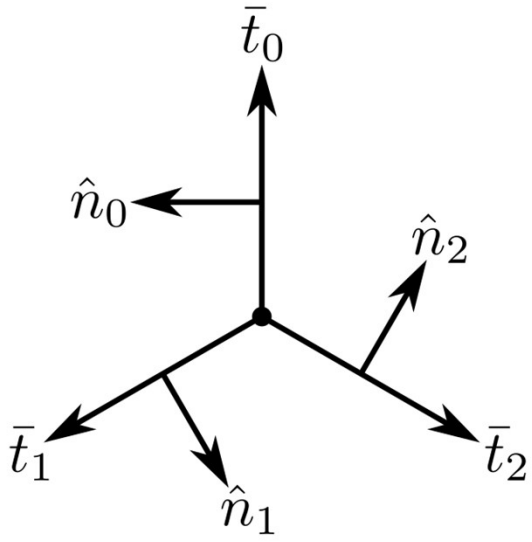
$$\omega = \left(\gamma + \frac{\partial^2 \gamma}{\partial \theta^2}\right)\kappa_1 + \left(\gamma + \frac{\partial^2 \gamma}{\partial \phi^2}\right)\kappa_2 \qquad \mathrm{d}\bar{F} = \hat{n}\omega \mathrm{d}A$$

The weighted mean curvature is the negative of the rate of change of surface energy with respect to the volume swept out

J.E. Taylor, Acta Metall et Mater **40**, 1475 (1992).

Equations of Motion: Part I

Given a 2D triangulation, search for local equations of motion for the general case



$$\mathrm{d}\bar{F} = \hat{n}\omega\mathrm{d}A$$

$$\bar{F} = \lambda \sum_i \hat{t}_i \gamma(\hat{n}_i) + \hat{n}_i \frac{\mathrm{d}\gamma}{\mathrm{d}\phi}\bigg|_{\hat{n}_i}$$

$$0 = \sum_i \hat{t}_i \gamma(\hat{n}_i) + \hat{n}_i \frac{\mathrm{d}\gamma}{\mathrm{d}\phi}\bigg|_{\hat{n}_i}$$

$$\bar{F} = \lambda \left[\delta_1 \bar{\bar{I}} + \frac{1}{2} \sum_i \delta_2(\hat{n}_i) \, \|\bar{t}_i\| \, \hat{n}_i \otimes \hat{n}_i \right] \bar{v}$$

This is an equation of motion for arbitrary grain boundary junction lines

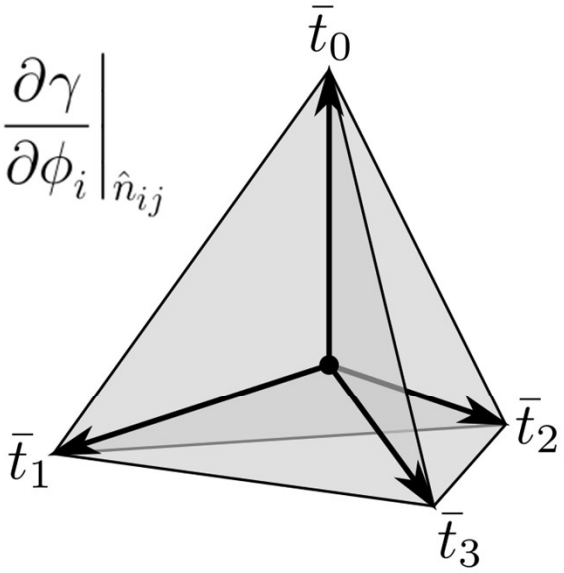
J.E. Taylor, Acta Metall et Mater **40**, 1475 (1992). J.K. Mason, Acta Mater 125, 286 (2017).

Equations of Motion: Part II

For arbitrary junction vertices, observe that the grain boundary energy has units of force per length

$$\bar{F} = \sum_i \hat{t}_i \tau(\hat{t}_i) + \frac{1}{2} \|\bar{t}_i\| \sum_{j:\{i,j\}\in\Delta} (\hat{n}_{ij} \times \hat{t}_i)\gamma(\hat{n}_{ij}) + \hat{n}_{ij} \frac{\partial \gamma}{\partial \phi_i}\bigg|_{\hat{n}_{ij}}$$

$$\bar{F} = \left[\delta_0 \bar{\bar{I}} + \frac{1}{2} \sum_i \delta_1(\hat{t}_i) \|\bar{t}_i\| (\bar{\bar{I}} - \hat{t}_i \otimes \hat{t}_i) + \frac{1}{6} \sum_{\{i,j\}\in\Delta} \delta_2(\hat{n}_{ij}) \left\|\bar{t}_i \times \bar{t}_j\right\| \hat{n}_{ij} \otimes \hat{n}_{ij} \right] \bar{v}$$



This is an equation of motion for arbitrary grain boundary junction vertices

J.K. Mason, Acta Mater **125**, 286 (2017).

The Reality of the Situation: Part II

The idealized grain structure is not often observed in practice

- Grain boundary properties are neither uniform nor isotropic
- Surfaces are not even once differentiable
- Cell valence conditions are not satisfied
- Cannot assume well-behaved initial conditions

Some of these difficulties can already be resolved

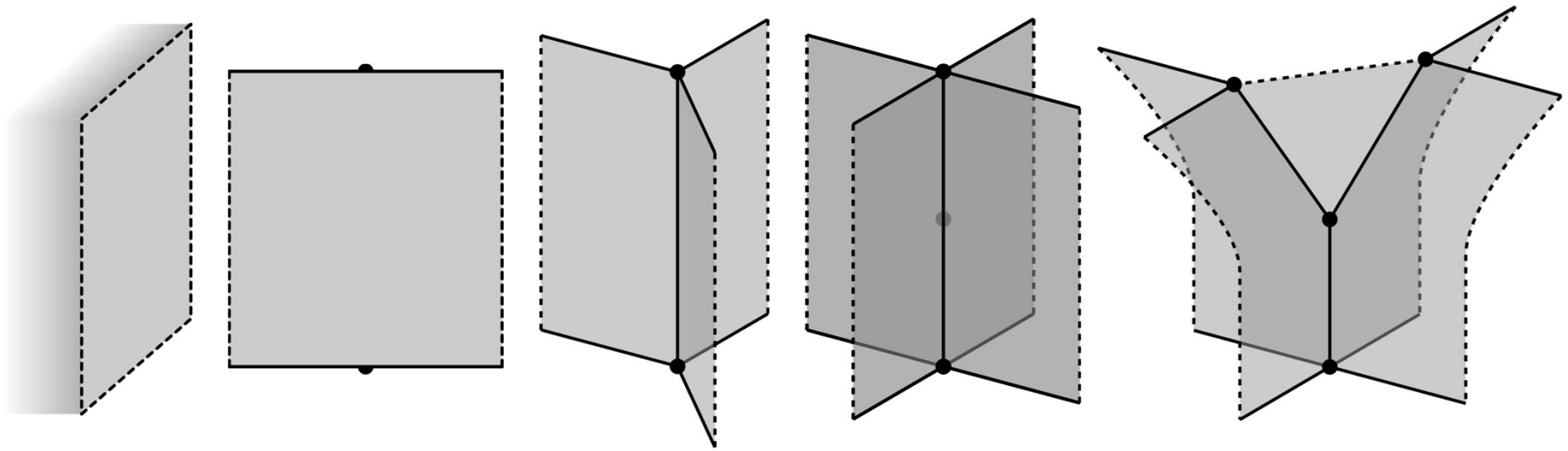
- Grain boundary properties can be extracted from 3D microstructures imaged by EBSD-FIB or 3DXRD
- Equations of motion can handle facets and relaxed valence conditions (every triangle is considered as a facet)

What is the set of singularities that can be expected to occur?
How can the topology of the resulting structures be described?

Relaxed Valence Conditions

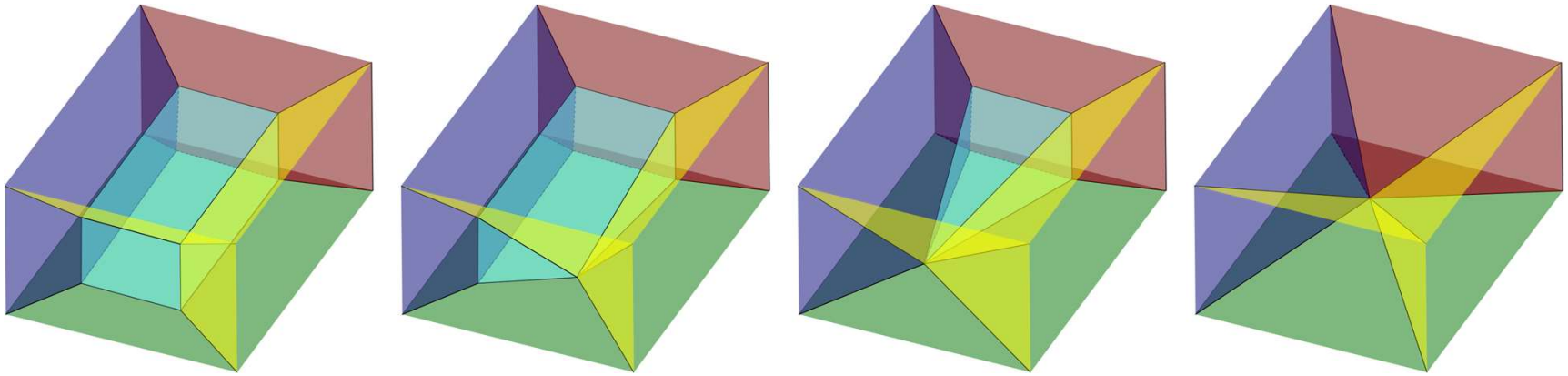
Valence conditions should be as permissible as possible while maintaining correspondence to physical system

- 2-cell must have one or more upper adjacencies
- 1-cell must have three or more upper adjacencies
- 0-cell must have three or more upper adjacencies
- No restrictions on number of lower adjacencies

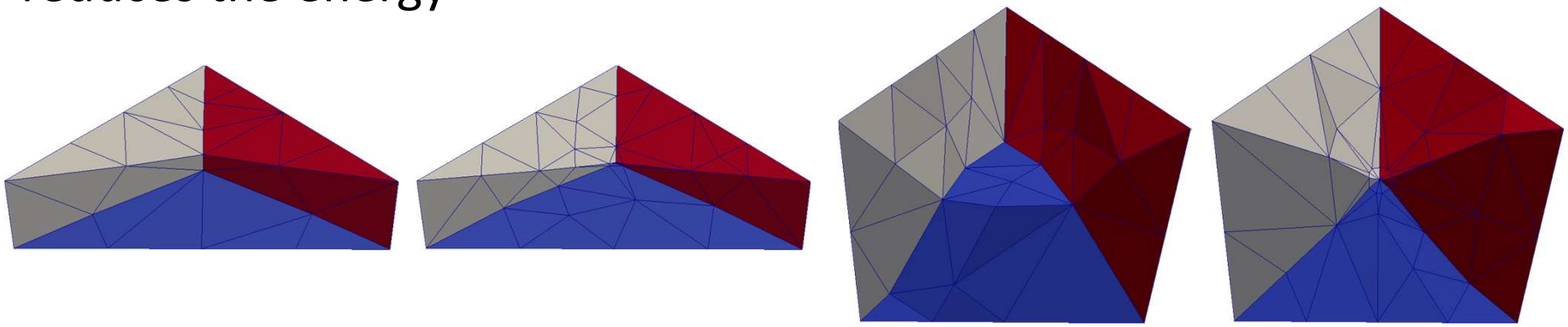


Singularities: Removal

Removal occurs when the Hausdorff measure of a cell vanishes



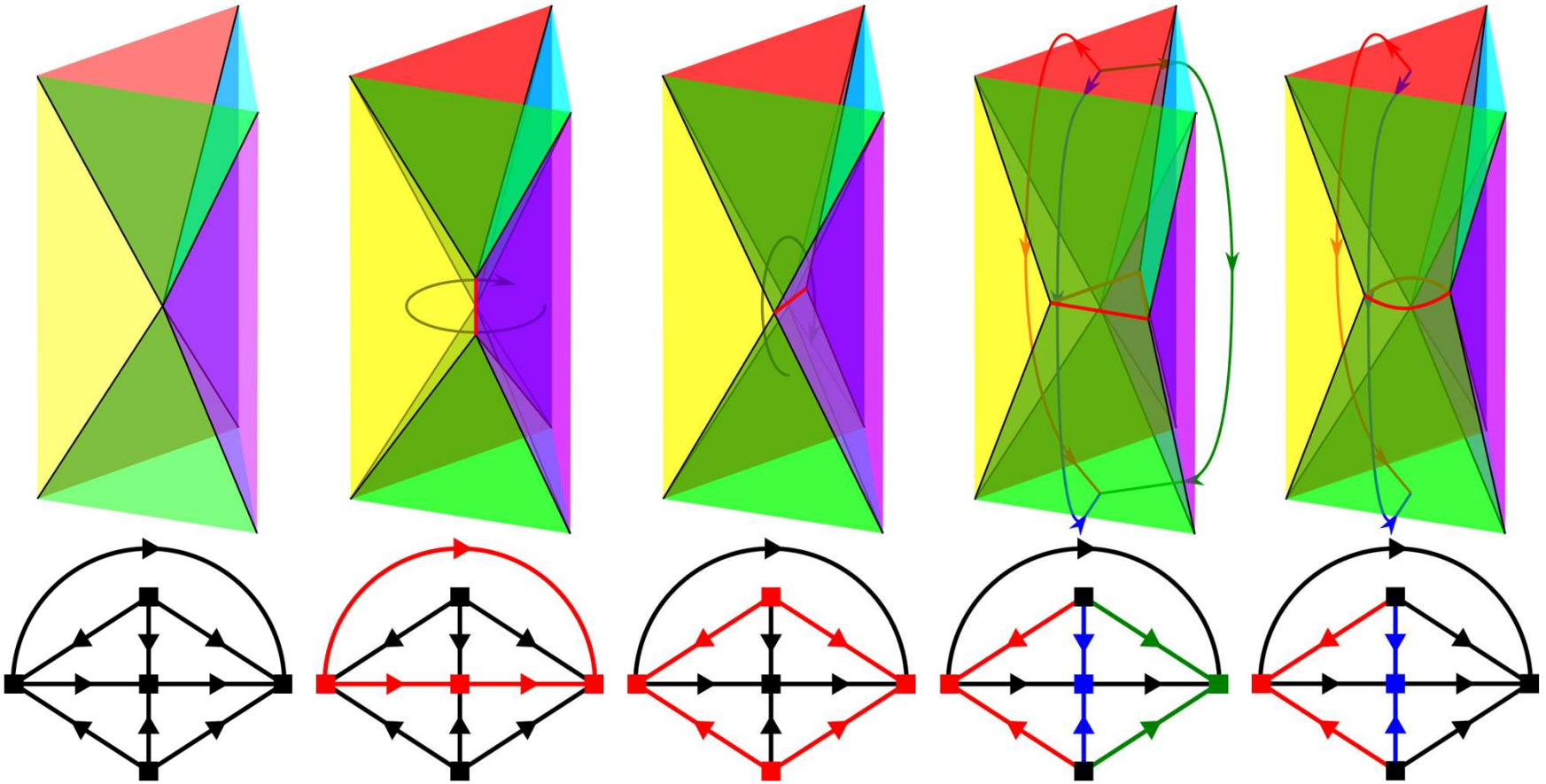
Implementation additionally requires that removal of mesh entities reduces the energy



Singularities: Creation

Initially assume that creation occurs only around a 0-cell

Relaxed valence conditions allow more types of cell creation



Singularities: Creation

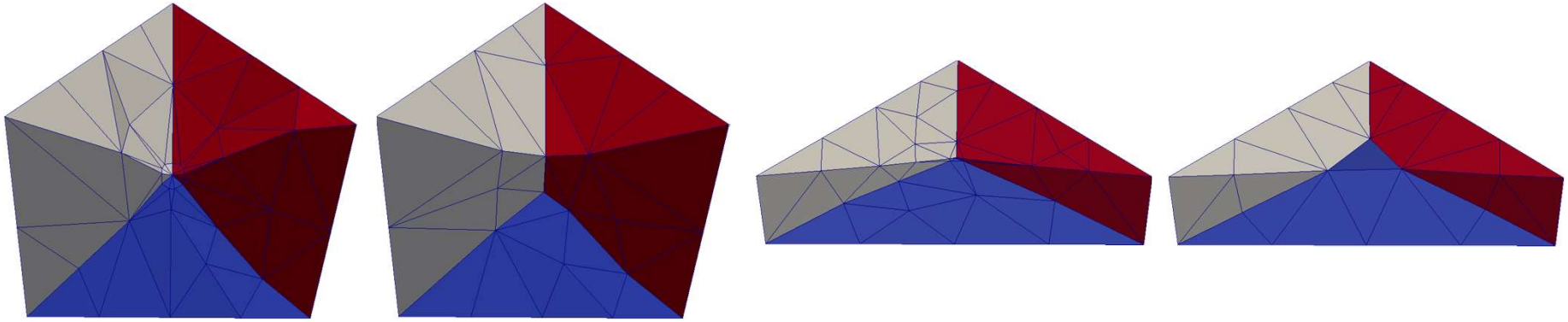
Construct adjacency graph of 2- and 3-cells

For the creation of a 1-cell

- Find a cycle that divides the graph into two nontrivial components

For the creation of a 2-cell

- Select two 3-cells that do not share a 2-cell
- Construct non-intersecting paths with the 3-cells as endpoints

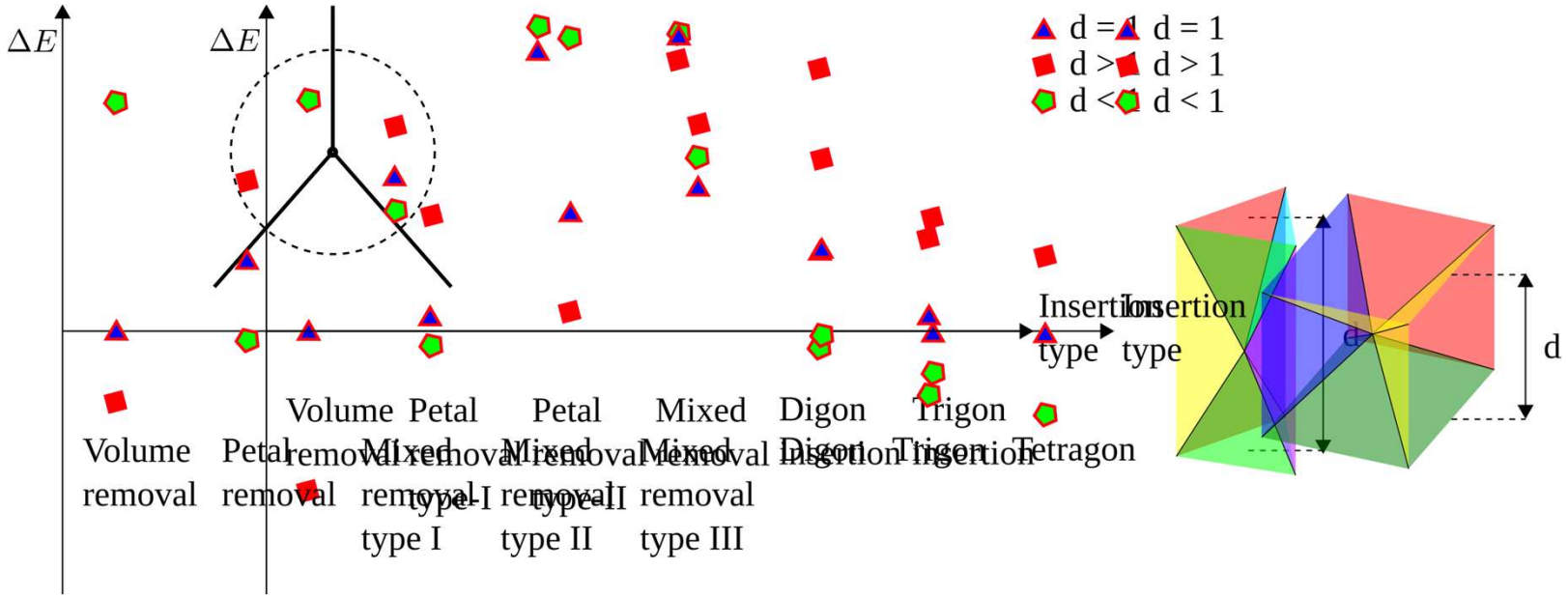


What is a reasonable criterion to select among allowed events?

Singularities: Energy Criterion

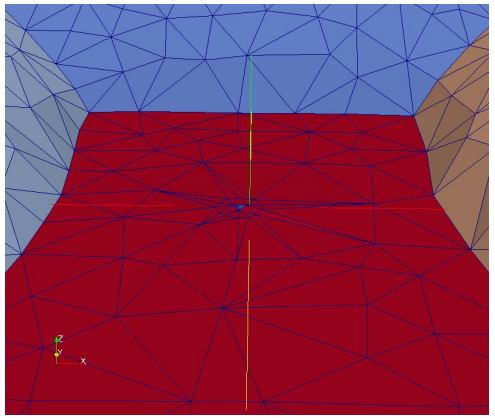
Principle: physical system selects the event that maximizes the rate of energy reduction (driving force)

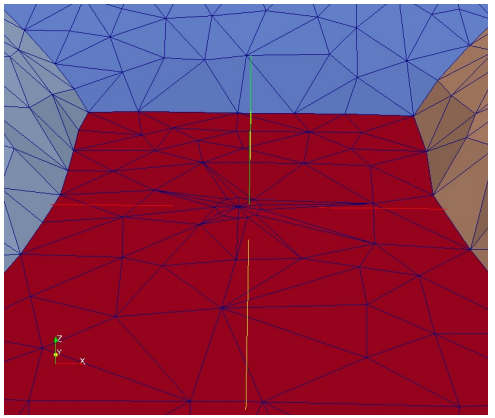
- Project initial triangulation to a sphere centered on 0-cell, relax vertices to locations where tangential forces vanish
- Force is derivative of energy change with respect to radius



Spurious Cells

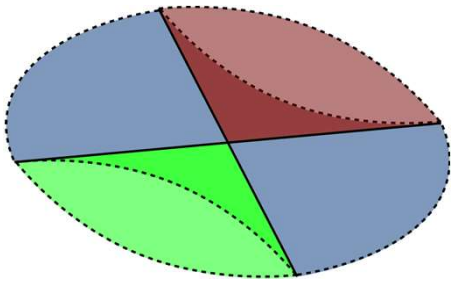
Numerical implementation integrates through singularities without substantially disturbing surrounding structure

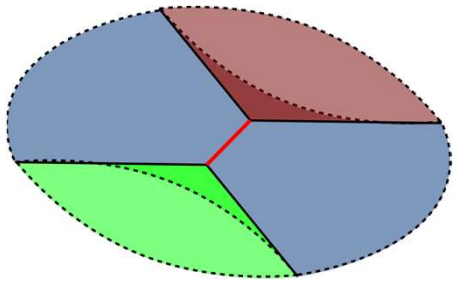


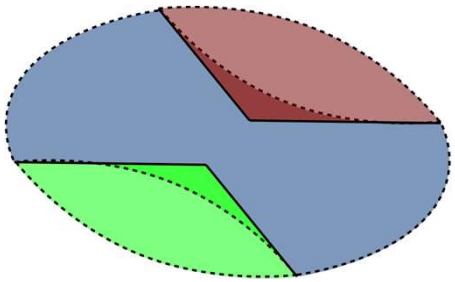


Observations

- Simulation generated a surface that is not a 2-cell
- Appearance of this surface involved a configuration that violated valence conditions, requires additional topological operation

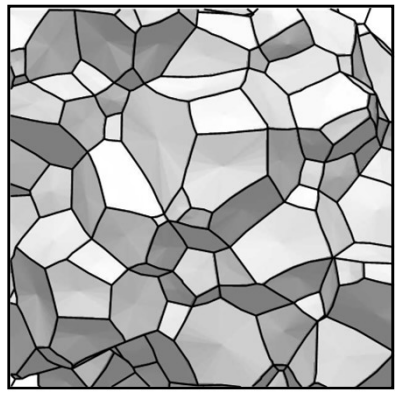


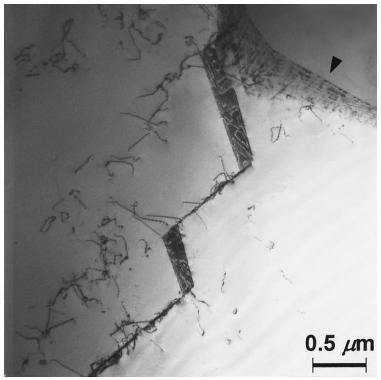




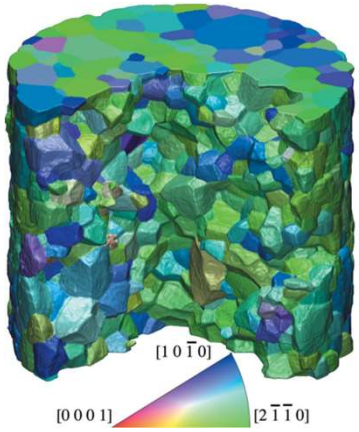
Conclusions

Ideal grain growth is the evolution of a regular pure CW-complex by gradient flow of the area functional





This is not a good approximation of the physical system where boundary properties are not uniform, surfaces are not smooth, etc.



Experimental limitations being resolved, require more accurate descriptions of these structures

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If these structures are not cell complexes, what is the correct description of the allowed topologies?

What other topological operations must be implemented to simulate evolution of the physical system?