SubStructure Dynamics

Dynamic recrystallization & Substructure Development

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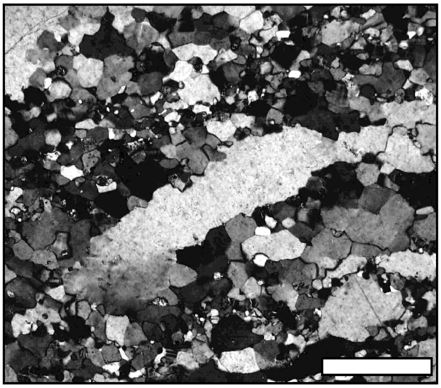
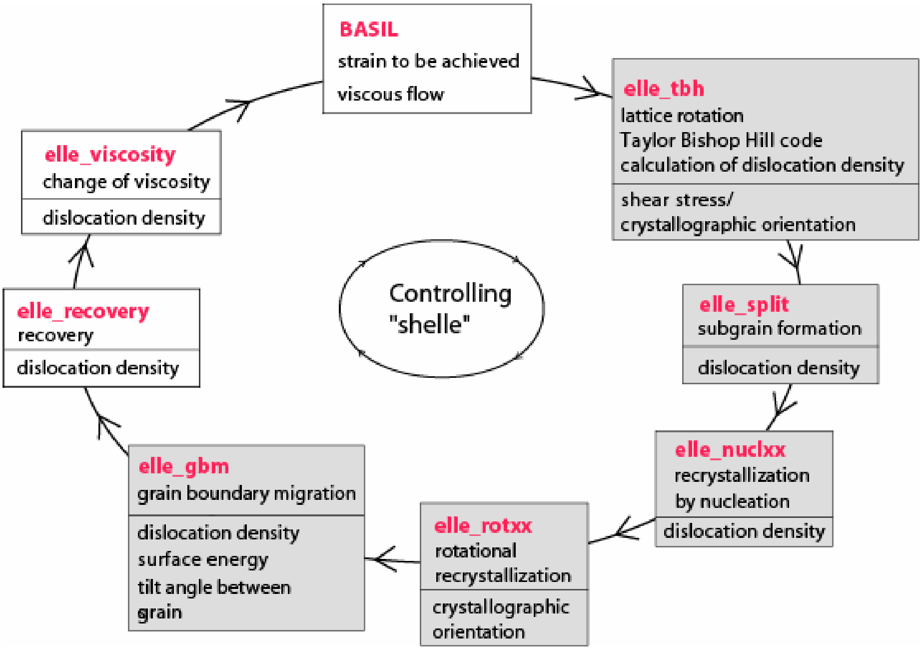
Mark Jessell, Lynn Evans, John Wheeler et al.

1) *Dynamic recrystallization: Short Review of what has been done*
2) *Dynamic recrystallization: how it should be done?*
3) *One part: Substructure development - practical*





BASIL
strain to be achieved
viscous flow

elle_tbh
lattice rotation
Taylor Bishop Hill code
calculation of dislocation density
shear stress/
crystallographic orientation

elle_split
subgrain formation
dislocation density

elle_nuclxx
recrystallization
by nucleation
dislocation density

elle_rotxx
rotational
recrystallization
crystallographic
orientation

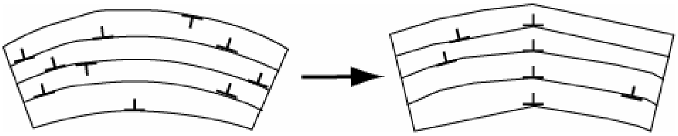
elle_gbm
grain boundary migration
dislocation density
surface energy
tilt angle between
grain

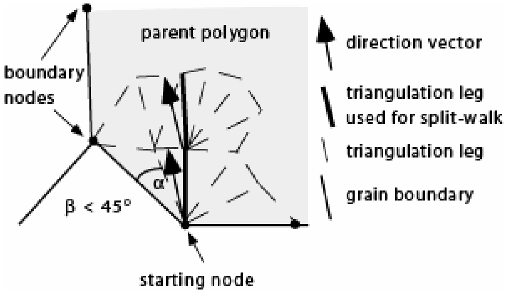
elle_recovery
recovery
dislocation density

elle_viscosity
change of viscosity
dislocation density

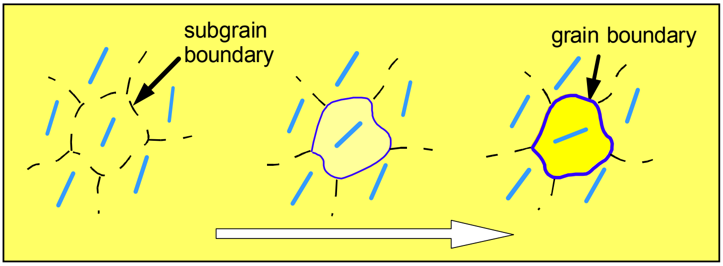
Controlling "shelle"

Formation of subgrains

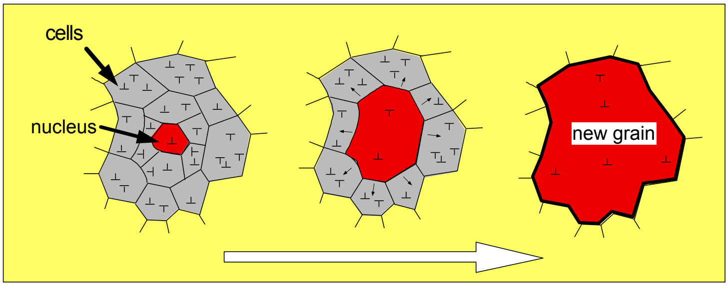




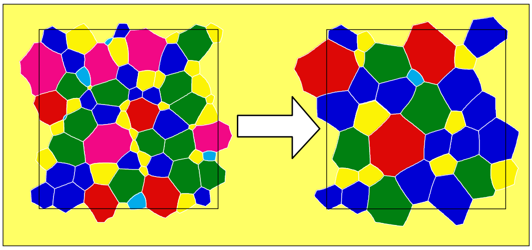
rotational recrystallization



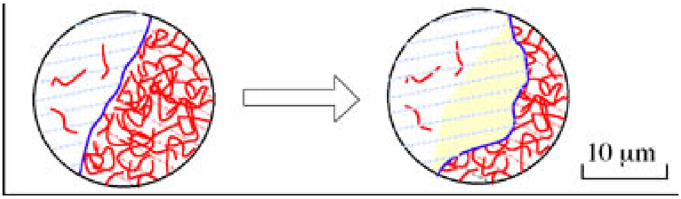
recrystallization due to nucleation



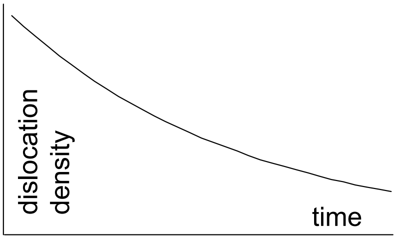
grain boundary migration due surface energy



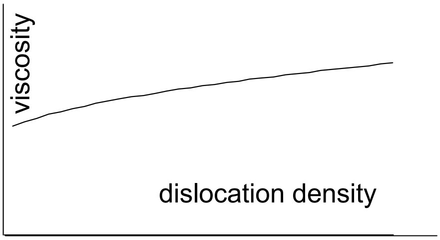
grain boundary migration due to dislocation density



recovery



viscosity



Results

Book: Example 16

Movie 1
Low GBMobility/low T

Movie 2
High GBMobility/ high T

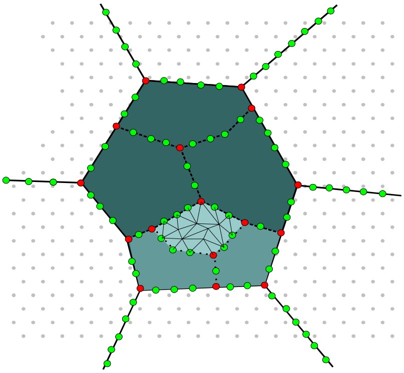
1) *Dynamic recrystallization: Short Review of whats has been done*

2) ***Dynamic recrystallization: how it should be done?***

3) *One part: Substructure development - practical*

Requirements

- Tracks & employs mechanical implications of dislocations
- Tracks & employs orientation implications of dislocations
- Multi-scale



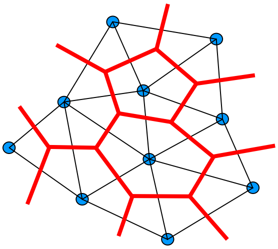
Parameters at unode level

- Strain Tensor
- Lattice Orientation
- Integrated Shear Activity of slip systems
- Voronoi cell area

Uses:

- BASIL (viscous deformation code)
- TBH/FFT – crystallographic reorientation
- Sub-grain evolution
- Recovery
- GBM
- Viscosity
- Kinking (?) e.g. ice

General Elements



Assumes voronoi cell boundaries consist of geometrically necessary dislocations and thus the energy level of each segment can be calculated from the misorientation

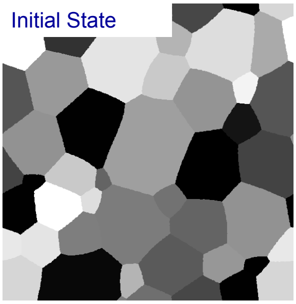
Comment: need to define scheme for Geometrically necessary dislocs -best using an reference orientation (not neighbouring unode) – otherwise problems with triple junction

Assumes: transformation of dislocations into Voronoi cell walls by recovery -> results in a change in misorientation

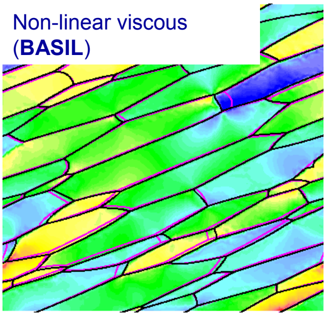
Assumes high angle GBM sweeps dislocations and loses orientation information

BASIL

- Outputs strain tensors at the unode level



Initial State



Non-linear viscous (**BASIL**)

TBH/FFT

- Uses strain tensors and orientations at the unode level, together with CRSS & crystallography information for the mineral

- Outputs:
  - New orientation at unode level
  - Adds activity of slip systems at unode level to existing values (?)

    (Comment: - “activity of slip systems” – does that mean to decide what kind of dislocations (screw, edge ..)
  - Calculate average dislocation density at unode level

    (use work term for that (as we had it) and then store what types we have (a) geometrically necessary ones, (b) free dislocations of different types– b1) type a due to activity on slip system 1, b2) type b due to activity on slip system 2 etc.)
  - Throws away strain tensor at unode level

Recovery

- Uses activity of slip systems and orientation at unode level

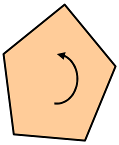
- A (temperature dependent) percentage of slip system activity is converted into voronoi cell walls. Good(?) option: geometrically necessary one!+ extra from free dislocation inventory

- We assume that the rotation associated with this percentage is used to reorient the cell (hopefully without regard to neighbours)

(difficult: look at lit. how to do this, design very simple case (where outcome is known) and check on scheme) – check with experiments

- We don't know how to calculate which dislocations to convert (most mobile, least mobile?)

(Lit? What does Raabe etc. do? Suggestions where to look)



- In addition a (temperature dependent) percentage of slip system activity is converted into thin air (here only look at free dislocation inventory)

Sub-grain Evolution

- Uses activity of slip systems at unode level, and misorientation

- Uses a Potts-type model with misorientation and activity of shear systems to modify unode level subgrain structure

Make a variety of schemes (as far as we know its not really known what to do, so best to try out several schemes and compare with experiments)

a) simple potts model, average orientation for both unodes involved

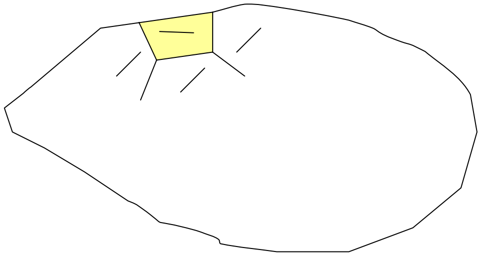
b)We assume the new orientation of the pair of Voronoi cells will be equal to the old orientation of the growing cell plus the rotation effect of the stored shear activity in the shrinking cell with area balanced?

c) We assume that the shear activity in the pair of Voronoi cells will be equal to the old shear activity in the growing cell divided ratio of growing cell area to combined area

Angle Recrystallisation

- Uses orientation of lattice at unode level

- If a voronoi cell is completely surrounded by high angle misorientations AND it is a cell adjacent to a grain boundary, it is promoted to a flynn with no change in orientation or internal energy

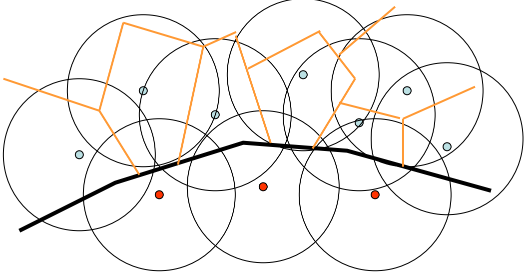


- If the same happens in the interior of a grain, it’s just too bad…

GBM

- Uses orientation of lattice at unode level, shear activity, surface energy of grain boundary
- Driving force for GBM is sum of:
  - Surface energy of High Angle Grain Boundary
  - Dislocation density or shear activity of slip systems

  (probably take whole dislocation inventory)
  - Swept length of Voronoi cell boundaries



GBM-2

- When a grain boundary passes over a unode region of interest, it removes a portion of the integrated shear activity

- When a grain boundary passes over a unode itself, the unode changes orientation, some energy should go into the growing grain, not mere redistribution of into "shrinking" grain

- If no neighbours remain, its orientation & shear activity is transferred to the parent flynn. Some dislocations should be just taken out of the system (go into boundary) and (?) change misorientation of high angle boundary accordingly.

- As grain boundary sweeps over unode regions of interest, the unode areas are updated

Viscosity

Options:

1) Attempt to standardise viscosity formulation

d=grain size

m=grain size sensitivity

n=stress exponent

B=d^{-m}.Σshear activity.$\exp^{(-Q/RT)}$

The viscosity is defined as: $\eta = \frac{1}{2} B \dot{E}^{\frac{n-1}{n}}$

and $\dot{E} = \sqrt{\sum_{ij} \dot{\varepsilon}_{ij}}$

Big problem with grain size: How do we define a grain, what reasoning do we have for it. Better to leave grain size out and use dislocation density

2) Function of disloc den.
But how to calculate? Only free Dislocs?

$\eta = (\eta\ \text{base} + \text{SQRT}(\rho))$

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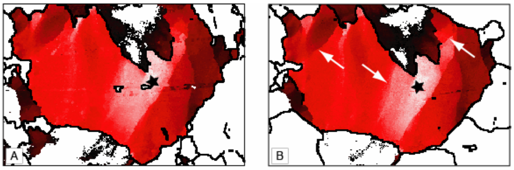
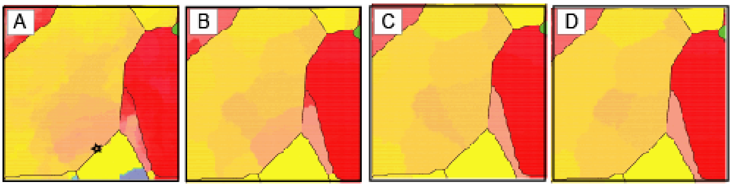
Subgrain growth/evolution



Subgrain growth has been modelled using two main modelling techniques:

1) discrete schemes mapped onto regular grids, in local change in subgrain boundaries position occur as a result of individual grid points switching their orientation, as a function of the local distribution of orientations. Here, the most common model types include Potts and Cellular Automata Models.
2) Continuous schemes mapped onto regular grids, where the local change in orientation property is a function of the properties of the whole system; here, the most common modelling type is the Phase Field Model.

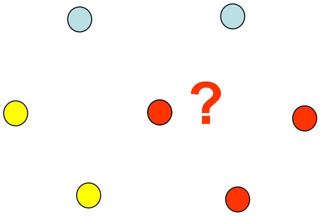
Subgrain growth



- Potts model
- probabilistisc subgrain growth

$$E = -J \sum_{i=1}^{NN}(\delta-1)$$

$$P=\begin{cases} \exp(-\Delta E(KT); & \Delta E>0 \\ 1 & \Delta E<0 \end{cases}$$



(Experiment 6)

1) start up the *Experiment Launcher* and select **Experiment 6** from the **Experiments menu**.

There are two possible sub-experiments: isotropic and anisotropic:
a isotropic,
b anisotropic

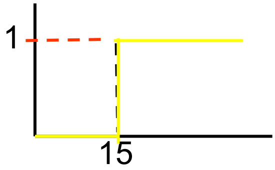
2) Load file
Note: ***Interface:*** These files will each load their appropriate preferences file automatically.

3) **Run** from the **Run menu** of the *Elle* window to watch the system evolve. You can display any of the three EULER orientations of the unodes.

Note on Input file: Input file with a highly strained grain of NaCl derived from EBSD measurements, which exhibit high grain lattice distortions.

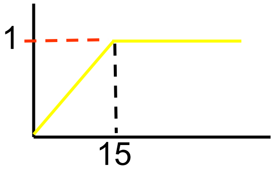
Note on example: We let the substructure of the grains evolve while the grain boundaries remain stable.

Example Elle Run:
Subgrain growth – isotropic



The driving force is the reduction of energy where the energy below the critical misorientation (between adjacent subgrains) of 15° is isotropic.

Example Elle Run: Subgrain growth – anisotropic
In this simulationwe take into account the anisotropy of surface energy and mobility of subgrain boundaries. Now, the calculation of the energy state differs as now the energy between data points below the critical misorientation of 10° is taken to be anisotropic.
Result: More subgrains remain at the end of the simulation, as the anisotropy has the effect of slowing down the microstructure evolution.



What else: changing parameters The user can vary 2 parameters:

1. *userdata[0] = max_angle*
gives the angle at which the maximum energy
is reached (e.g. 15° for salt)

2. userdata[1] = slope.

Slope=1 signifies that all energies are the same, while another value allows differences in energy according to misorientation.

Slope=2 signifies that the energy changes linearly, as afraction of the max_angle. This means that at a misorientation of 10 and max_angle is 15, the energy is 10/15=0.66667. The energy reaches unity when misorient is equal or larger than max-angle.

Slope=3 signifies a Shockley equation change between 0 and max_angle misorientation, with:

$$\text{energy} = \left(\frac{\text{orient}}{\text{max\_angle}}\right)\left(1-\ln\left(\frac{\text{orient}}{\text{max\_angle}}\right)\right)$$

If the value for slope is not 1, 2, 3 it is set by default to 1.

For example:
elle_sub_gg -u 15 3 means that the max_angle is 15 (here the energy is 1), and the Shockley equation is used to calculate the energy.