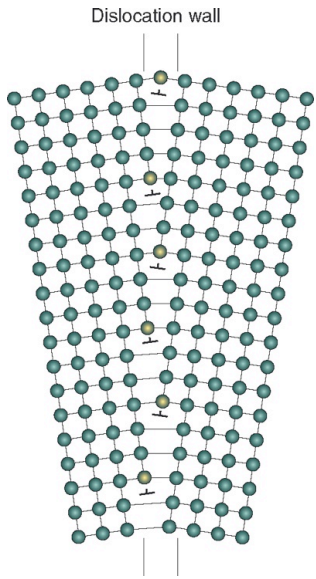


Working towards the 5 parameter model (misorientation & plane) of grain boundaries: overview & preliminary results on Ice



MTEX Users workshop
TU Chemnitz, 9th February 2017

David Mainprice

(david.mainprice@gm.univ-montp2.fr)



Outline of this presentation

- Some conclusions about GBCD
- 5 parameter grain boundary description in **M**TEX ?
- CMU stereology analysis FORTRAN programs
- Exporting boundary traces from **M**TEX
- Towards phase boundaries ?
- Coincident Site Lattice (CSL) in **I**ce ?
- Evolution of **I**ce with annealing

Low & high angle boundaries - Motivation

- Boundaries are typically characterized as **tilt** and **twist** type with ***misorientation vector parallel or normal to*** the boundary plane.
- **Tilt boundaries** have reported to migrate one or two orders faster the **twist** in metals.
- Can the grain boundary migration in Ice be also characterized by **fast tilt boundary migration**?
- What are limits of boundary characterization in 2D EBSD?
- What can they tell us **locally** (e.g. boundary profile) or **globally** (e.g. EBSD map scale) about deformation and migration processes ?
- It has been reported despite the complexity of polycrystals that boundaries have same crystallographic (habit = low index hkl) as single crystals grown from a magma or other liquid.

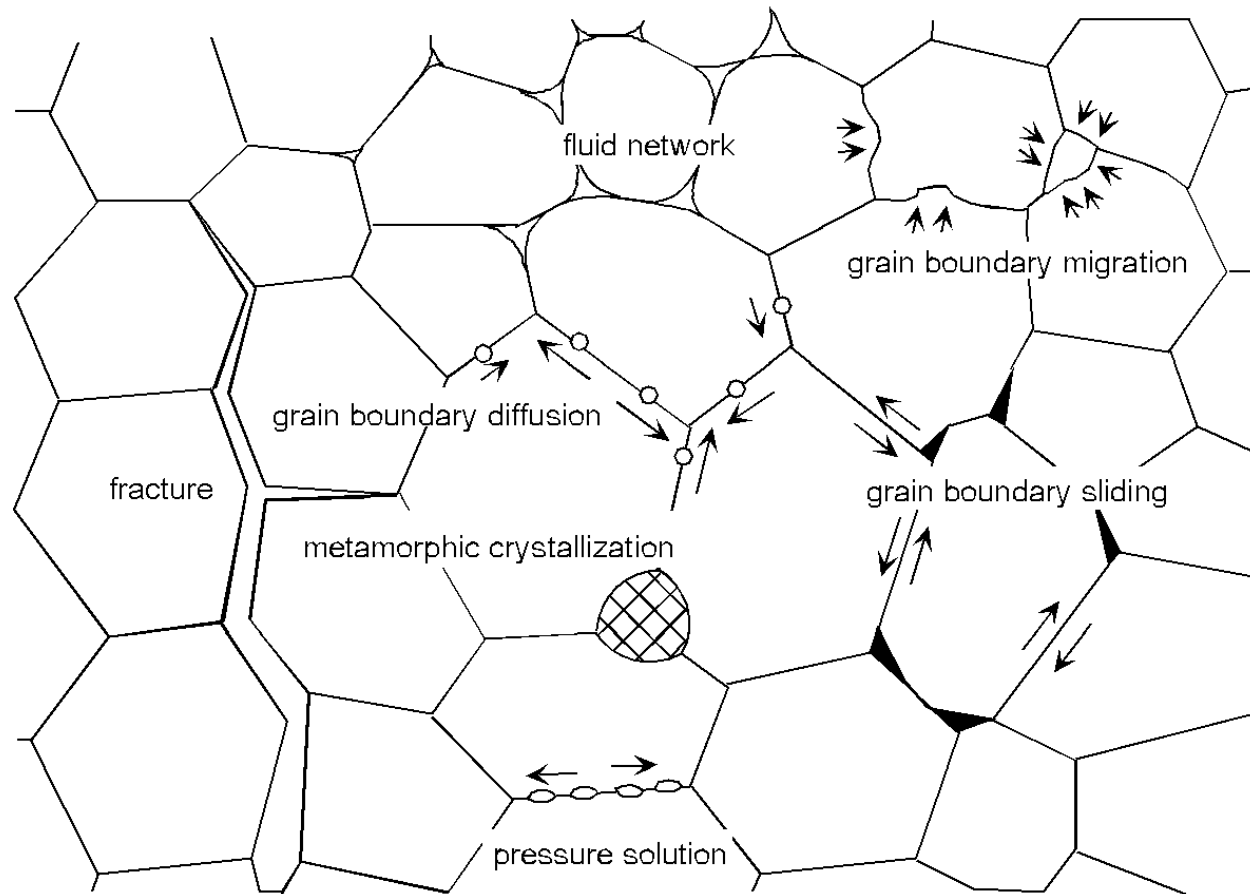
Anisotropy of boundaries properties

- The influence of the **boundary plane orientation** is greater than **misorientation angle between grains**.
- The Read-Shockley (dislocation) model (1950) for low misorientations θ is **reliable for relative energies** $\gamma_{gb} = E_0\theta[A - \ln\theta]$
- Coincidence Site Lattice (CSL) models are **poor predictors of boundary energies**.
- There is an **inverse correlation** of between the grain **boundary energy** and grain **boundary frequency**. (i.e. low energy boundaries are the most frequent boundaries).
- **Isostructural crystals** (e.g. MgO, NiO & NaCl) have **similar grain boundary energy anisotropy**.

Based on G.S. Rohrer (2011) J. Mater. Sci.

Importance of **grain** and **interphase** boundaries

Interface as a place for geodynamics



Schematic illustration of interfacial processes in rocks

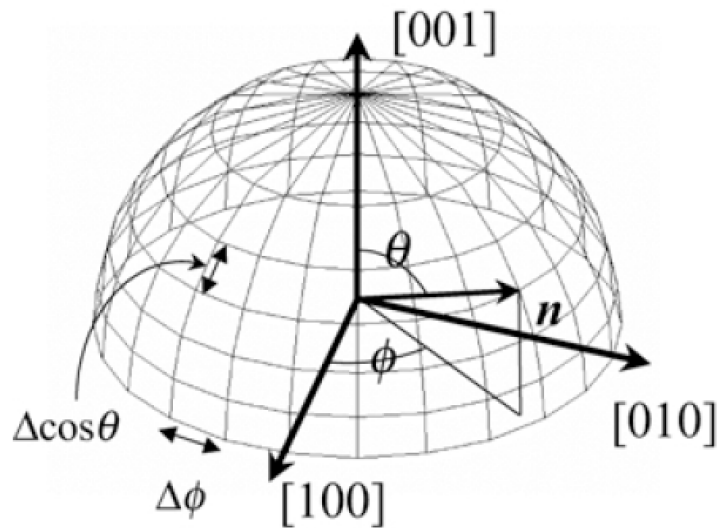
Credit : Takehiko HIRAGA

Some conclusions about GBCD

grain boundary character distribution (GBCD)

PF-specimen coordinates

Boundary plane orientation (θ, ϕ)

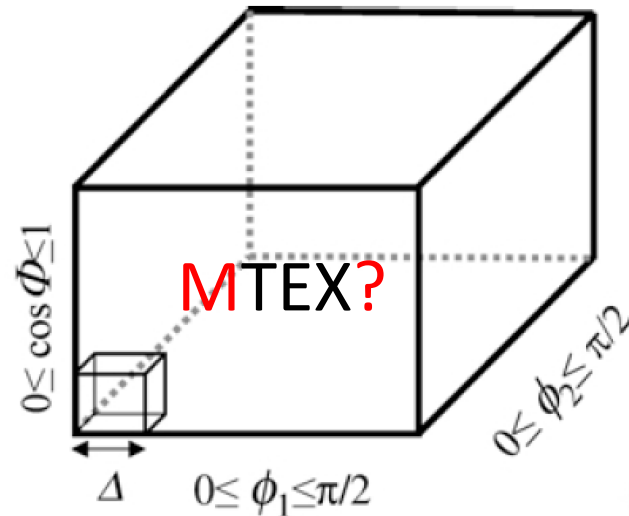


(a)

MTEX -> Kernel density estimation

MDF-crystal coordinates

Boundary misorientation (ϕ_1, Φ, ϕ_2)



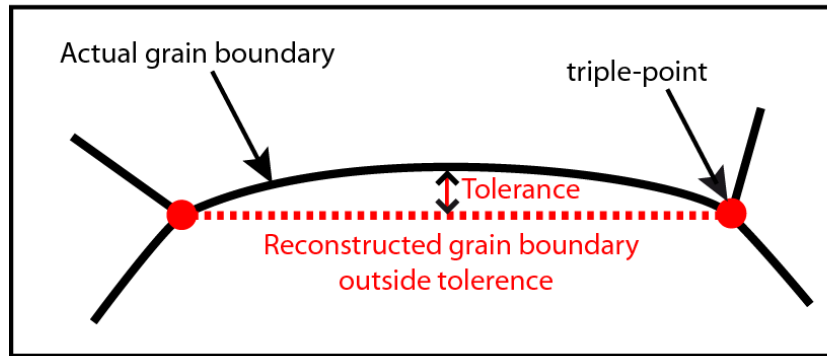
(b)

Conclusions about GBCD

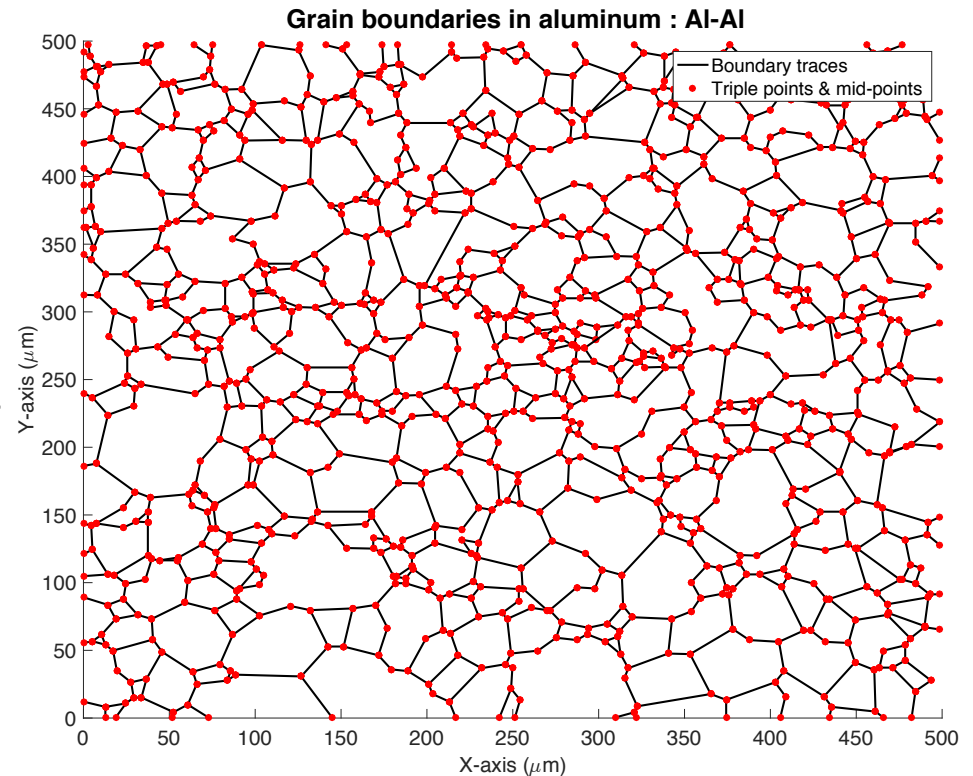
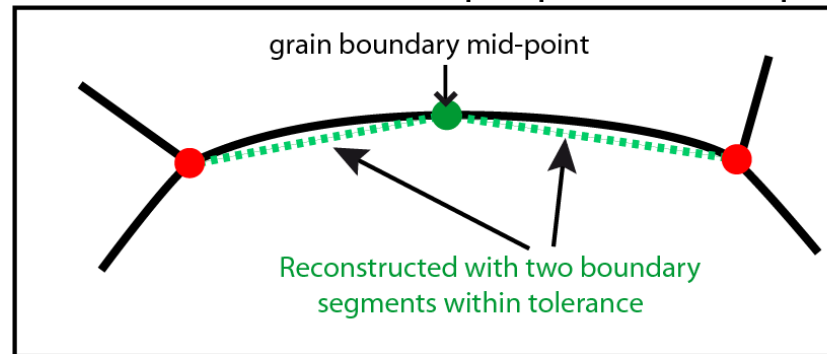
- The resolution of the EBSD mapping should be **at least 10 points per grain diameter**.
- When comparing two GBCDs, **differences of less than 10% should be considered insignificant**.
- **At least 5×10^4 grain boundary traces should be recorded** to determine the GBCD. This estimate assumes that they are relatively evenly distributed (*i.e.* weak texture).
- Note that if too many of the segments arise from a single type of misorientation, then there will be grain boundary configurations that are not sampled.
- For example, if one third of all the boundaries are coherent twins, then 1.7×10^4 traces will fall in one cell and 3.3×10^4 will be distributed among the remaining 6560 cells.
- While the grain boundary plane distribution will be well determined for the twin misorientation, it will be underdetermined for all of the other misorientation types.

TSL grain boundary trace construction

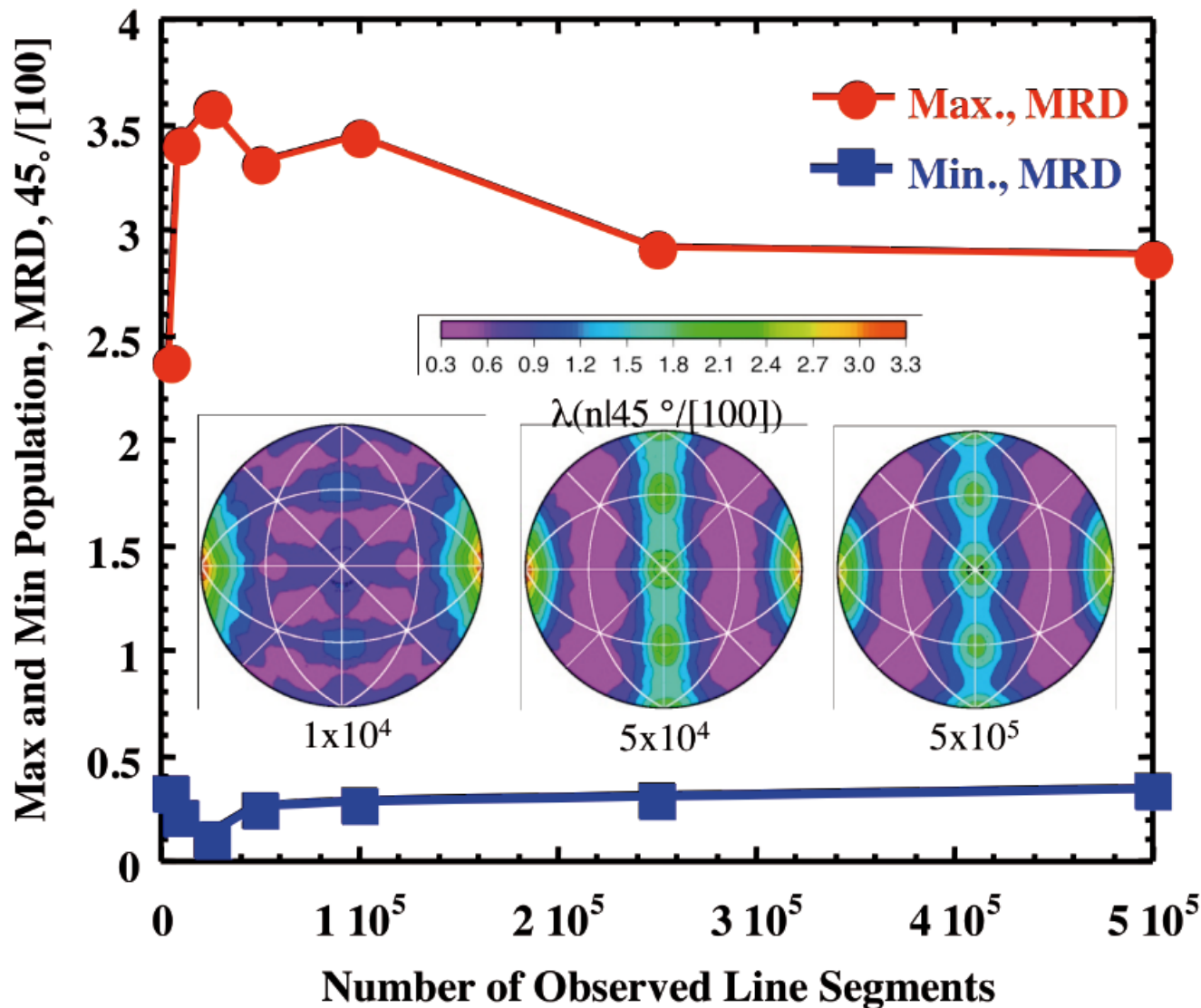
Initial construction : triple-point to triple-point



Revised construction : triple-point to mid-point



1. To minimise errors a small EBSD map step size is recommended
2. The segmentation process must aim to reproduce the true boundary trace
3. The tolerance should be 2x the step size
4. Expected error for boundary of length 6x greater than the step size is $\pm 2^\circ$ (Wright and Larsen, 2002)



The distribution computed from 5×10^4 traces is not significantly different from that determined from 5×10^5 traces. (Saylor et al.2004)

5 parameter grain boundary description in MTEX ?

- You can use this description to model individual boundaries
- Study the distribution of random boundaries for a given crystal symmetry
- Alternatively you can use GBtoolbox, Windows, Mac OS and Linux
- You can use the Gbtoolbox to check your own calculations

Application in MTEX

1) Transform symmetry operations to a specific matrix form for proper or rotational point groups

`CS_high_cubic_432 = CS_high_cubic_m_3m.properGroup`

Symmetry operations in matrix form using proper symmetry elements

$$C_n = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & R_{11} & R_{12} & R_{13} \\ 0 & R_{21} & R_{22} & R_{23} \\ 0 & R_{31} & R_{32} & R_{33} \end{pmatrix} \quad C_1 \ 0^\circ/[100] = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad C_2 \ 180^\circ/[100] = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

Application in MTEX

2) Create the B matrix of your grain boundary

Grain boundary B matrix

$$B = \left(\begin{array}{c|ccc} 0 & n2(1) & n2(2) & n2(3) \\ \hline n1(1) & M(1,1) & M(1,2) & M(1,3) \\ n1(2) & M(2,1) & M(2,2) & M(2,3) \\ n1(3) & M(3,1) & M(3,2) & M(3,3) \end{array} \right) = \left(\begin{array}{cc} 0 & \mathbf{n}_2^T \\ \mathbf{n}_2 & \mathbf{M} \end{array} \right)$$

$M = gB$ Misorientation matrix defined as $O1 \text{ transpose}(O2)$ $O2$ wrt $O1$

$n1 = gB$ Plane normal vector wrt $O1$

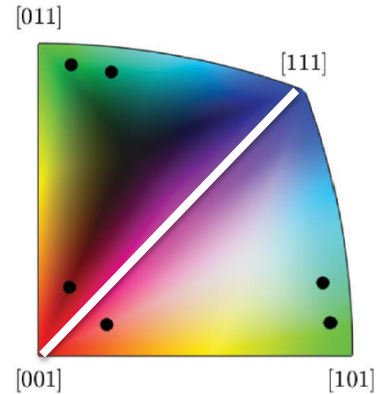
$n2 = gB$ Plane normal vector wrt $O2$

Application in MTEX

2) Create the B matrix of your grain boundary

Grain boundary B matrix

$$B = \begin{pmatrix} 0 & n2(1) & n2(2) & n2(3) \\ n1(1) & M(1,1) & M(1,2) & M(1,3) \\ n1(2) & M(2,1) & M(2,2) & M(2,3) \\ n1(3) & M(3,1) & M(3,2) & M(3,3) \end{pmatrix} = \begin{pmatrix} 0 & \mathbf{n}_2^T \\ \mathbf{n}_1 & \mathbf{M} \end{pmatrix}$$



$\mathbf{M} = \mathbf{g}_B$ Misorientation matrix defined as $O_1 \text{ transpose}(O_2)$ O_2 wrt O_1

$\mathbf{n}_1 = \mathbf{g}_B$ Plane normal vector wrt O_1

$\mathbf{n}_2 = \mathbf{g}_B$ Plane normal vector wrt O_2

**Need 2 triangles
to represent boundary
if not exchange symmetry**

3) Create B^T and B^-

Three types of B , B^T and B^- due the presence of exchange symmetry and center of symmetry

$$B = \begin{bmatrix} 0 & \mathbf{n}_2^T \\ \mathbf{n}_1 & \mathbf{M} \end{bmatrix} \quad \text{exchange symmetry } B^T = \begin{bmatrix} 0 & \mathbf{n}_1^T \\ \mathbf{n}_2^T & \mathbf{M} \end{bmatrix} \quad \text{center of symmetry } B^- = \begin{bmatrix} 0 & -\mathbf{n}_2^T \\ -\mathbf{n}_1 & \mathbf{M} \end{bmatrix}$$

Application in MTEX

Generate all symmetrically equivalent forms of **B**

For loop over symmetry operations

$$B_{\text{SYMM}} = C_1 B C_2^T \quad \text{apply crystal proper elements of groups with } C_1 \text{ and } C_2$$

$$B_{\text{SYMM}}^- = C_1 B^- C_2^T \quad \text{use } B^- \text{ due to presence of inversion symmetry}$$

Remove for phase boundaries: $C_1 \neq C_2$

$$B_{\text{SYMM}}^T = C_1 B^T C_2^T \quad \text{use } B^T \text{ due to exchange symmetry of O1 and O2}$$

$$B_{\text{SYMM}}^{T^-} = C_1 B^{-T} C_2^T \quad \text{use } B^{-T} \text{ due to exchange symmetry of O1 and O2}$$

Application in MTEX

Generate all symmetrically equivalent forms of **B**

For loop over symmetry operations

$$B_{\text{SYMM}} = C_1 B C_2^T \quad \text{No exchange symmetry or } B^- \quad 1 \times 24 \times 24 = 576$$

$$B_{\text{SYMM}}^- = C_1 B^- C_2^T \quad \text{With } B^- \quad 2 \times 24 \times 24 = 1152$$

$$B_{\text{SYMM}}^T = C_1 B^T C_2^T \quad \text{With } B^T \quad 3 \times 24 \times 24 = 1728$$

$$B_{\text{SYMM}}^{-T} = C_1 B^{-T} C_2^T \quad \text{With } B^{-T} \quad 4 \times 24 \times 24 = 2304$$

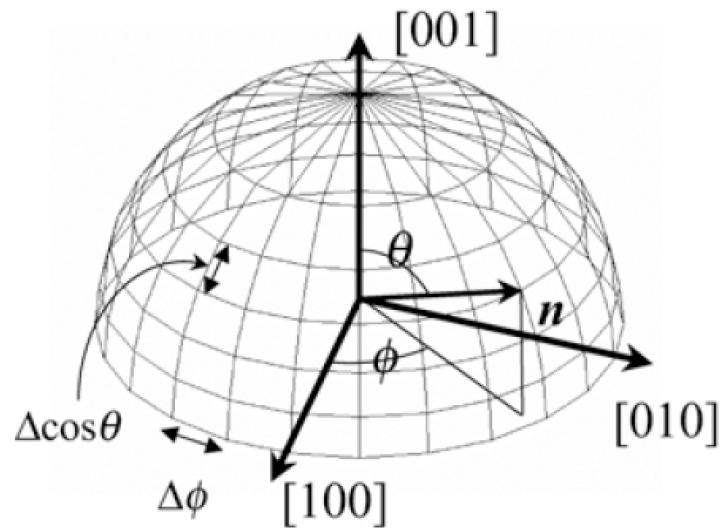
CMU stereology analysis FORTRAN programs

Greg Rohrer's CMU stereology analysis

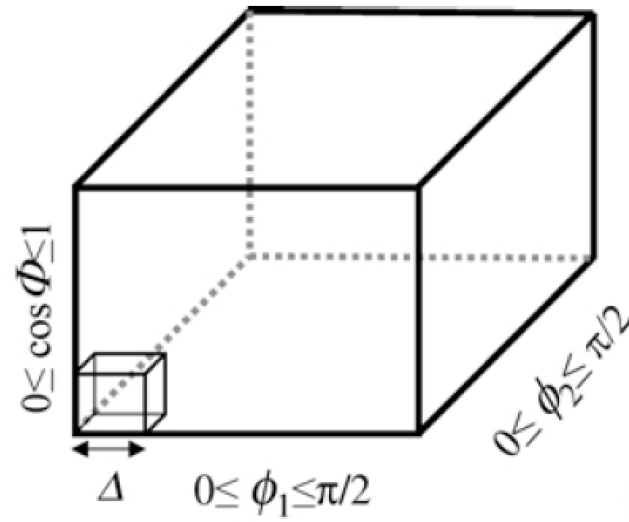
FORTRAN programs

- http://mimp.materials.cmu.edu/~gr20/Grain_Boundary_Data_Archive/
- Uses probability of boundary inclination and GB traces to estimate 5-parameter grain boundary characterization from large data sets from 2D EBSD.
- Recently modified additional orthorhombic crystal symmetry.
- A series of programs for the calculations, but graphics produced using free and open source GMT or other alternatives
- Not really user friendly programs...

- The most important part of the package is `calc_gbcd_stereo_fd` which generates the grain boundary character distribution (gbcd)



(a)

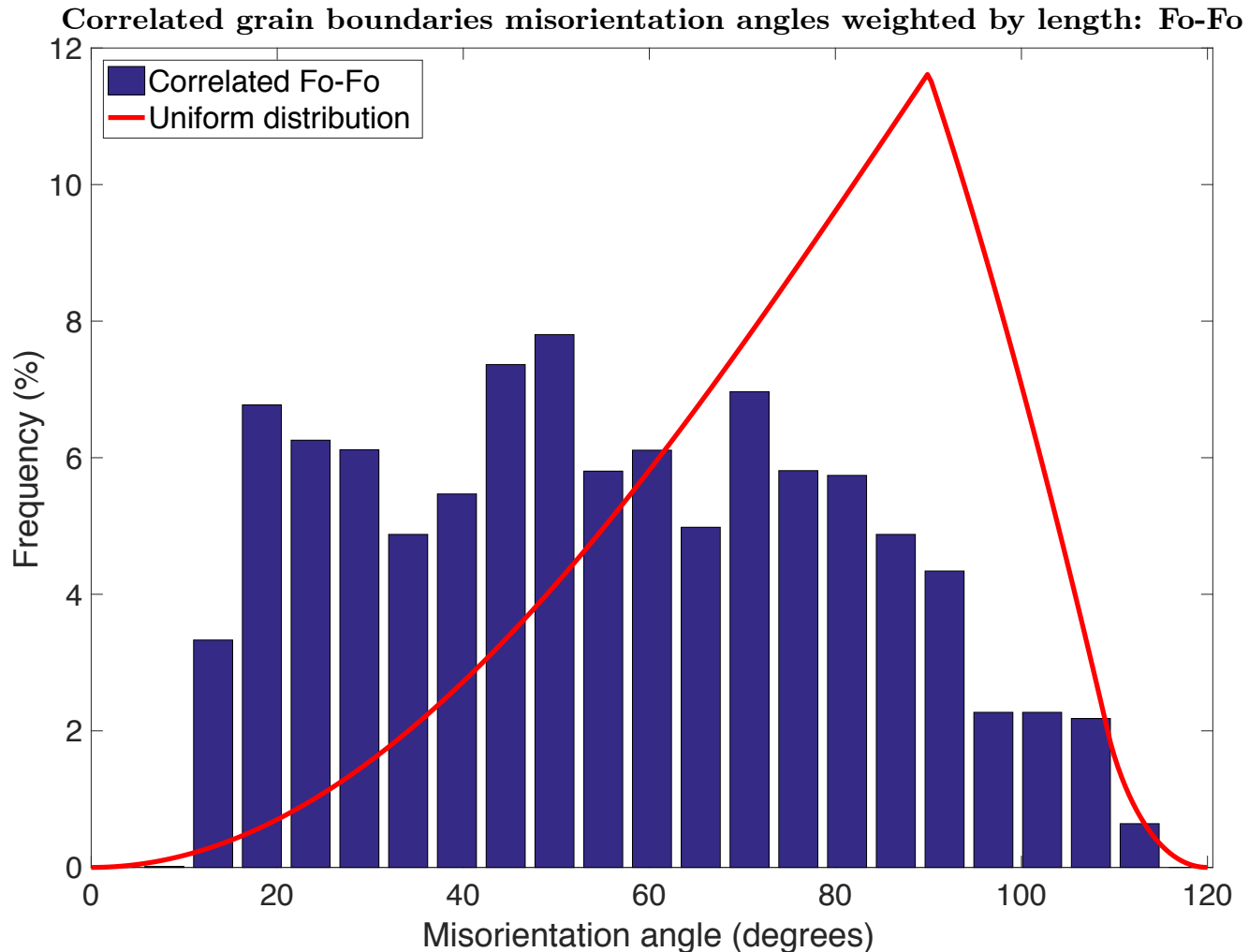


(b)

Disor functionality can be replaced by MTEX calculations & plots

Disor : calculates a one-dimensional distribution of grain boundaries as a function of disorientation (minimum misorientation) angle.

MTEX dataset forsterite coarse grained (~813 μm) with EBSD stepsize = 50 μm
Sample clearly has a texture ! **Poor correlation with uniform distribution**

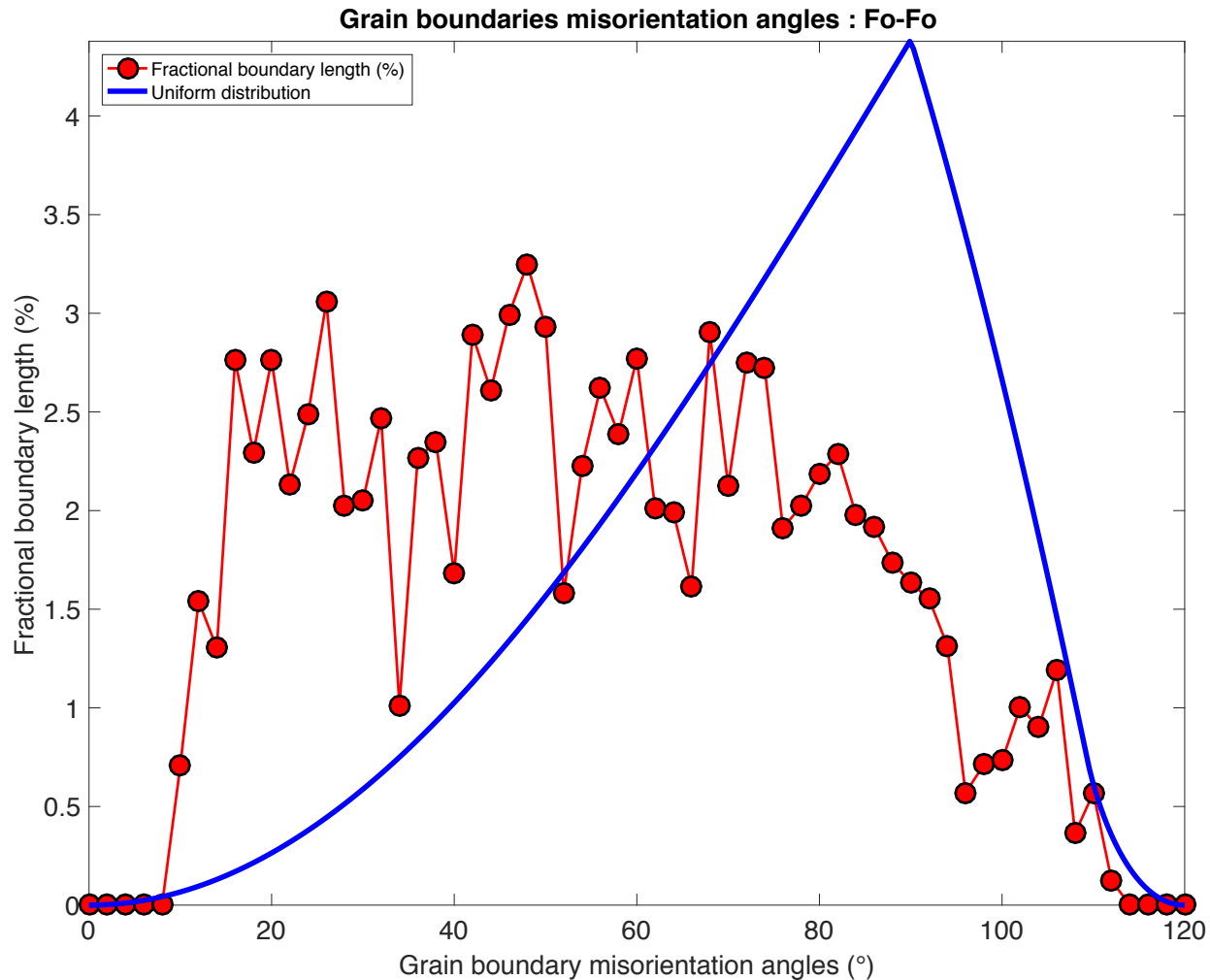


Disor functionality can be replaced by MTEX calculations & plots

Disor : calculates a one-dimensional distribution of grain boundaries as a function of disorientation (minimum misorientation) angle.

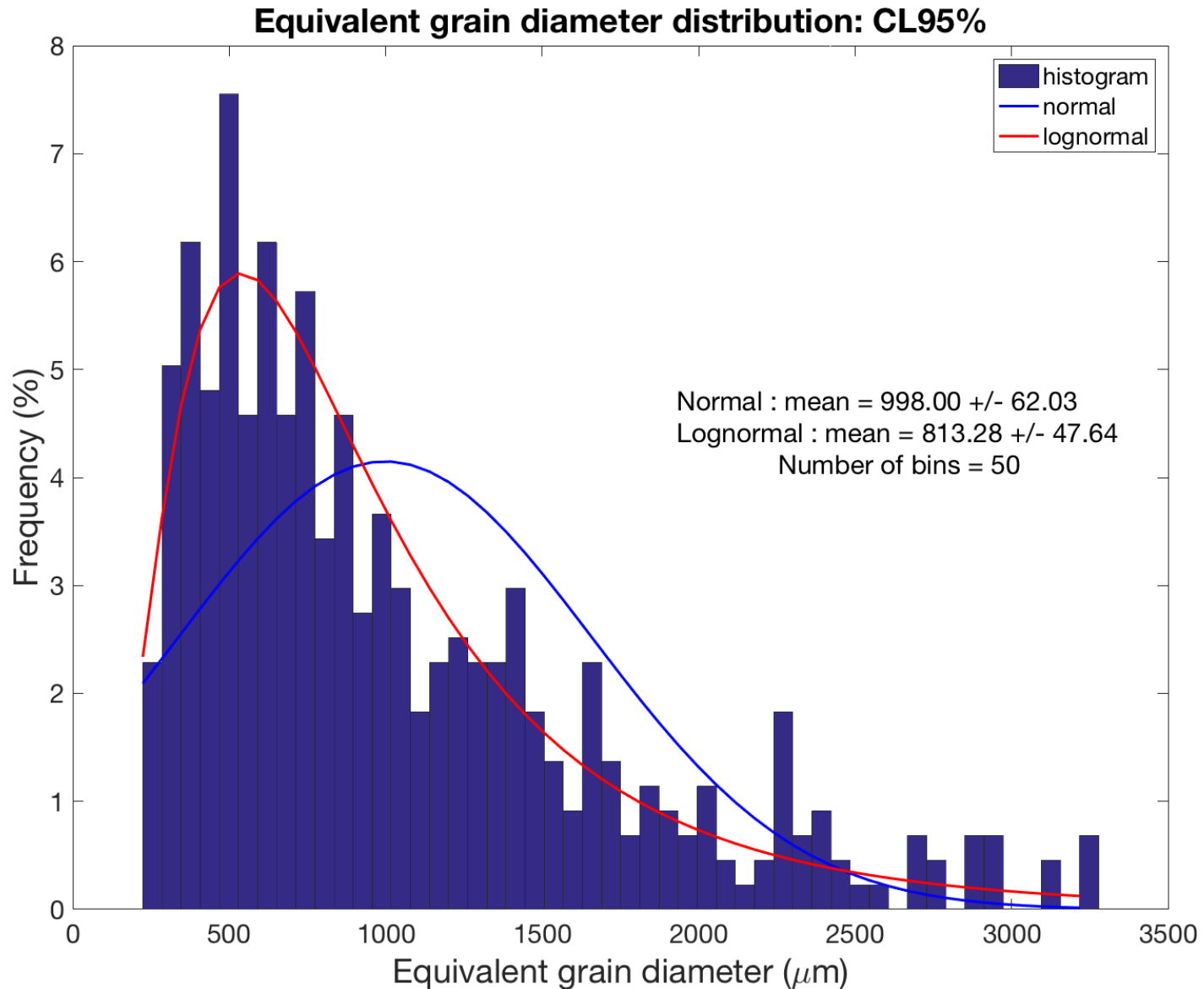
MTEX dataset forsterite coarse grained with EBSD stepsize = 50 μ m

Sample clearly has a texture ! **Poor correlation with uniform distribution**



MTEX plot without additional toolboxes

Natural forsterite large grained ($813.28 \pm 47.64 \mu\text{m}$) with EBSD step size = $50 \mu\text{m}$

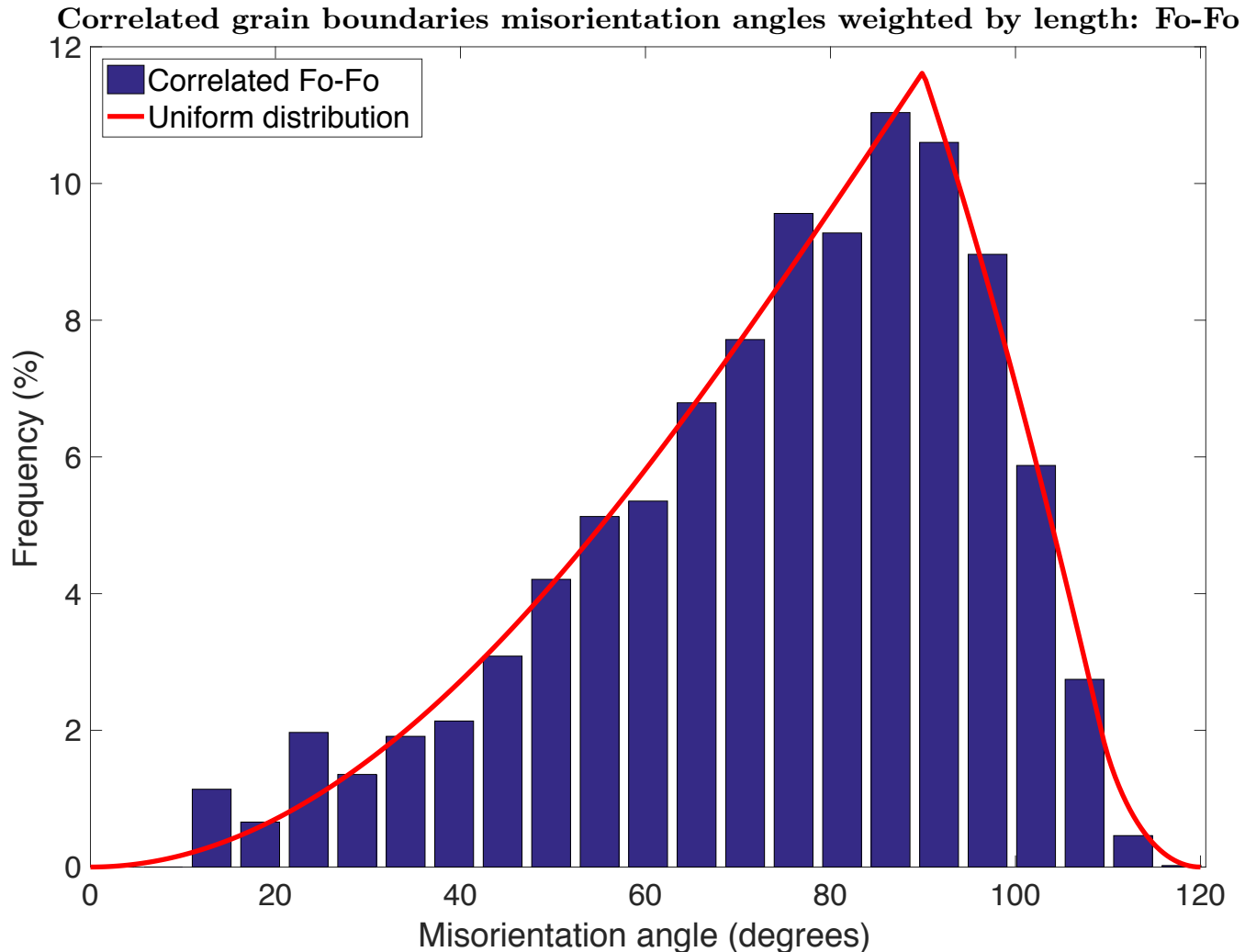


Disor functionality can be replaced by MTEX calculations & plots

Disor : calculates a one-dimensional distribution of grain boundaries as a function of disorientation (minimum misorientation) angle.

Sol-gel forsterite fine grained ($\sim 2.6\mu\text{m}$) with EBSD step size = $0.4\mu\text{m}$

Sample clearly has no texture ! **Very good correlation with uniform distribution**

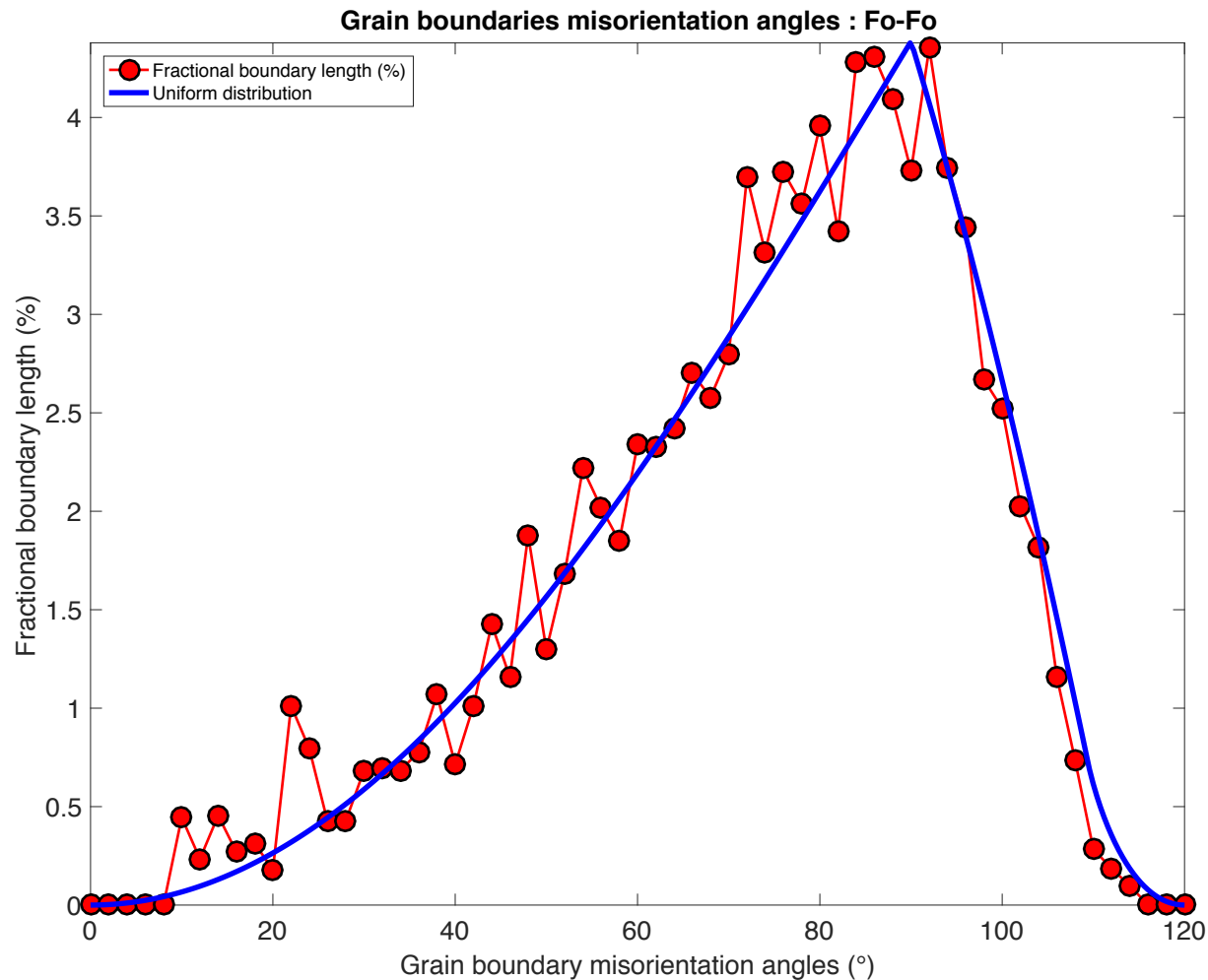


Disor functionality can be replaced by MTEX calculations & plots

Disor : calculates a one-dimensional distribution of grain boundaries as a function of disorientation (minimum misorientation) angle.

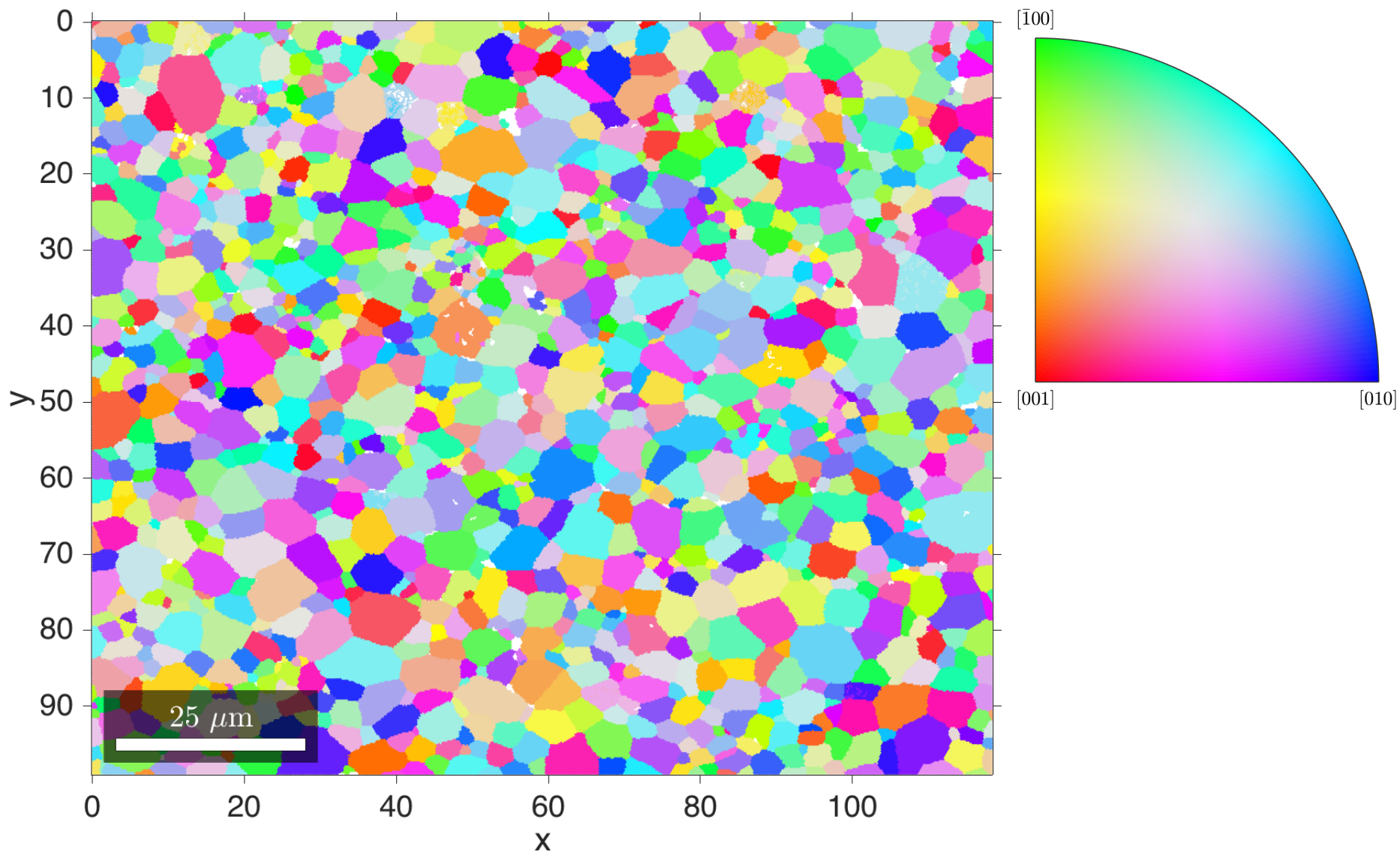
Sol-gel forsterite fine grained ($\sim 2.6\mu\text{m}$) with EBSD step size = $0.4\mu\text{m}$

Sample clearly has no texture ! **Very good correlation with uniform distribution**



Sol-gel forsterite fine grained ($2.58\pm 0.07\mu\text{m}$) with EBSD
step size = $0.4\mu\text{m}$

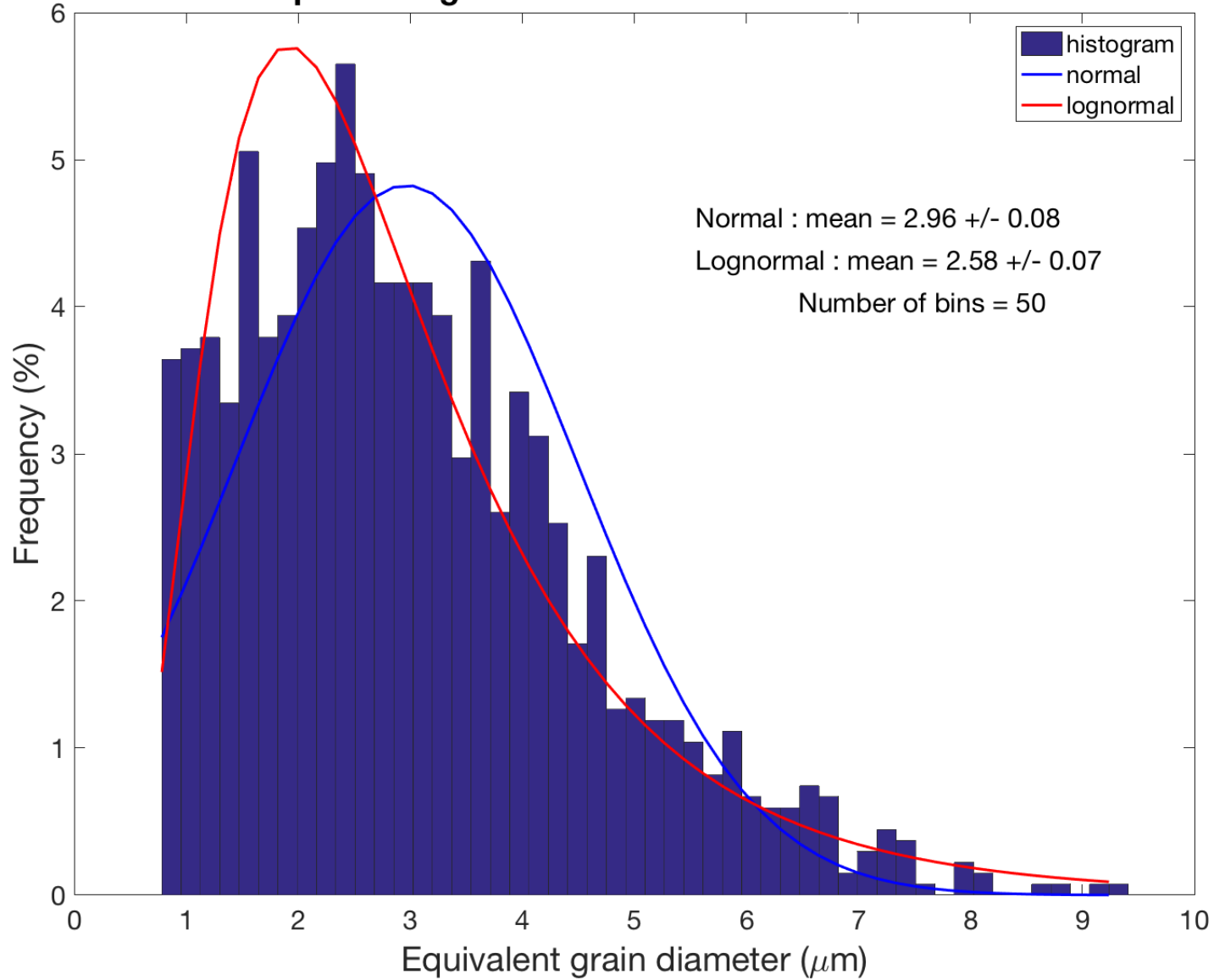
IPF-Z



MTEX plot without additional toolboxes

Sol-gel forsterite fine grained ($2.58 \pm 0.07 \mu\text{m}$) with EBSD step size = $0.4 \mu\text{m}$

Equivalent grain diameter distribution: CL95%



Stereology (3.85) versus 3D EBSD (2.21)

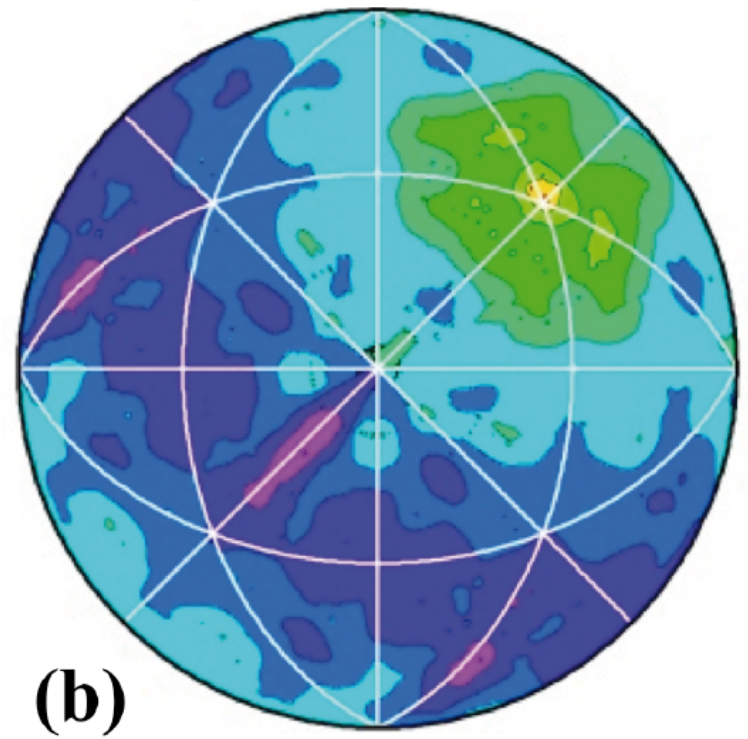
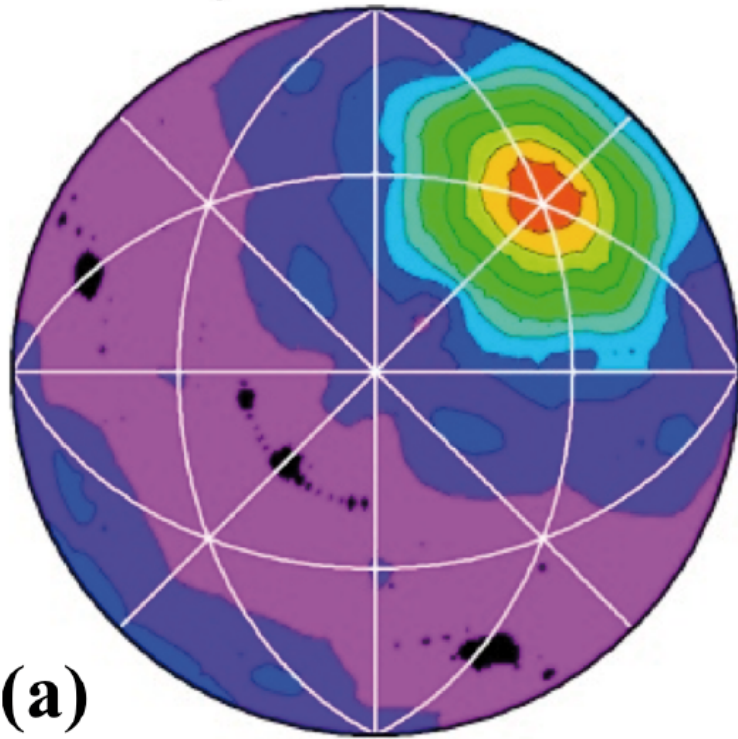
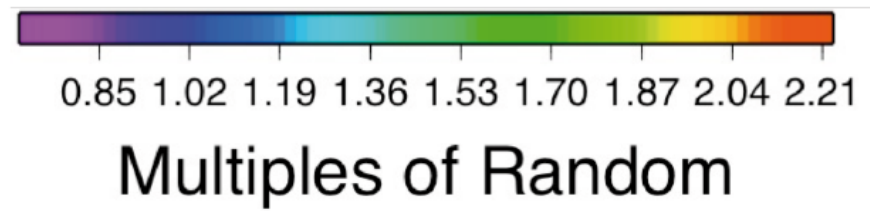
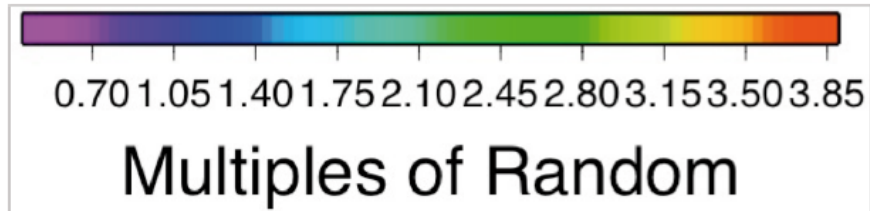
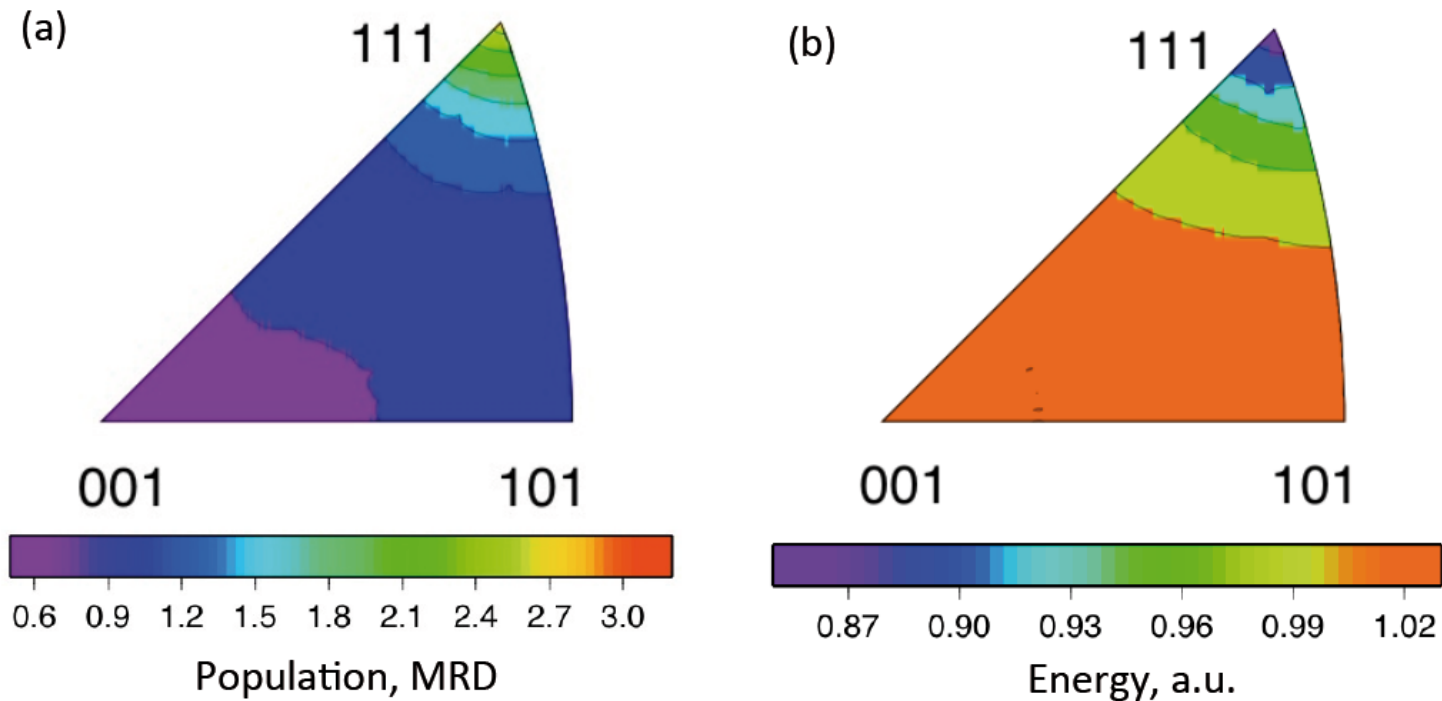


Figure 10. The distribution of grain boundary planes for the $\Sigma 3$ ($60^\circ/[111]$) grain boundary in Y_2O_3 computed (a) using the conventional stereology and (b) from 3D data.

Distribution of GB planes and energies in the crystal reference frame



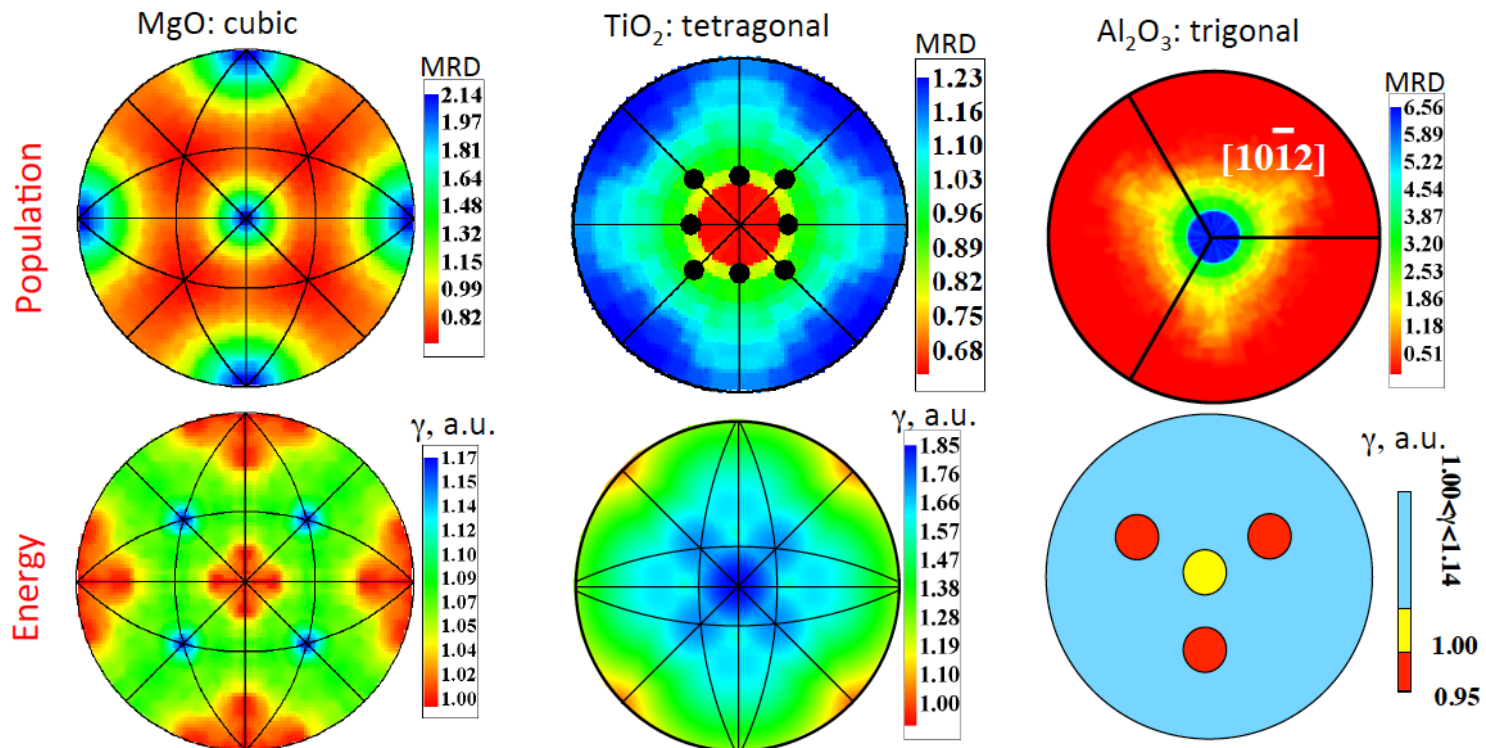
(111) planes have the highest population and the lowest relative energy (computed from dihedral angles)

Li et al., *Acta Mater.* **57** (2009) 4304

Effect of crystal symmetry on gBs

Energy-Population (Inverse) Relationship

Non-random grain boundary plane distributions, $\lambda(n)$, independent of misorientation (Δg), were found for all materials investigated



GB plane populations are inversely correlated to known **interfacial** energies.

MgO and TiO₂ distributions: Saylor et al., *J. Amer. Ceram. Soc.*, 87 (2004) 724.

MgO surface energy: Saylor & Rohrer, *Interface Science*, 9 (2001) 35.

Titania surface energy: Pang & Wynblatt, *J. Amer. Ceram. Soc.*, 89 (2006) 666.

Alumina surface energy: Kitayama and Glaeser, *J. Amer. Cer. Soc.*, 85 (2002) 611.

Exporting boundary traces from MTEX

- Function called “Export_gb_traces_CMU”
- Mean grain Orientations left and right of boundary
- Misorientation angle
- Misorientation axis wrt to Orientation left
- Misorientation axis wrt to Orientation right
- Trace lengths
- Trace azimuths
- Trace end-points
- Grain Ids
- Currently single phase (grain) boundaries
- Can be modified for phase boundaries, which are very common in rocks

- %
- % MTEX export file for grain boundary traces and associated gB parameters
- % in the format used by CMU stereology analysis programs written and
- % maintained by Greg Rohrer et al.
- %
- % You can find the stereology FORTRAN programs and ebsd data sets at
- % http://mimp.materials.cmu.edu/~gr20/Grain_Boundary_Data_Archive/
- %
- % INPUT
- %
- % export_filename = file name like 'CMU_gB_segments.txt'
- %
- % ebsd = MTEX ebsd object
- %
- % seg_angle = segmentation angle for grain model e.g. 10 or 15 degrees
- % may be material dependent.
- %
- % min_points = minimum number of indexed points per grain e.g. 10 points
- %
- % n_gB_smooth = Laplacian smoothing of grain boundaries to remove the
- % stair-case effect of the EBSD grid.
- % n_gB_smooth = 0 NO smoothing, a value of 1 to 2 recommended
- %
- % phase_name = e.g. 'Forsterite' to limited the boundaries
- % between the same phase e.g. Forsterite-Forsterite
- %
- % plot_option = 1 to save plots to graphics file allow checking
- % saving plots to file may take some time to transfer
- % graphic file to the hard drive
- % plot_option = 0 do NOT save plots to file
- %
- % Fig_size_maps = 'huge','large','medium' or 'small' recommend 'large'
- %
- % Fig_size_trace = try 800 or 1500 length and width of the gB trace plot
- %
- % plot_file_path = example '/MatLab_Programs/' saves plots in folder

- % output_format = 12 for 12-columns or 21 for 21-columns
- %*****
- % 12-columns format
- %*****
- % Column 1-3: o_right right hand average orientation (phi1, PHI, phi2 in radians)
- % Column 4-6: o_left left hand average orientation (phi1, PHI, phi2 in radians)
- % Column 7: trace_length length (in microns)
- % Column 8: trace_azimuth trace angle (in degrees)
- % Column 9-12: X1,Y1,X2,Y2 x,y coordinates of trace endpoints (in microns)
- %
- %*****
- % 21-columns format
- %*****
- % Column 1-3: o_right right hand average orientation (phi1, PHI, phi2 in radians)
- % Column 4-6: o_left left hand average orientation (phi1, PHI, phi2 in radians)
- % Column 7: m_angle misorientation Angle (in degrees)
- % Column 8-10: m_axis_right misorientation Axis in Right Hand grain
- % Column 11-13: m_axis_left misorientation Axis in Left Hand grain
- % Column 14: trace_length length (in microns)
- % Column 15: trace_azimuth trace angle (in degrees)
- % Column 16-19: X1,Y1,X2,Y2 x,y coordinates of endpoints (in microns)
- % Column 20-21: Id_grain_R,Id_grain_L IDs of right hand and left hand grains
- %
- To do add number of segments : Number_segs = length(gB.segLength)
- To do add EBSD step size : I have written function for this

Grain modelling – segmentation angle

Segmentation angle defines the misorientation limit between low-angle boundaries (sub-grains, innerboundaries) and high-angle boundaries (grain boundaries) using indexed EBSD points

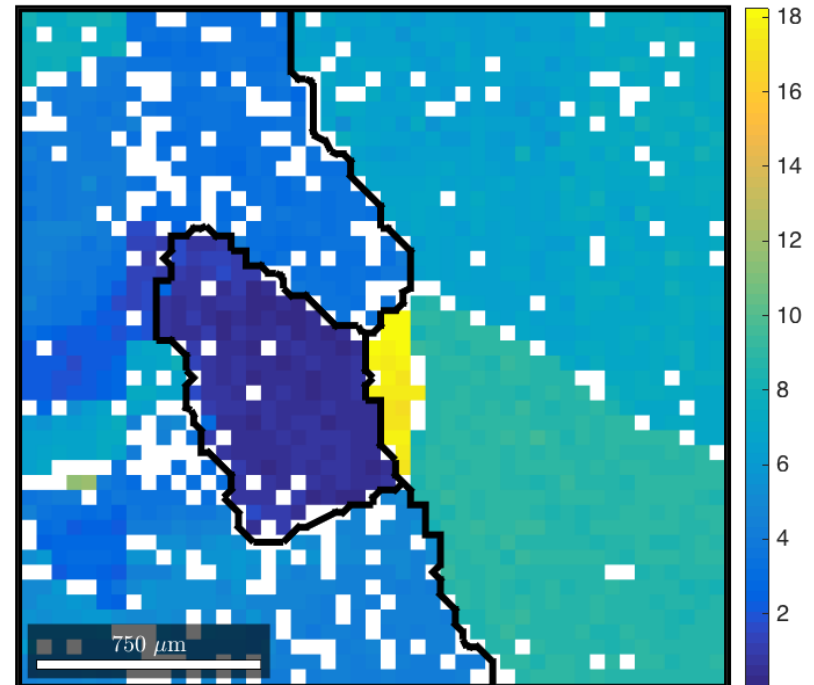
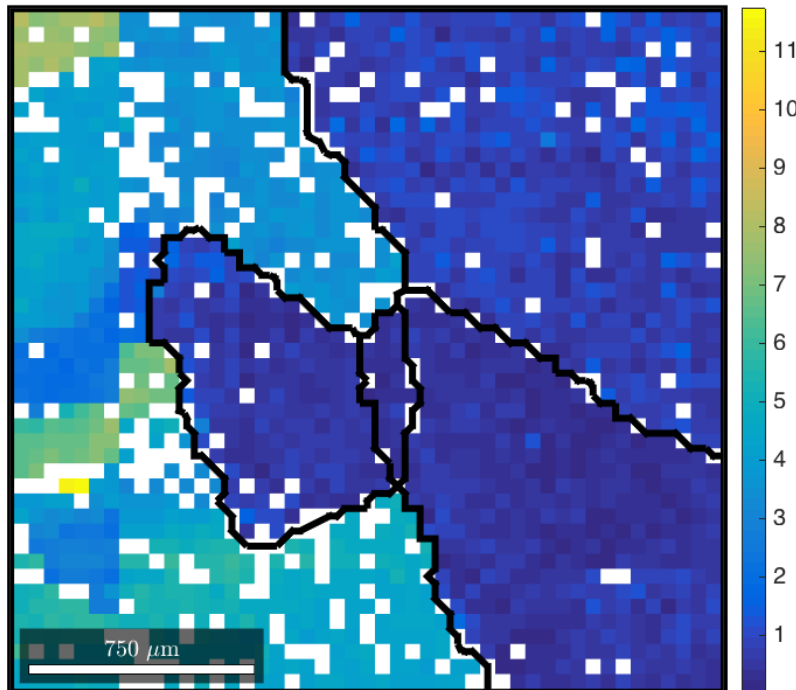
The choice of the angle has strong impact on modelled grain microstructure

```
grains = calcGrains(ebsd('indexed'),'angle',10*degree)
```

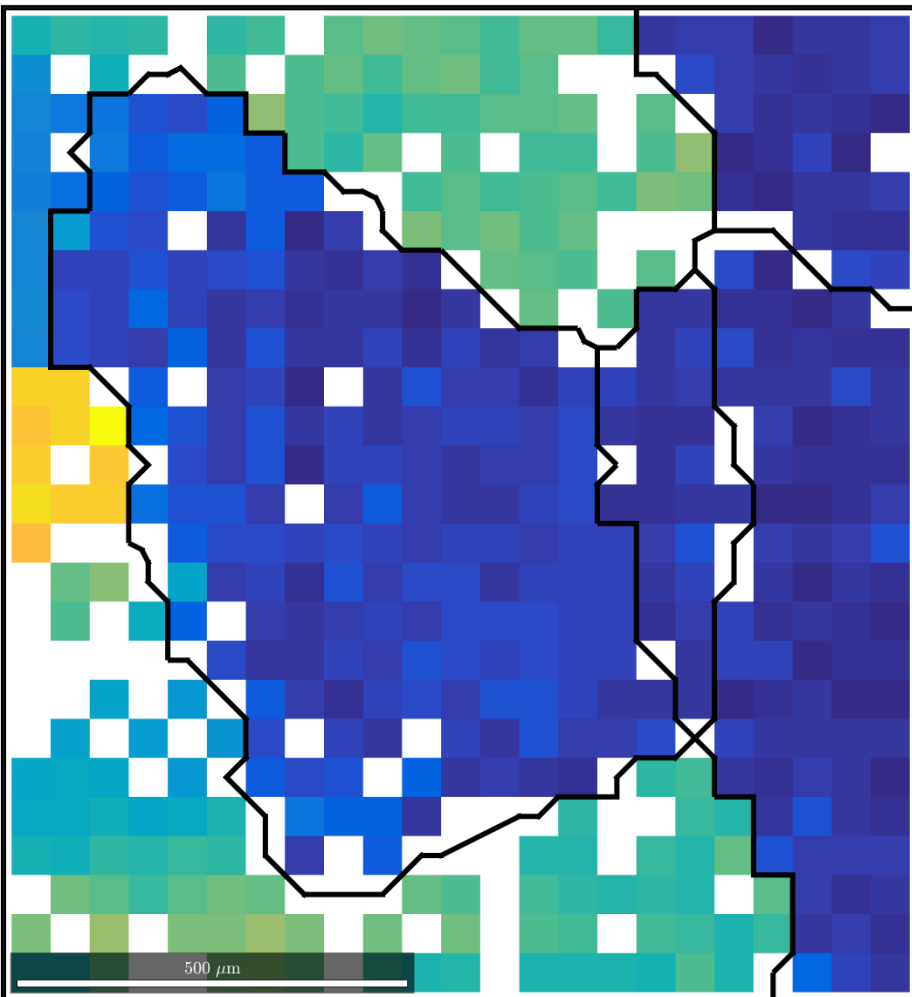
```
grains = calcGrains(ebsd('indexed'),'angle',15*degree)
```

```
grains = calcGrains(ebsd('indexed')) undefined angle uses default value of 15°
```

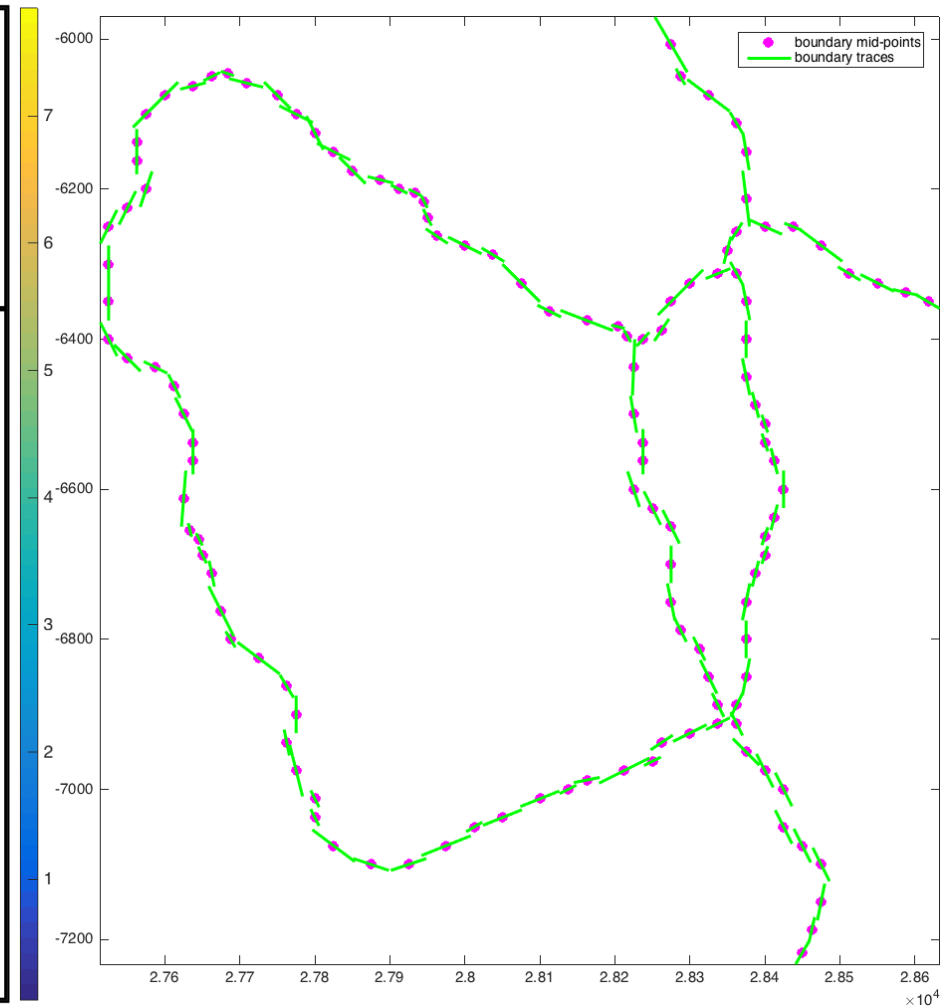
10°-> smaller grains Mis2mean maps 15°-> larger grains



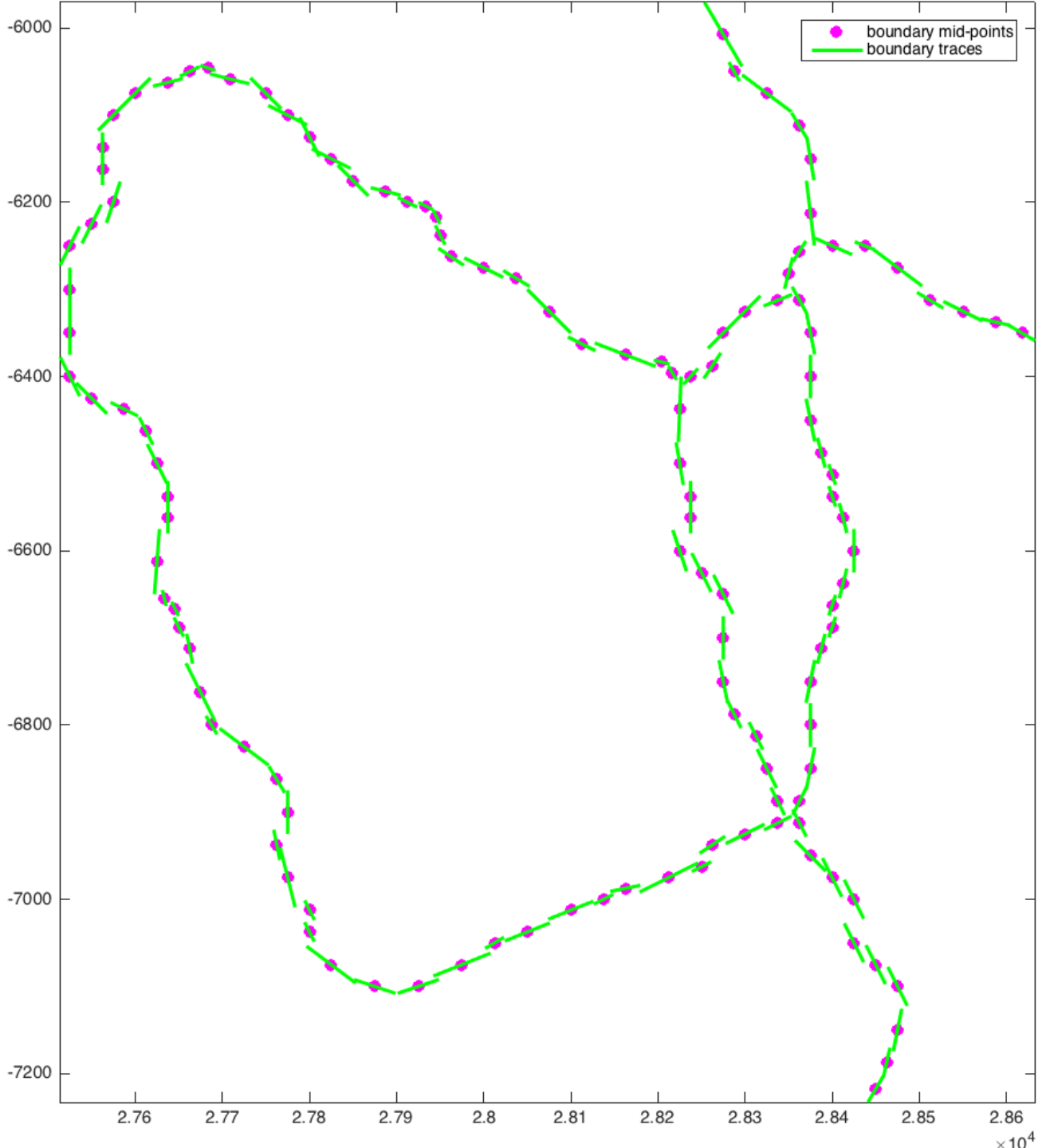
GB Laplacian Smoothing = 0



mis2mean

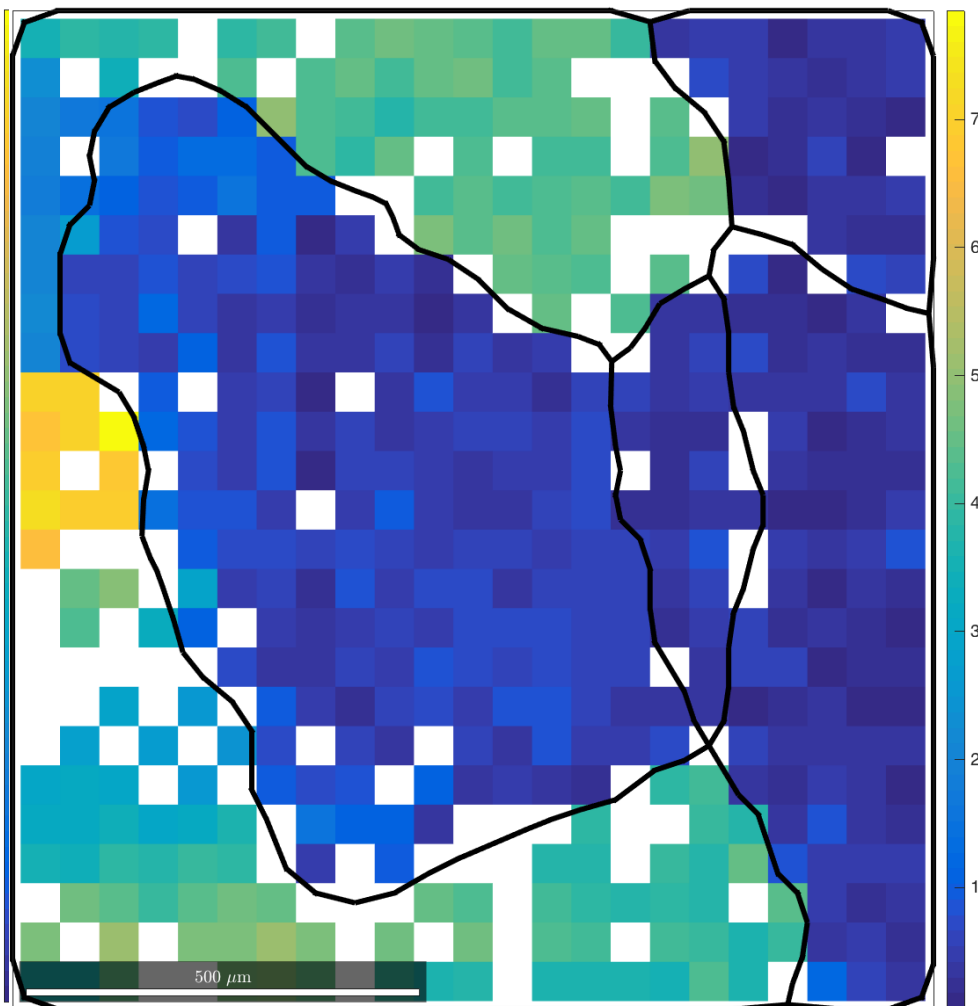
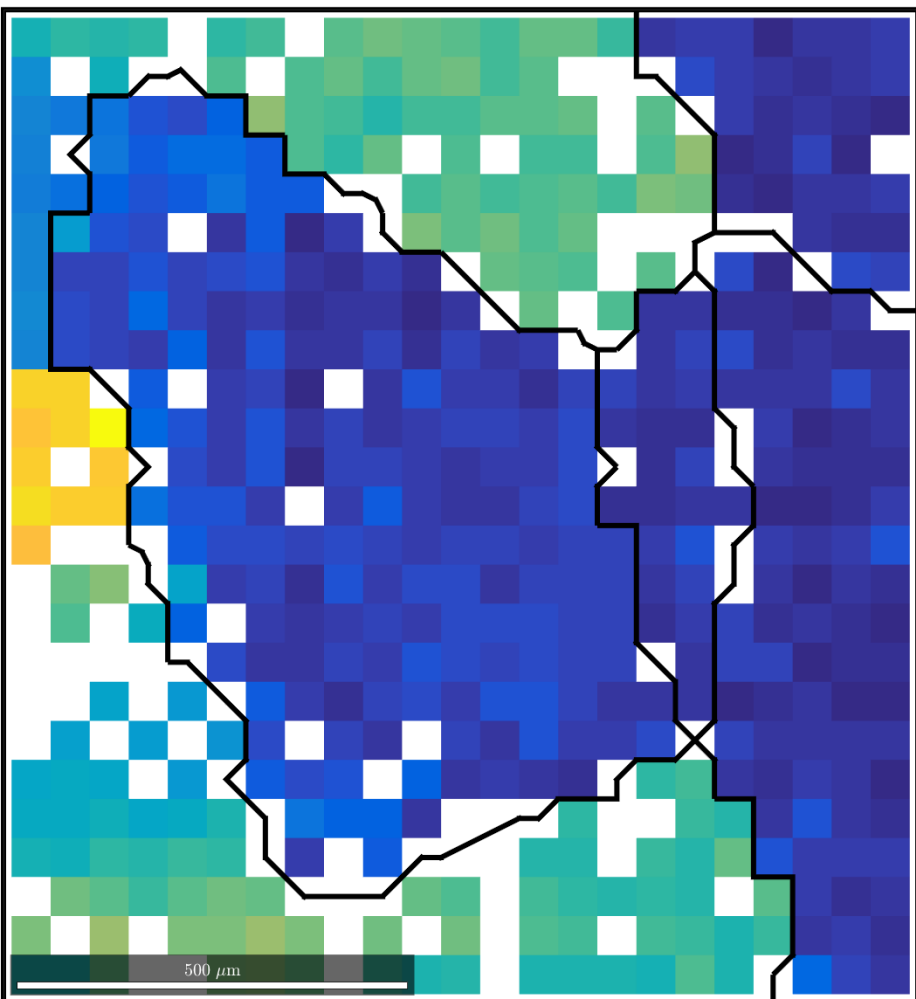


Boundary traces



Smoothing=0

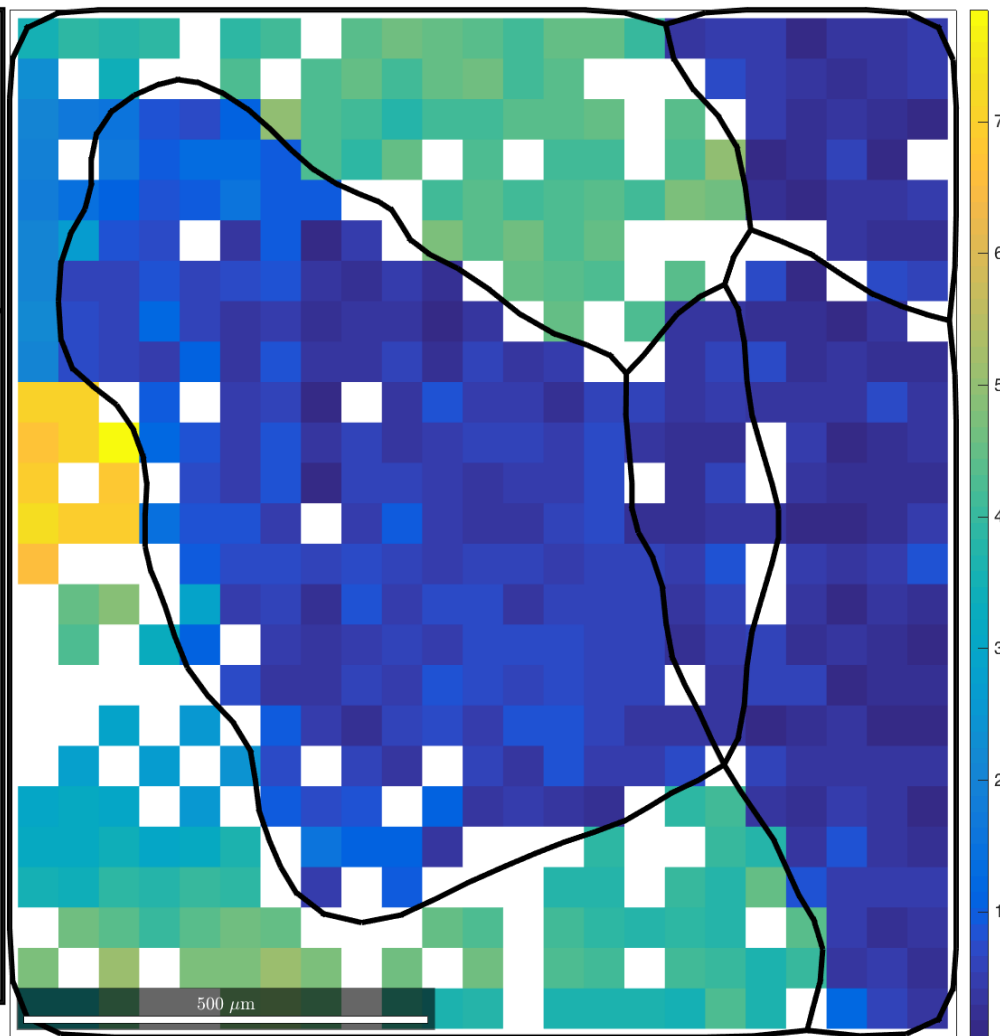
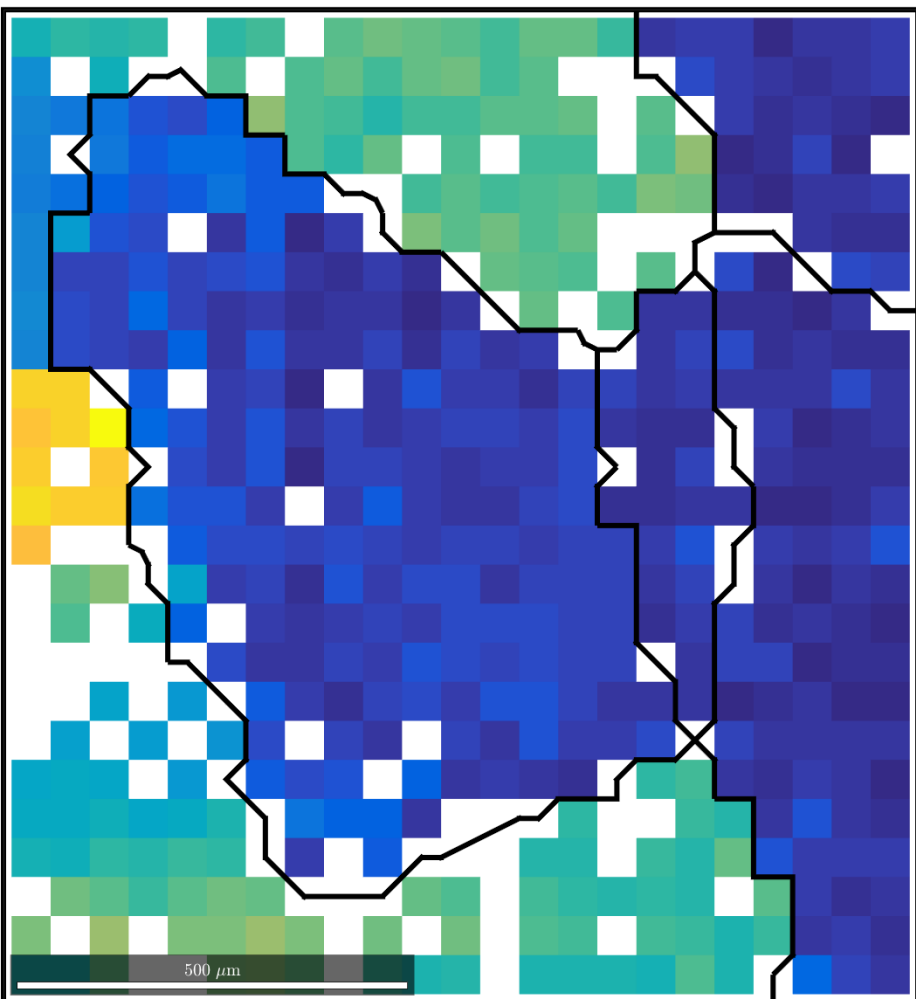
Smoothing=1



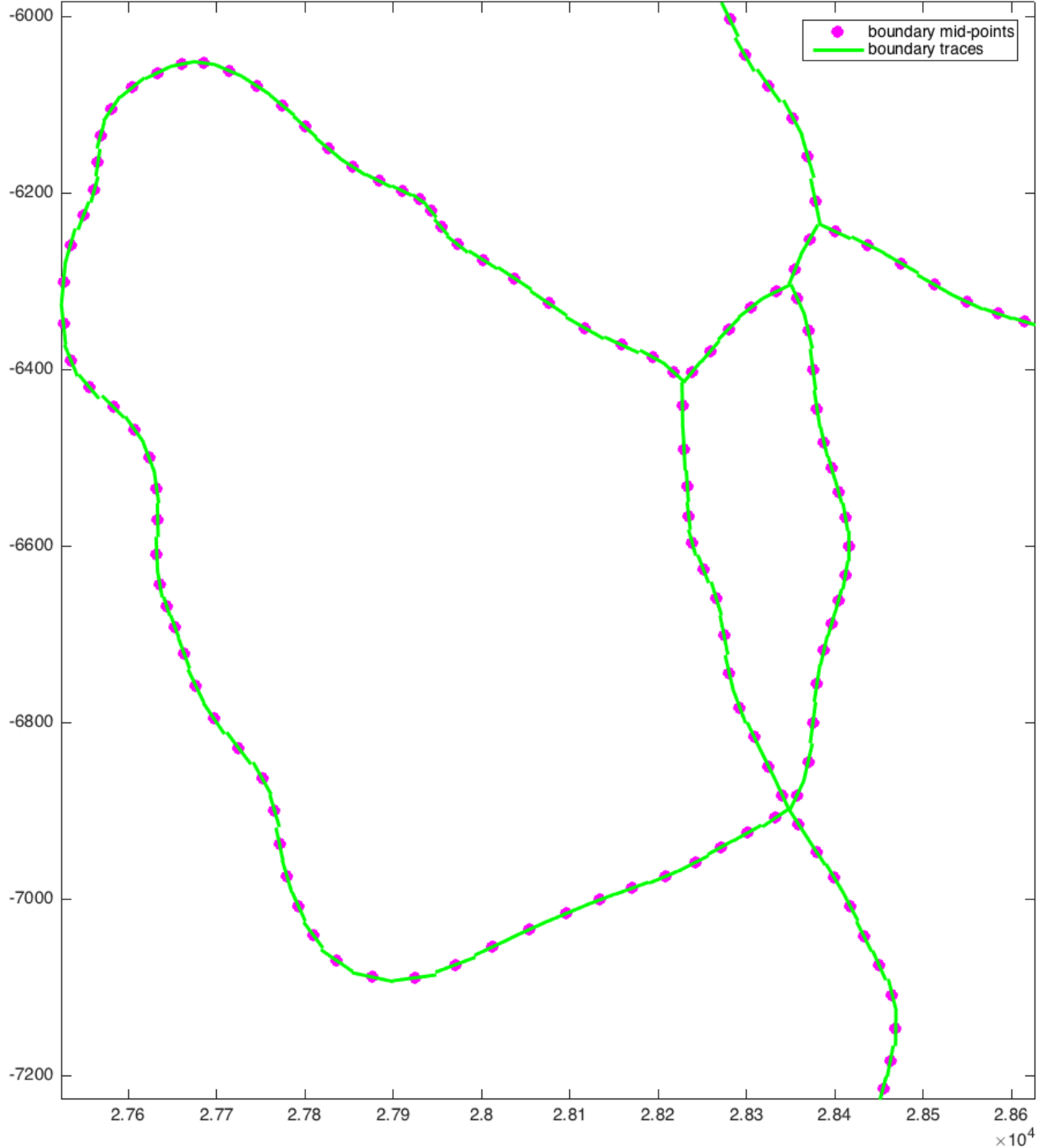
mis2mean

Smoothing=0

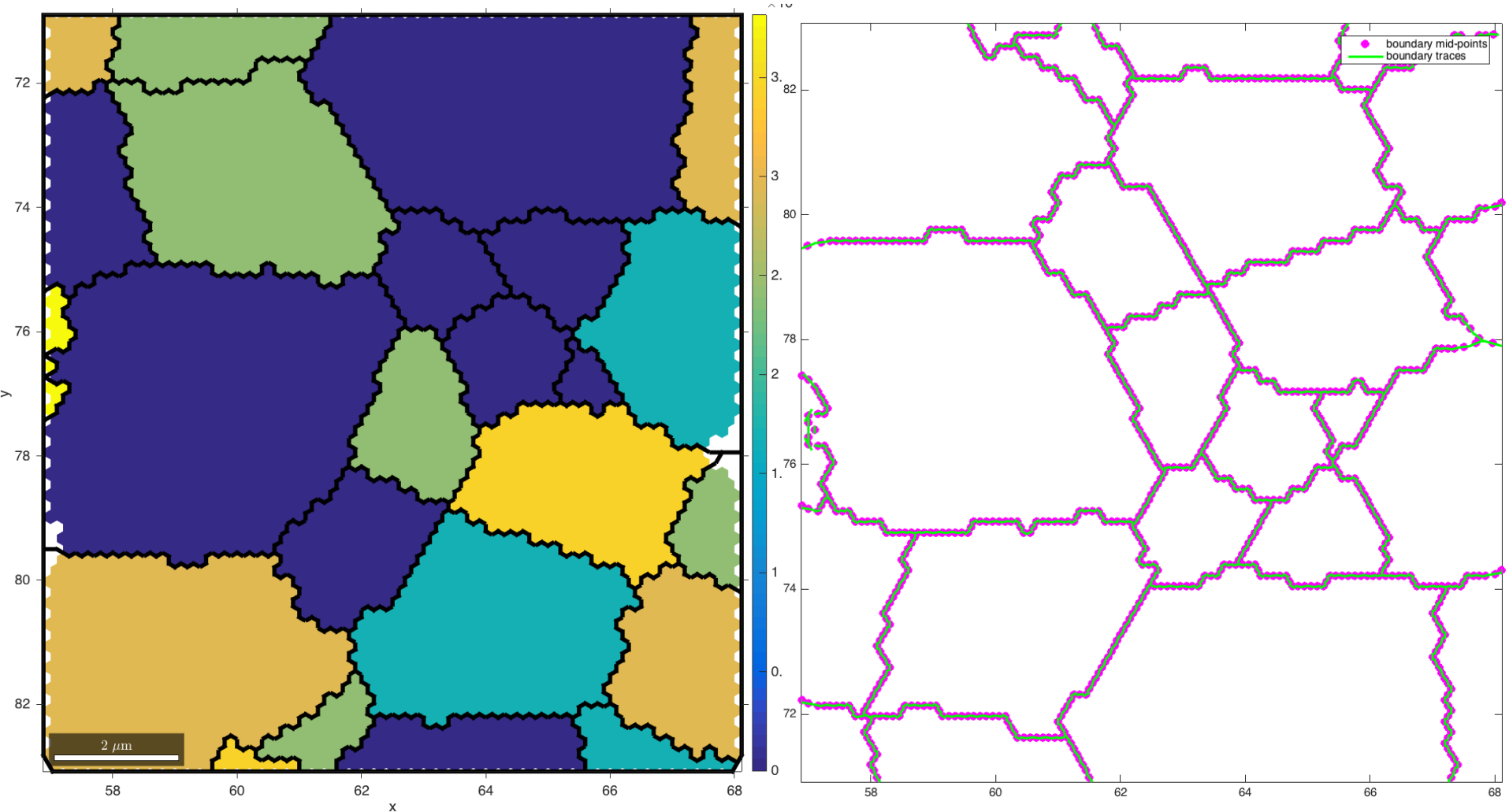
Smoothing=2



mis2mean



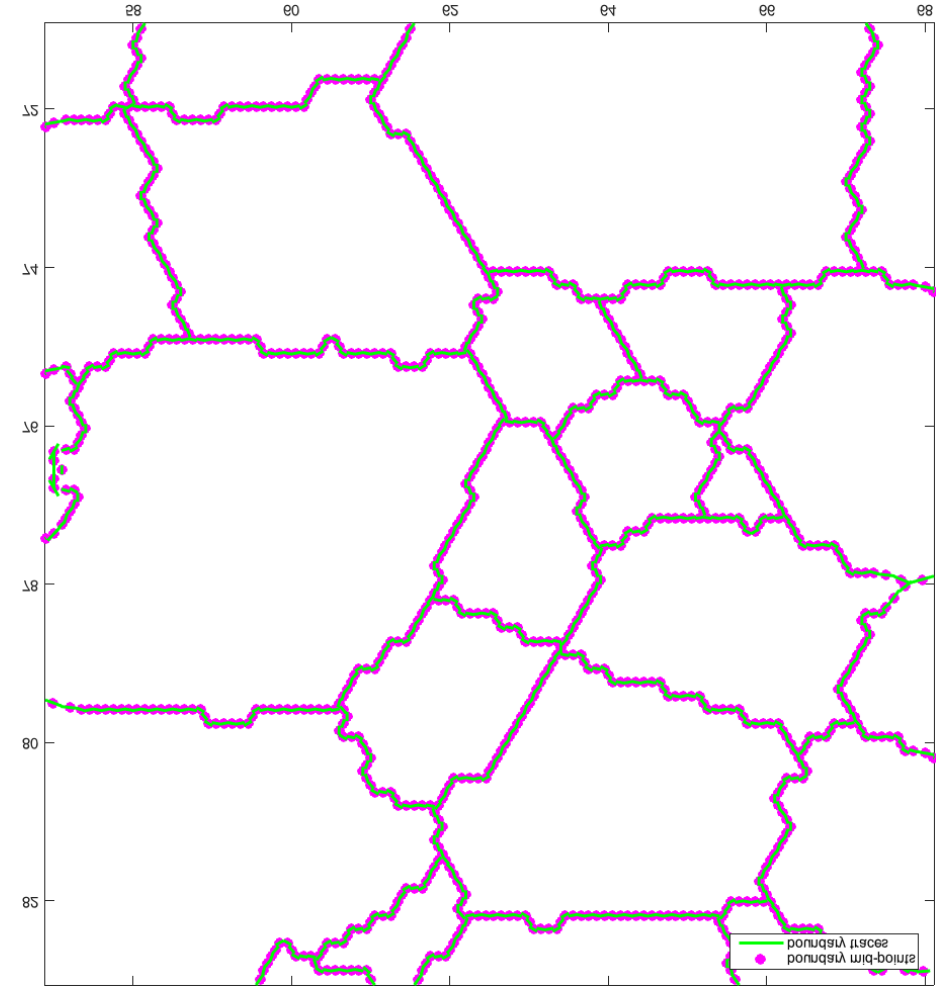
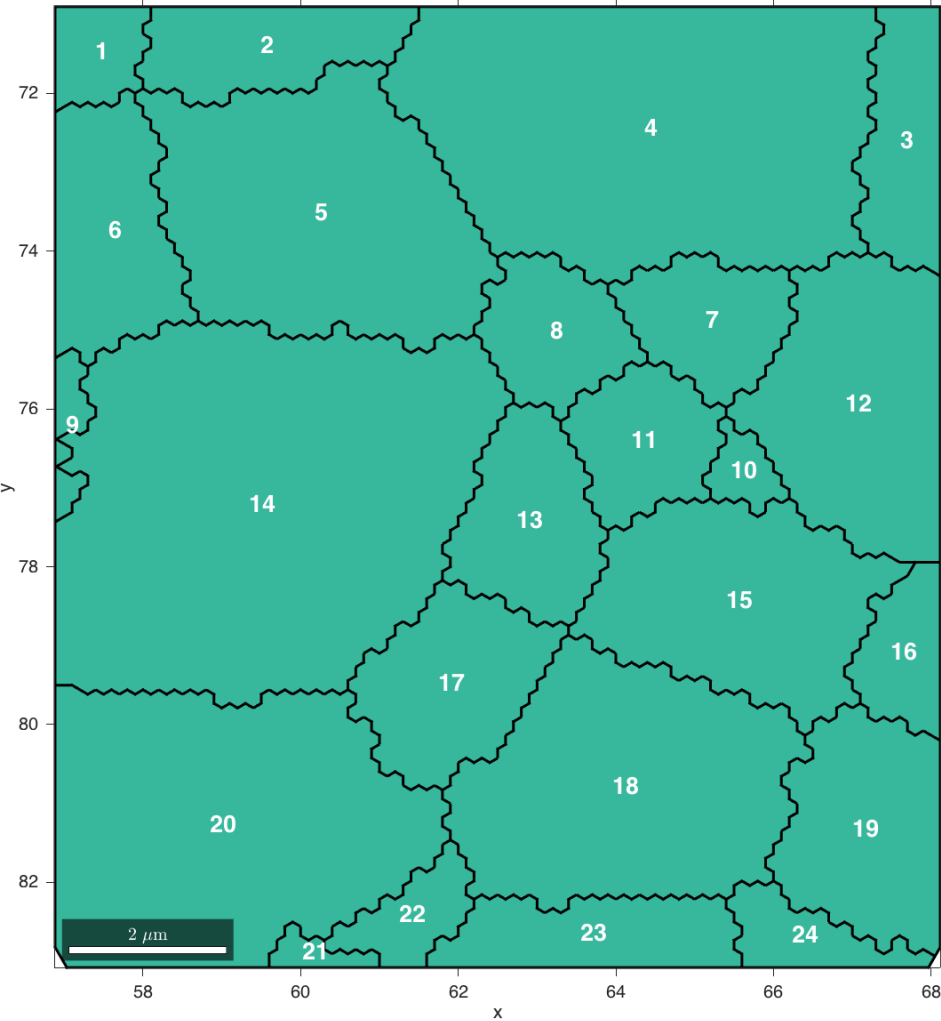
GB Smoothing = 0



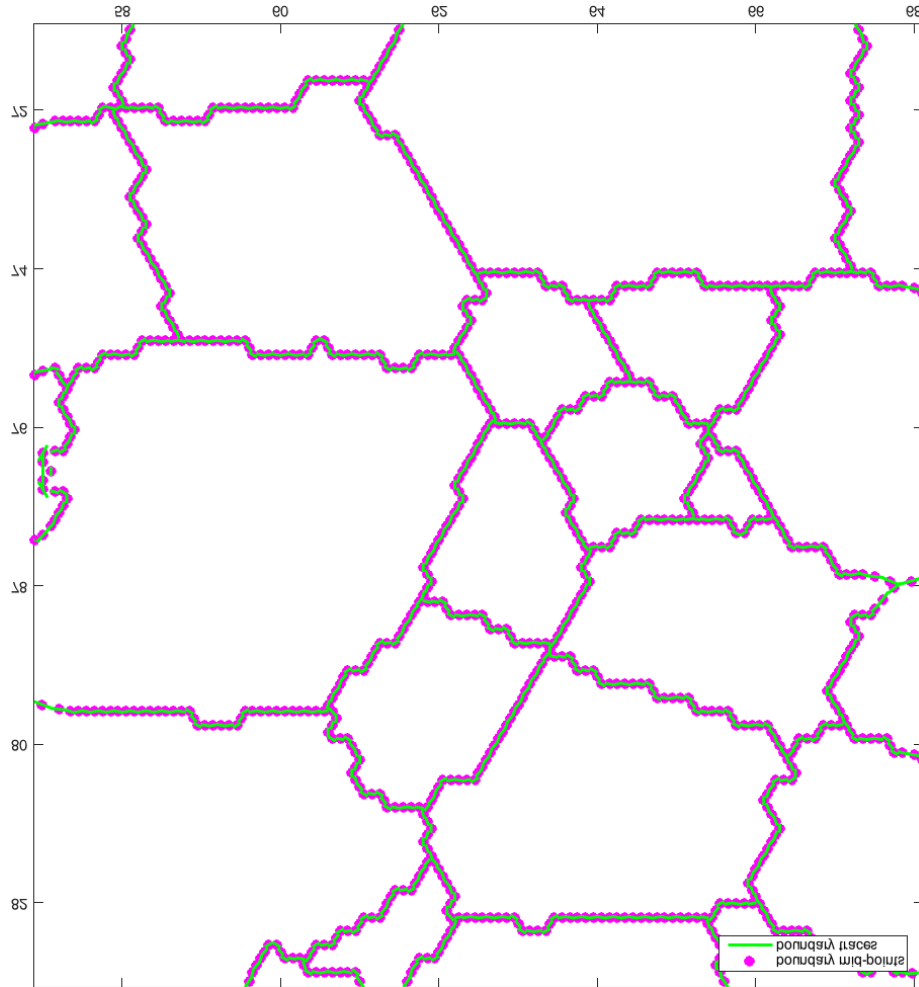
mis2mean

Boundary traces

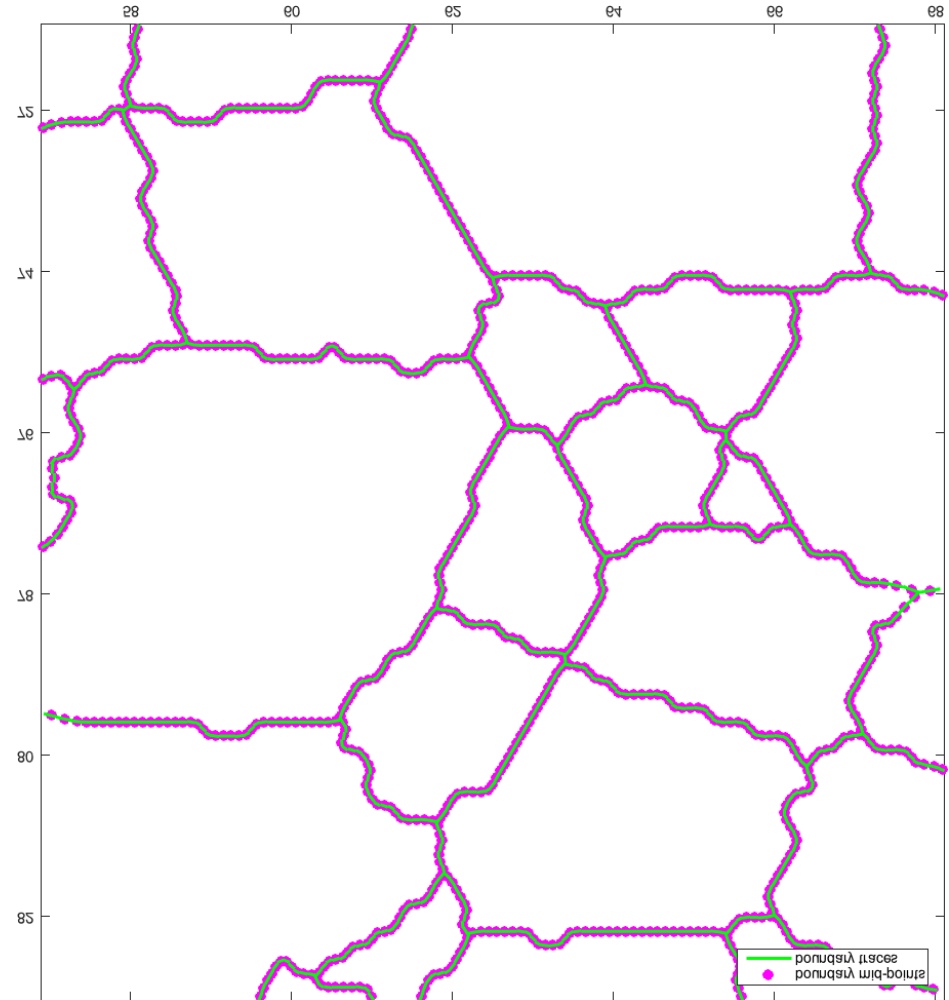
Grain Ids N.B. trace map is flipped



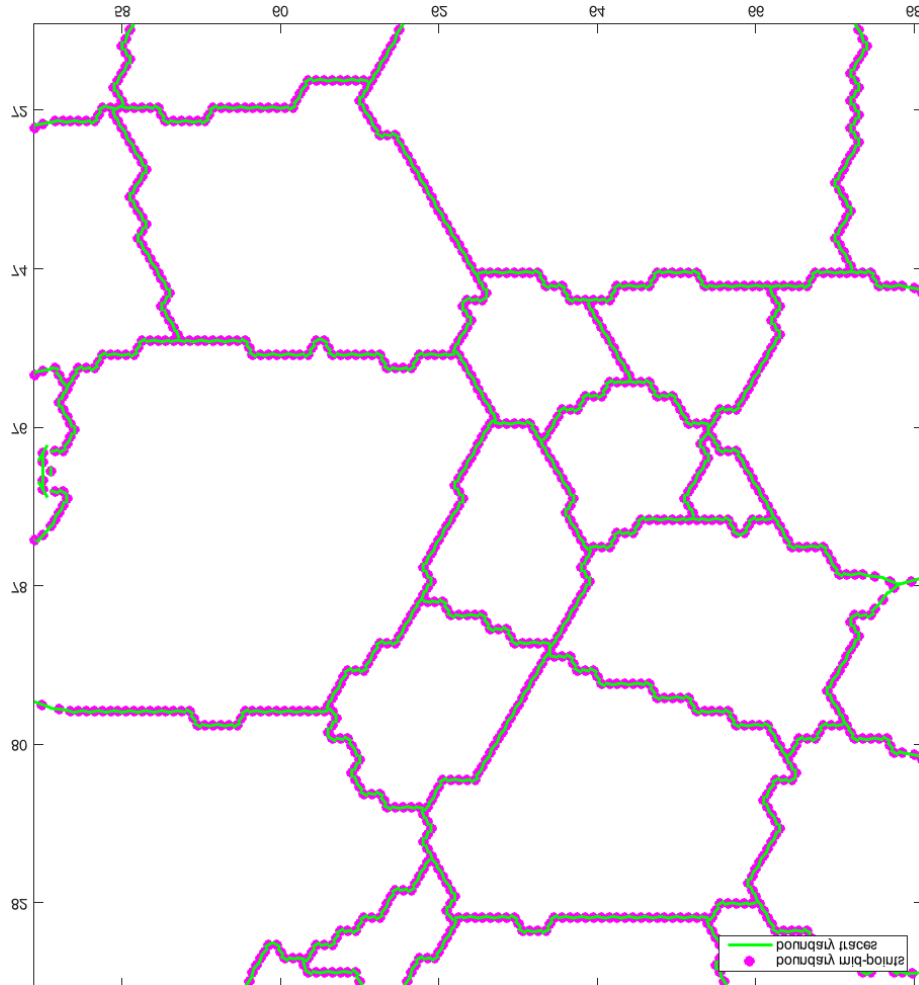
Smoothing=0



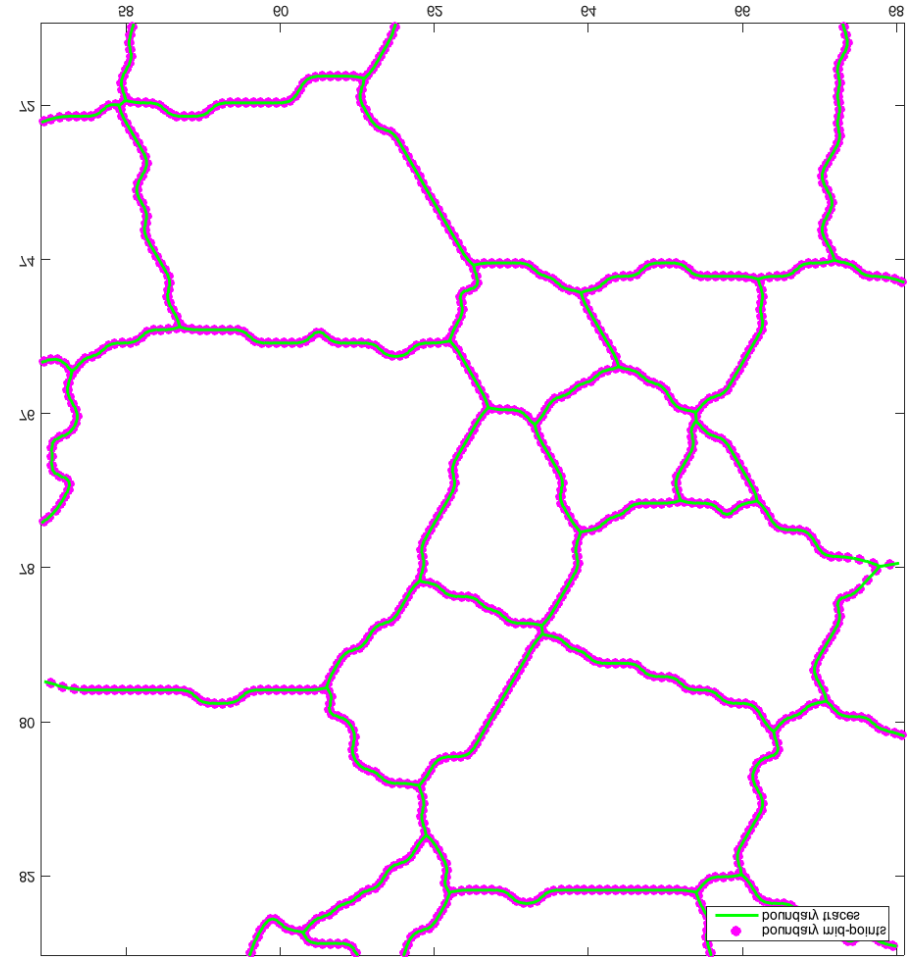
Smoothing=1

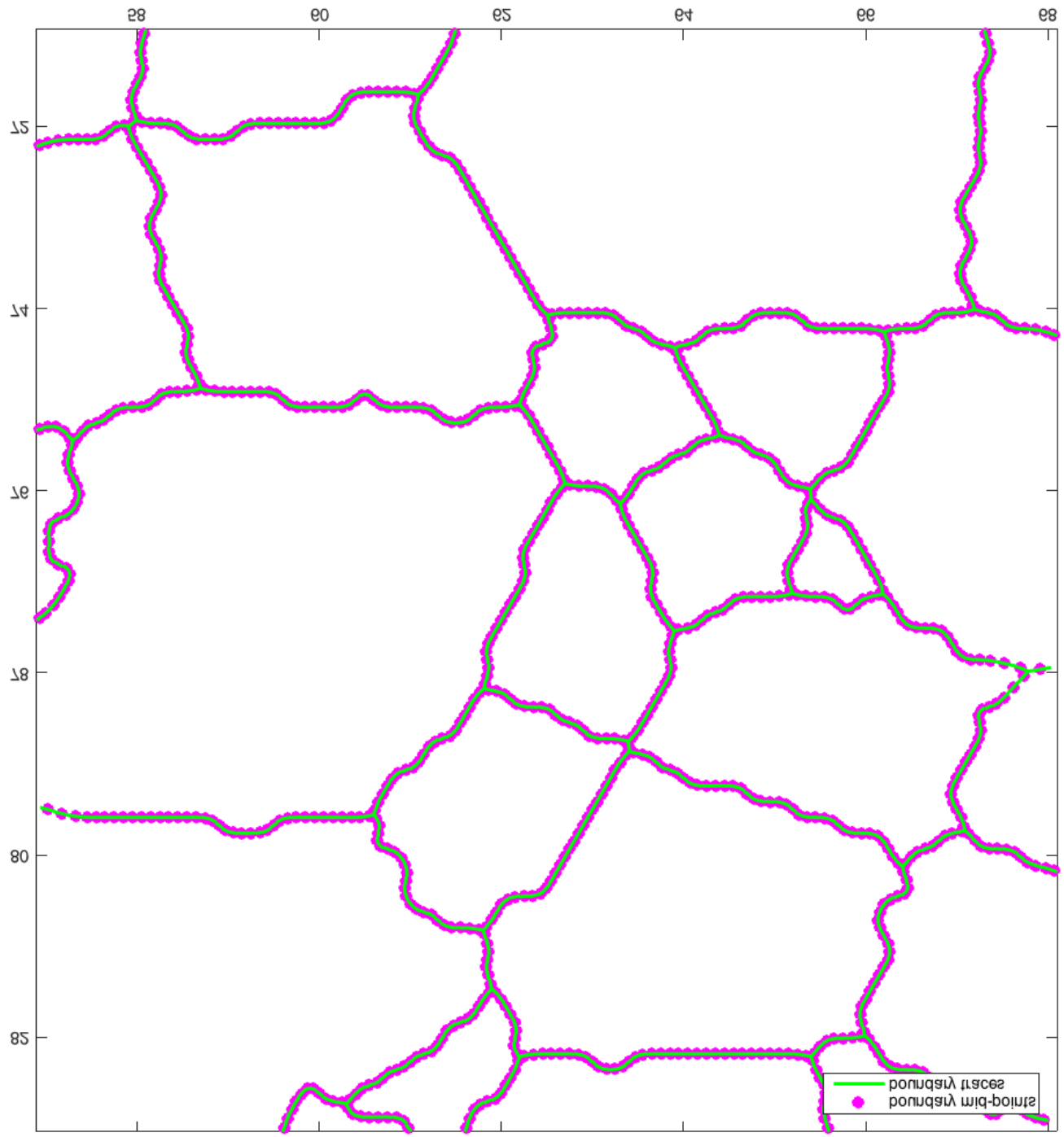


Smoothing=0



Smoothing=2

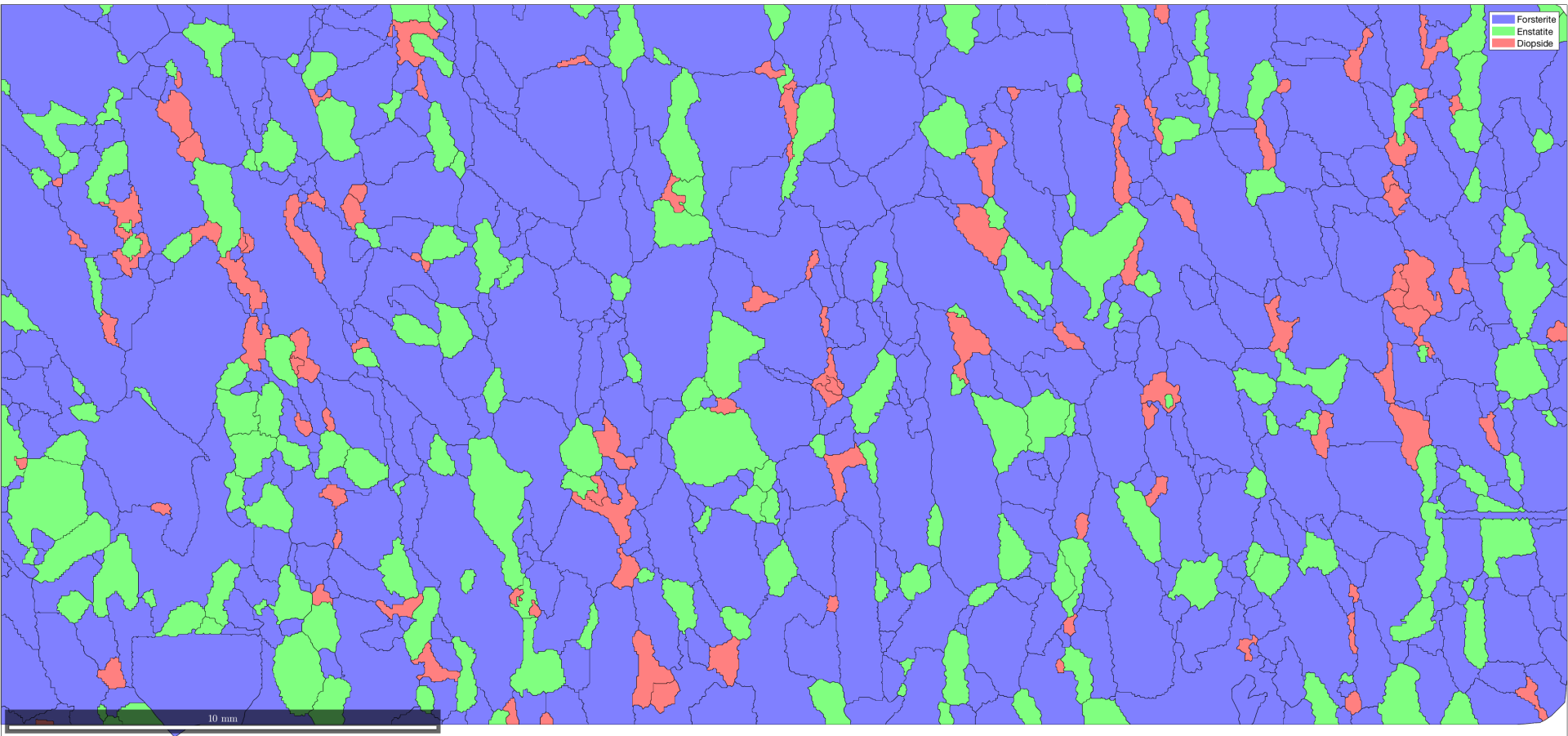




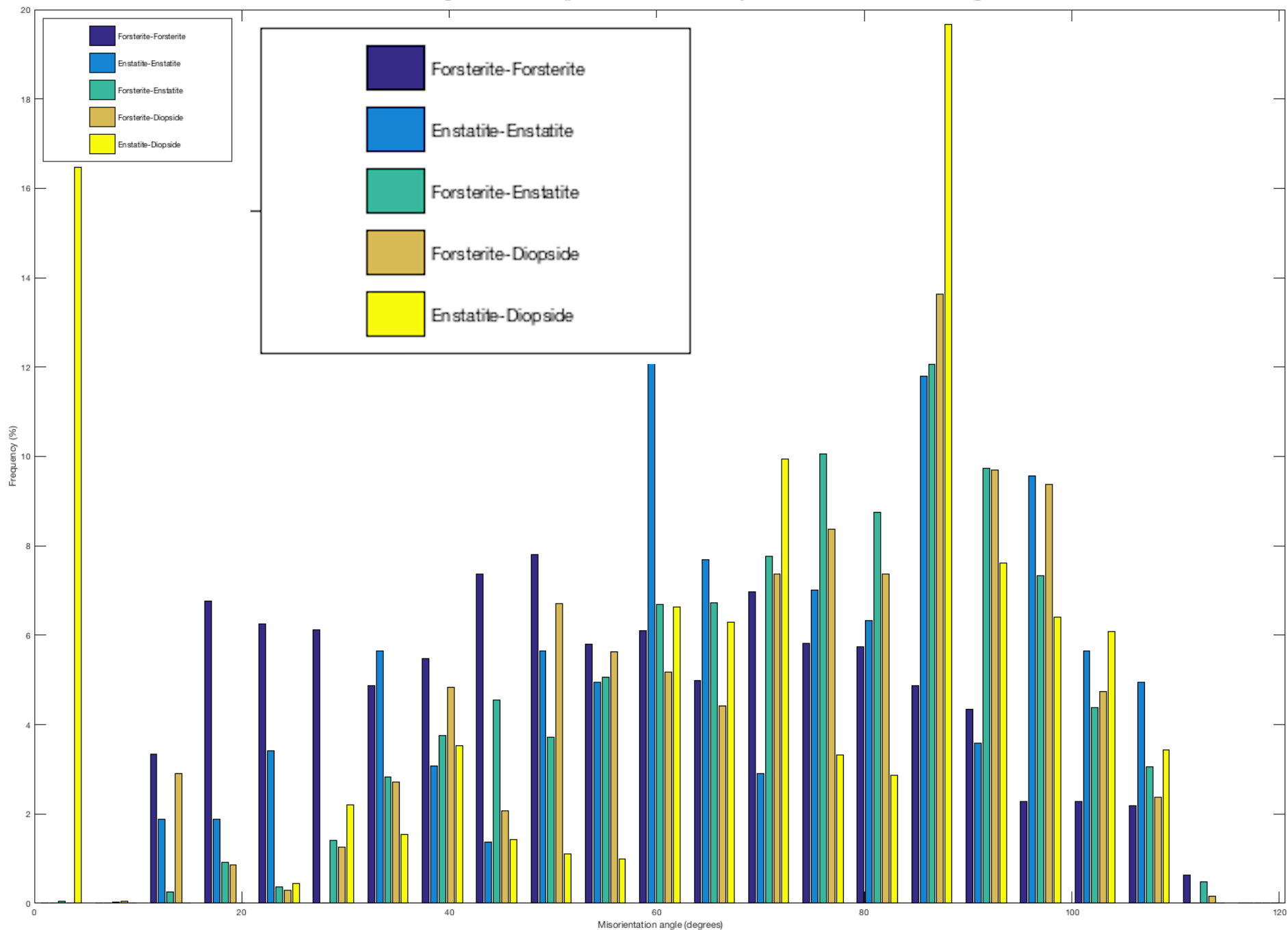
Towards phase boundaries ?

- Phase transitions : olivine-antigorite
- Polyphase rocks : Peridotite (Olivine, Enstatite, Diopside, Garnet, Spinel...).

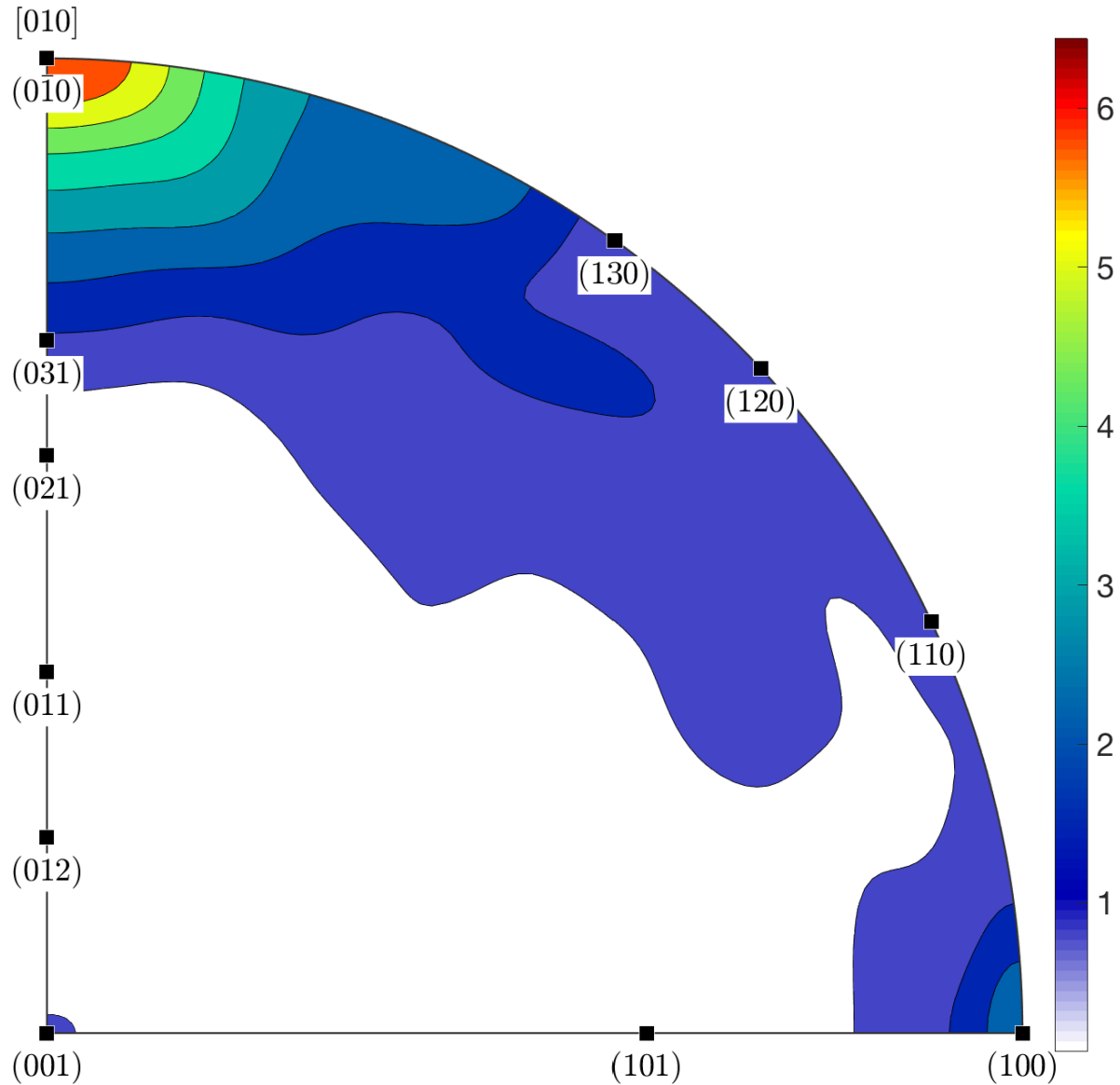
MTEX data set “forsterite”



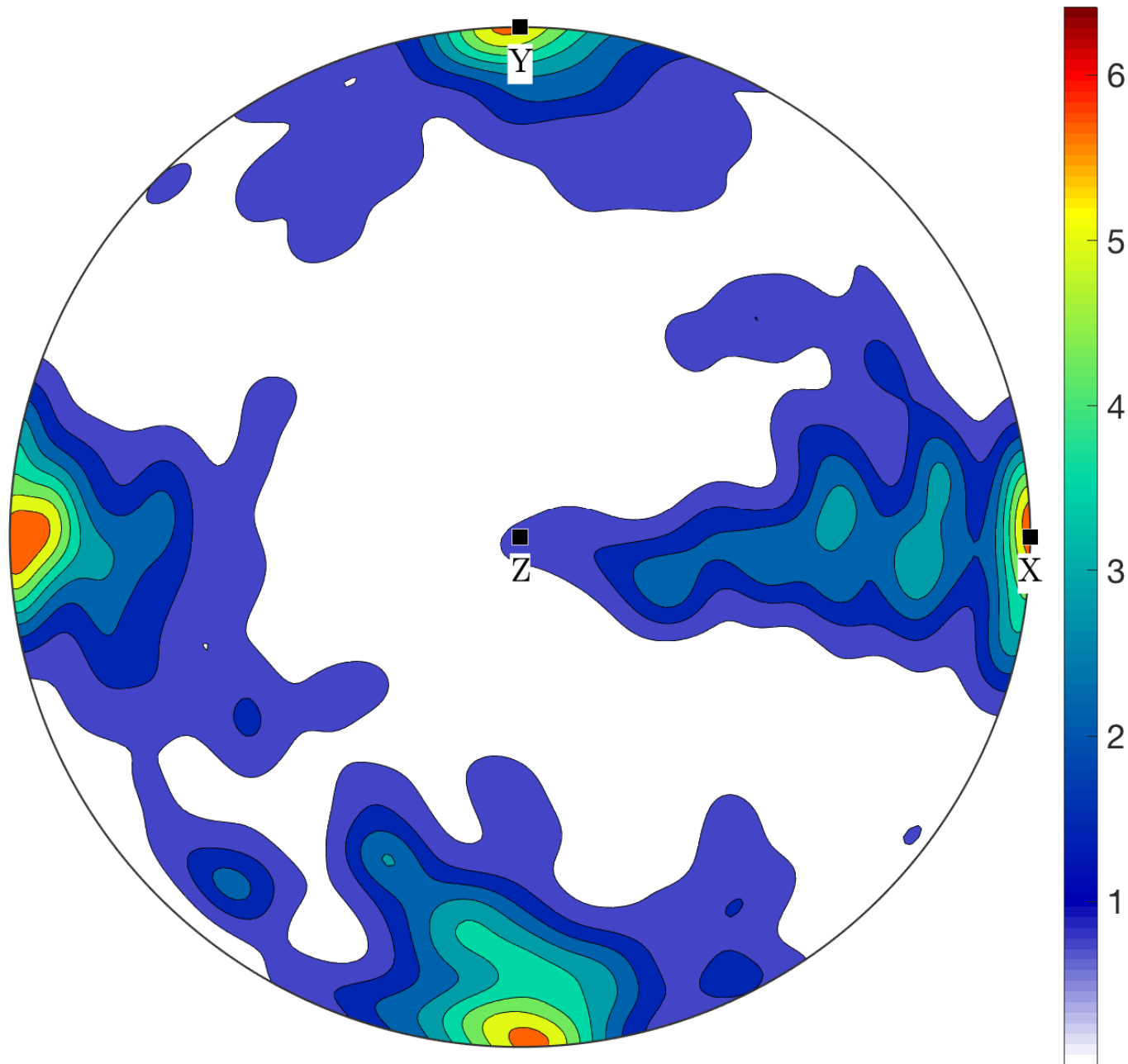
Correlated grain and phase boundary misorientation angles



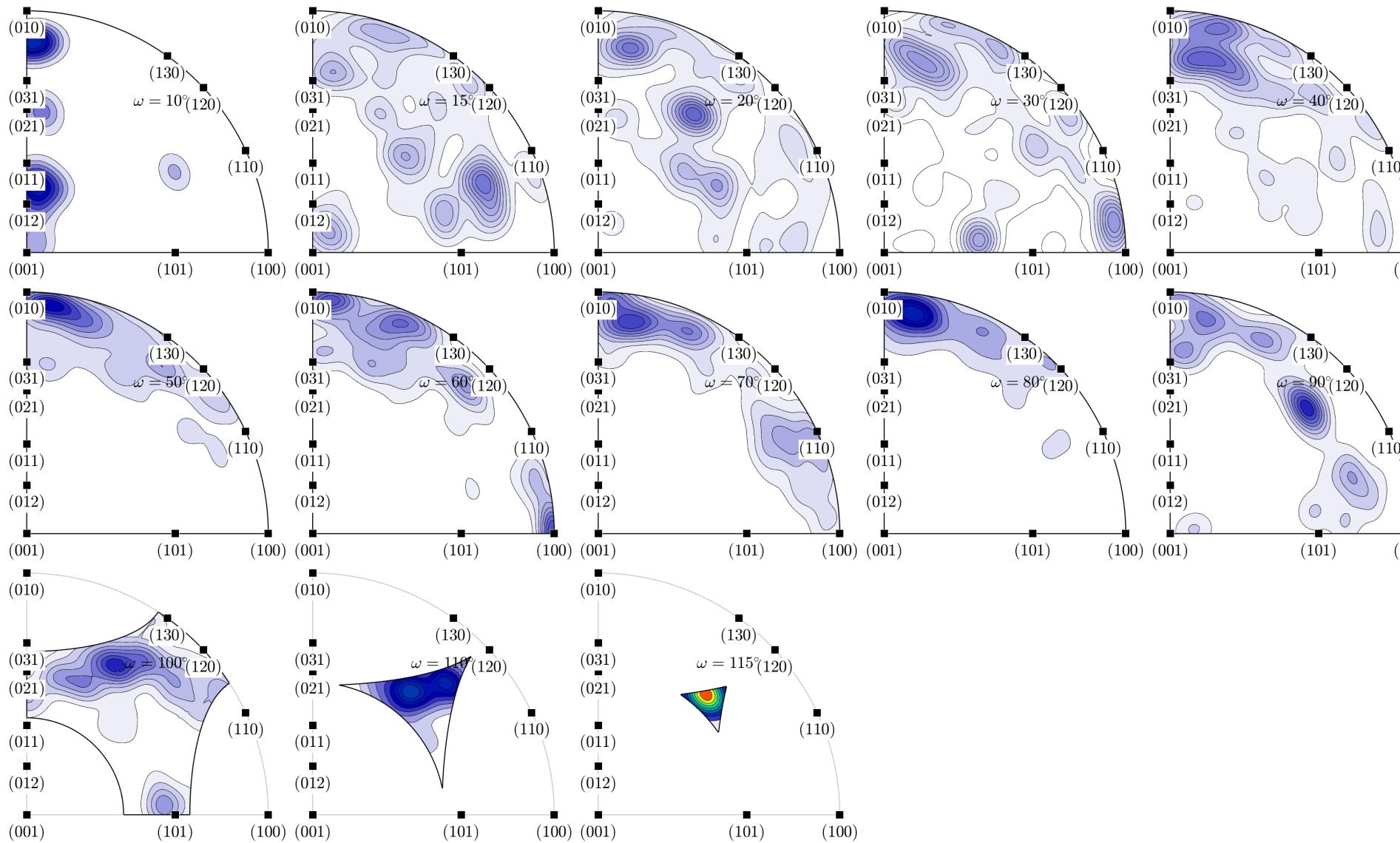
Fo-Fo boundaries misorientation axes



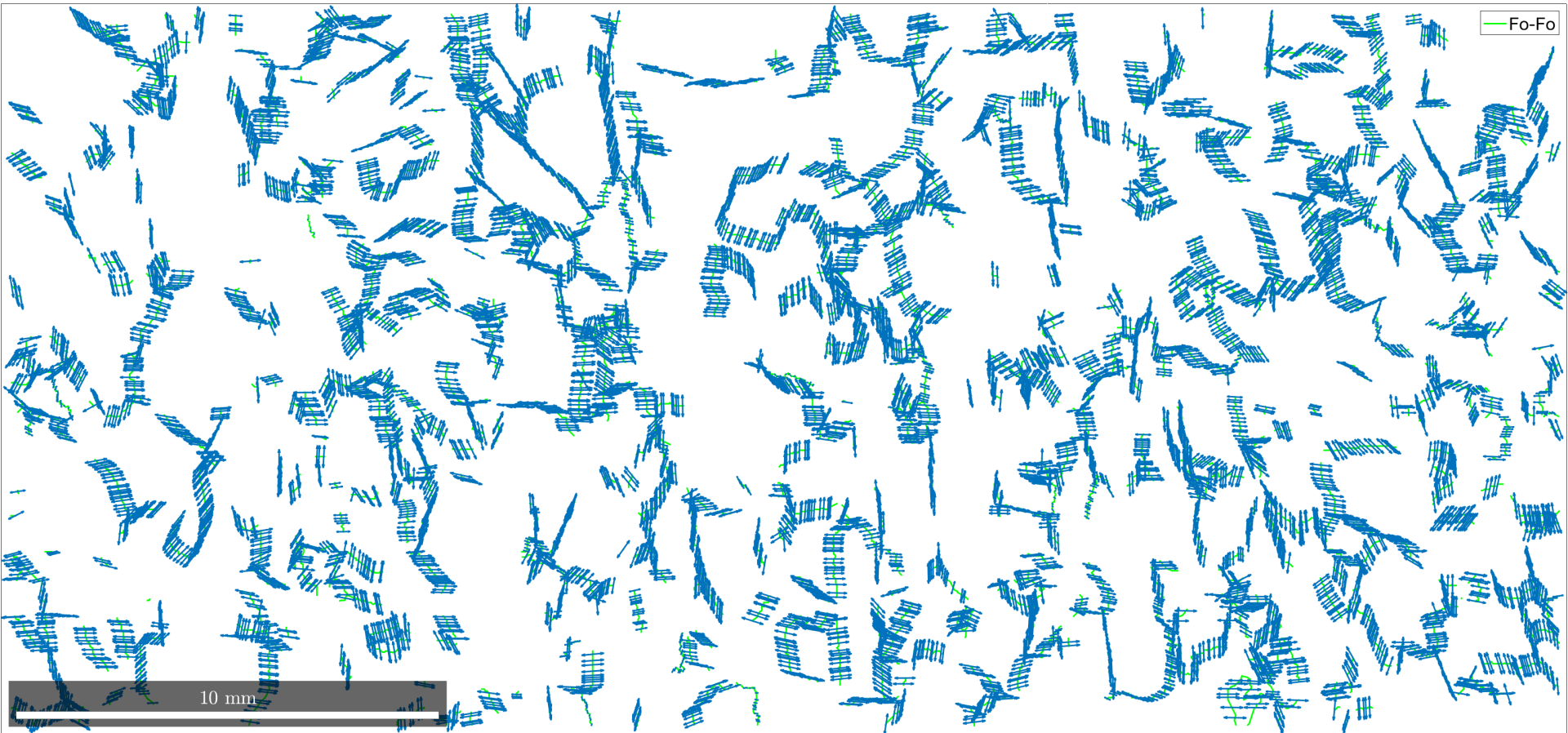
Correlated grain Fo-Fo boundary misorientation axes



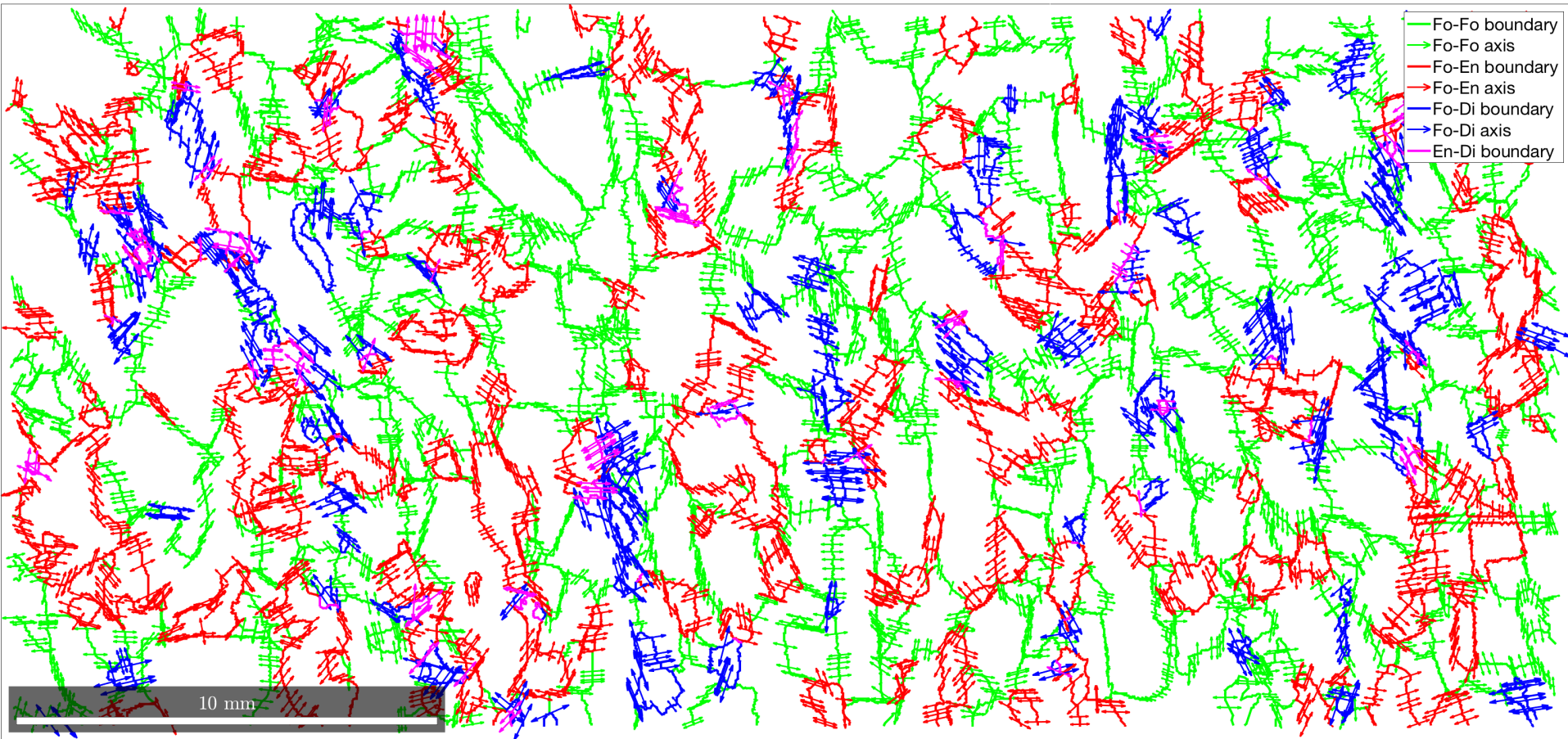
Fo-Fo boundary misorientation axes



Fo-Fo boundary misorientation axes



All phases misorientation axes



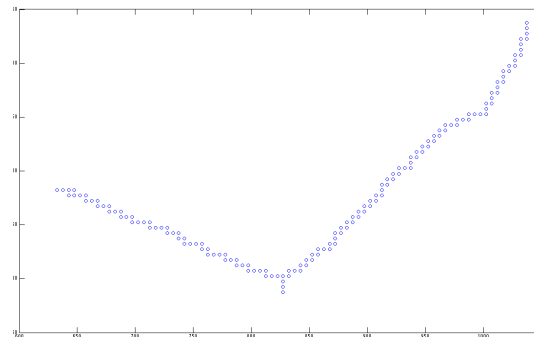
New global gB analysis : *map scale*

- Pole figures in specimen coordinates of the orientations in the boundary region.

Plot of boundary orientation locations.

Plotted PFs of habit (low index),

which are potential boundary plans



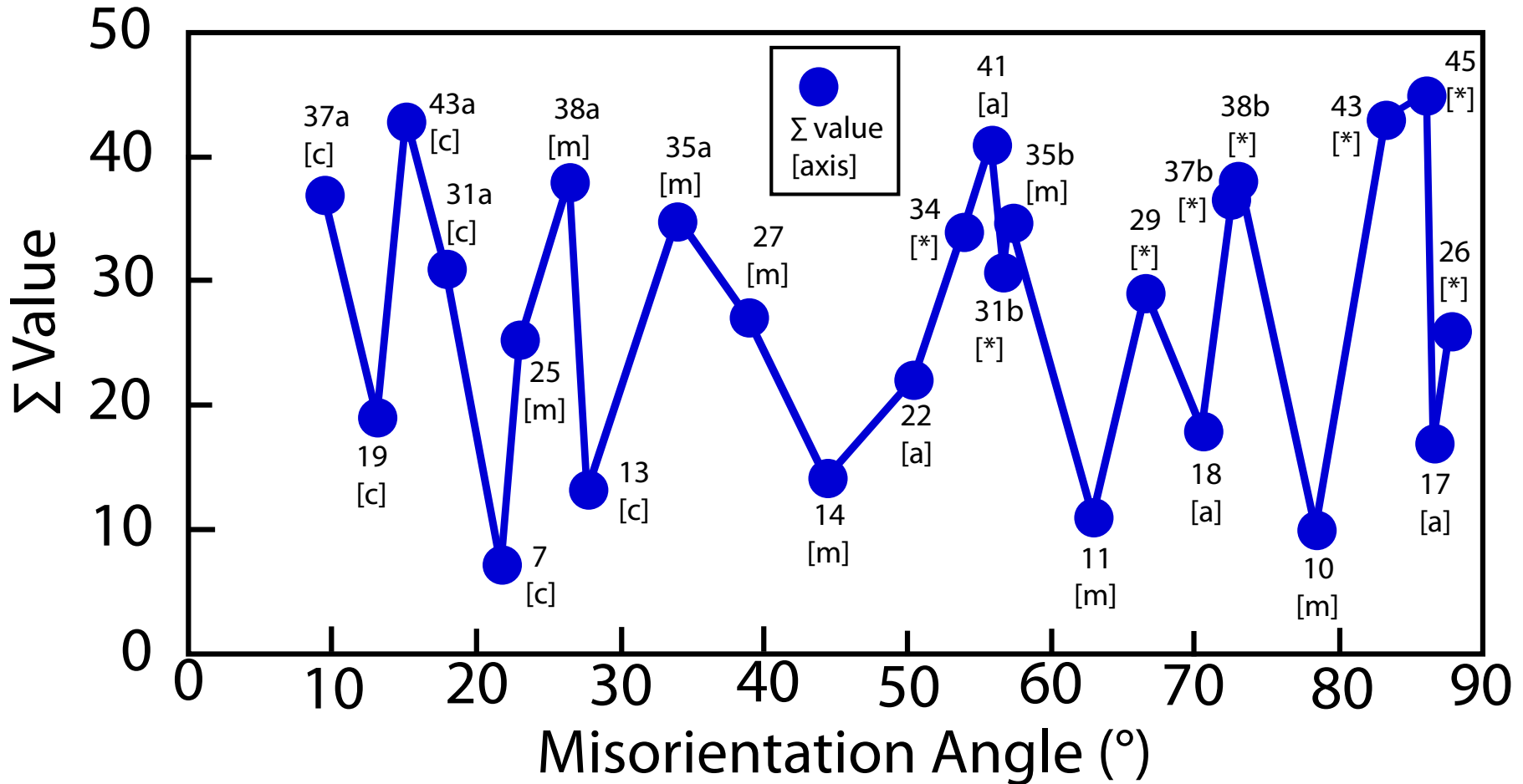
- Pole figure in specimen coordinates of *boundary misorientation axes*.
- Misorientation Distribution Function (MDF) of *boundary misorientation axes* in crystal coordinates.

Coincident Site Lattice (CSL)

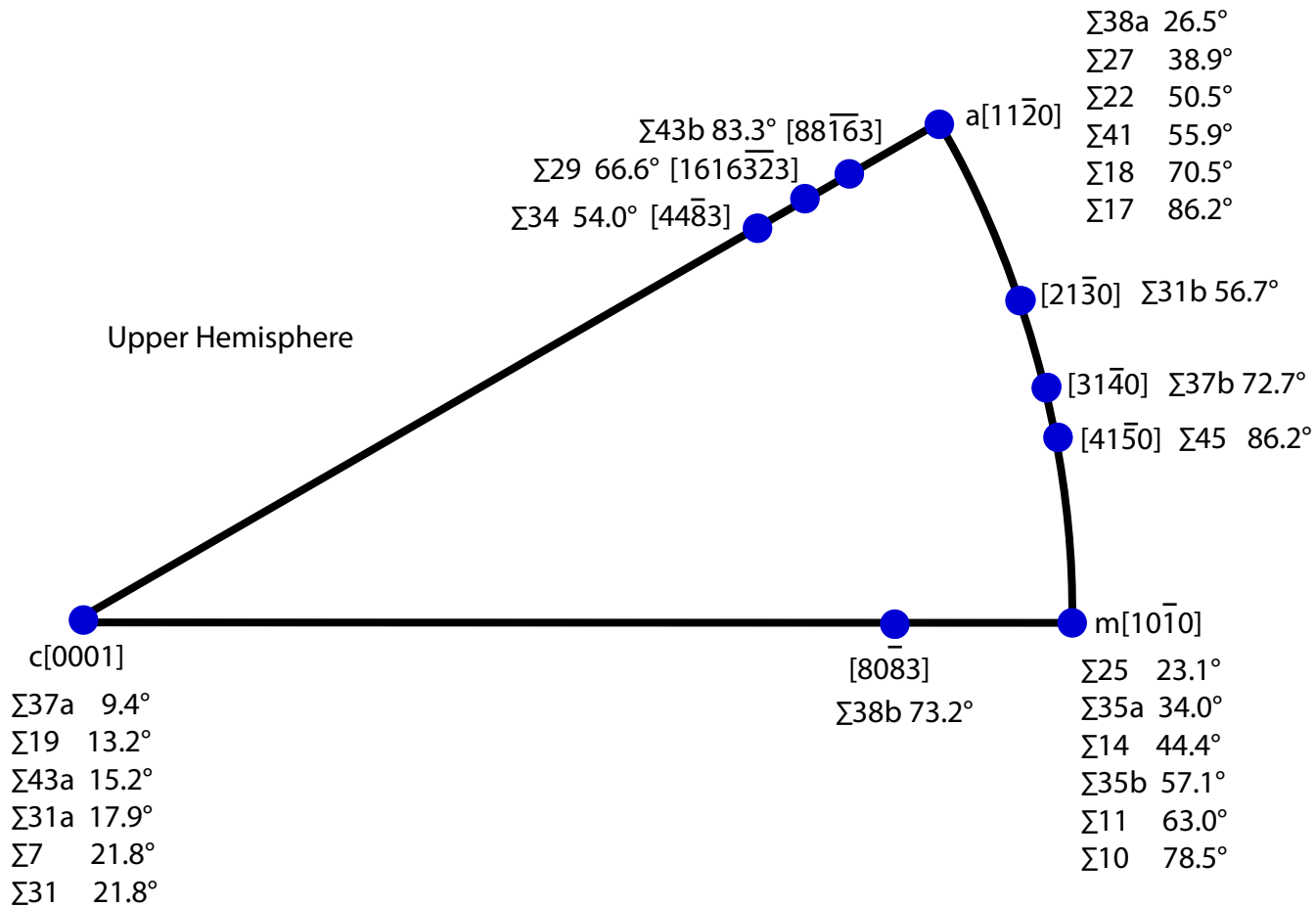
- Useful in FCC ? Hexagonal ?
- Lattice, but not atomic structure
- CSLs on the boundary of fundamental region.
- Twins planes on boundary of fundamental region – *also more likely to have slip transmission from host to twin*
- Probably pure tilt and twist plus special boundaries on boundary of fundamental region.

CSL for a hexagonal lattice with $c/a = 1.6270$

Ice Ih = $c/a = 1.6330$



CSLs for c/a ratio of Ice Ih



Quantitative study of fabric & microstructure development in Ice Ih



Compression, annealing

Work in progress



Laboratoire de Glaciologie et Géophysique de l'Environnement

Collaboration Geosciences Montpellier

David Mainprice, Andrea Tommasi, Fabrice Barou, Karoly Hidas

and Le Laboratoire de Glaciologie et Géophysique de l'Environnement Grenoble

Maurine Montagnat, Thomas Chauve, Baptiste Journaux

EBSD Orientation map measured at -100°C and 1 Pa (no post-treatment 98% indexed)

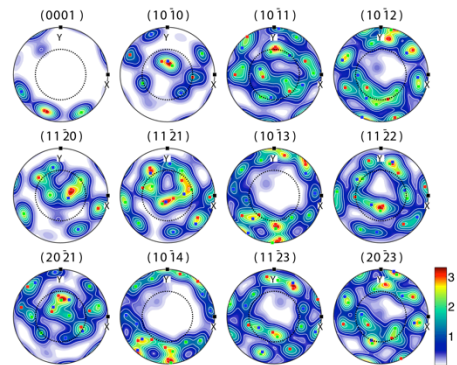


New global gB analysis : map scale

Annealing time = 0 minutes

Pole figures of
in the boundary region

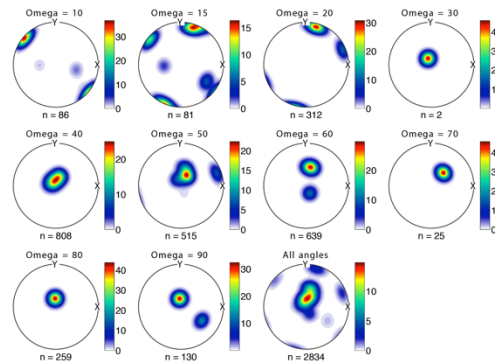
Pole figures of orientations in boundary regions



Pole figure of Boundary
misorientation axes

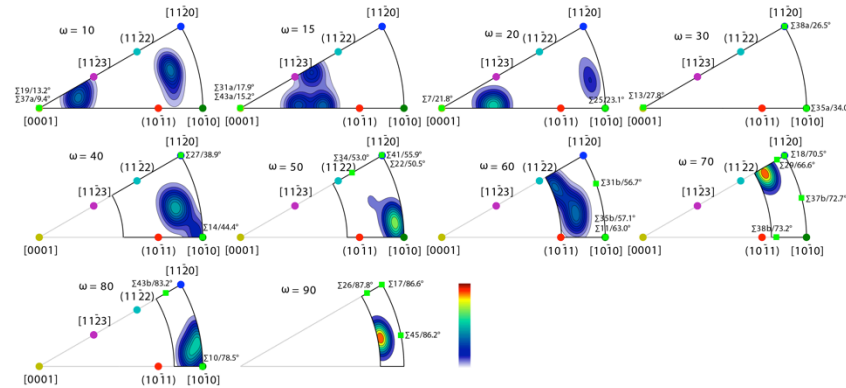
Z6 Deformed Sample : T=0

Pole figures misorientation axes in specimen ref



MDF of grain boundaries
in crystal coordinates

MDF Misorientations of orientations along grain boundaries



Line = 100-70% Probability

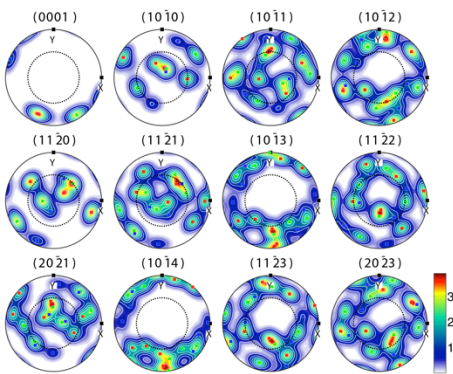
Colour dots on MDF sections are hexagonal Ice CSL boundary misorientation axes
Note all PF misorientation axes and MDF IPF of axes are data,
except MDF section at $\omega=30^\circ$

Z6 T = 4680 minutes

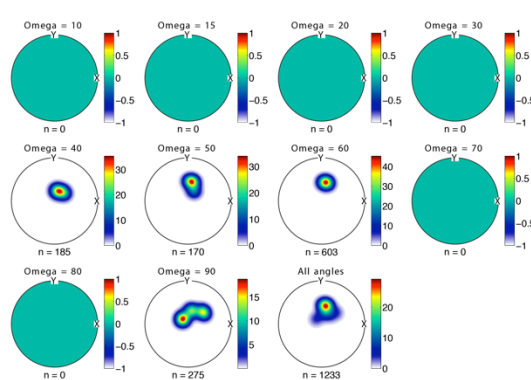
Note many PF misorientation axes and MDF IPF of misorientation axes are empty

Z6 Deformed Sample : T=4680m

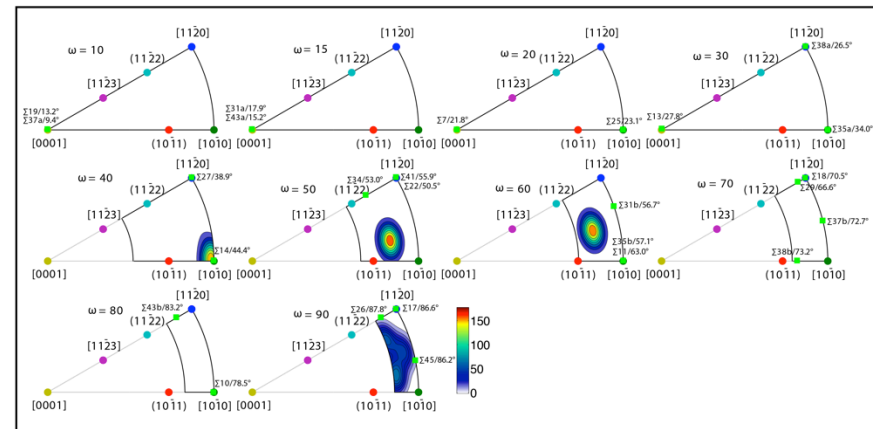
Pole figures of orientations in boundary regions



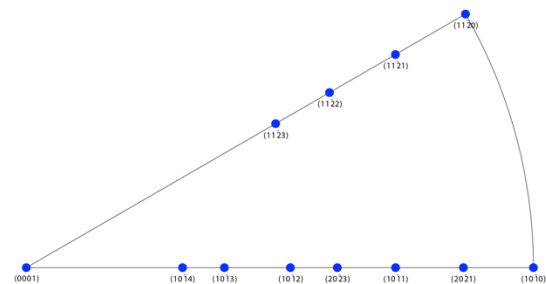
Pole figures misorientation axes in specimen ref



MDF Misorientations of orientations along grain boundaries



Planes with d-spacing greater than 1.5 Angstroms - should be habit planes



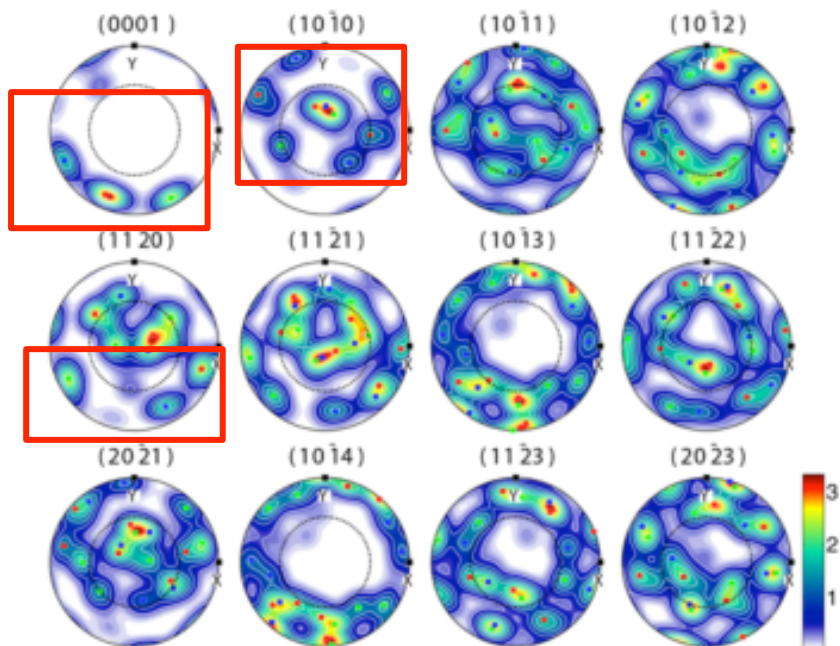
Z6 : PFs of potential boundary planes

1. Very little evolution of the potential boundary planes; except $c(0001)$ $m(10\bar{1}0)$, $a(11\bar{2}0)$, ... ?

2. **Little evolution of boundary planes during annealing, a common observation**

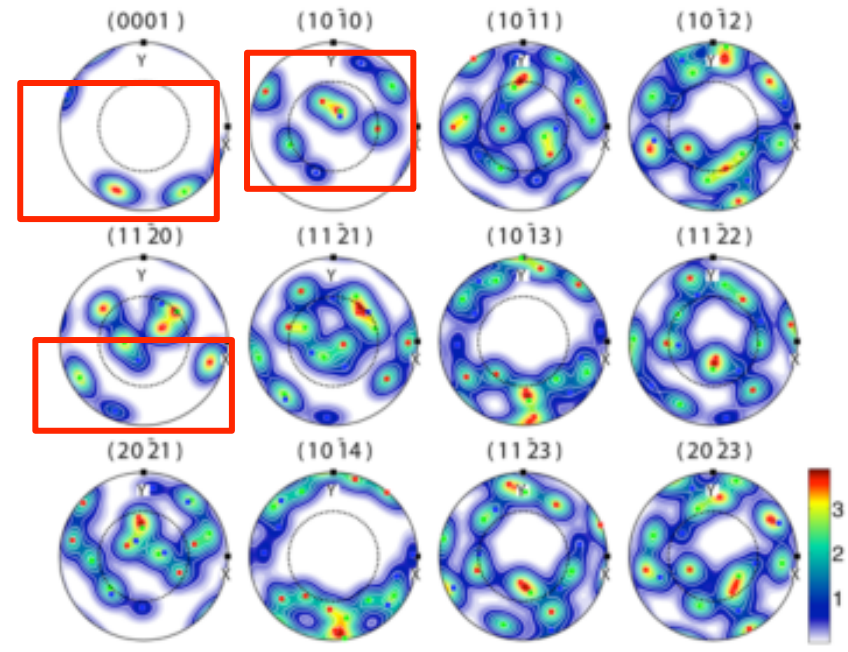
T = 0 minutes

Pole figures of orientations in boundary regions



T = 4680 minutes

Pole figures of orientations in boundary regions



The most common boundary planes in hexagonal symmetry are $m(10\bar{1}0)$, $c(0001)$, $a(11\bar{2}0)$. In this sample likely grain boundary planes are have pole normal to Z on edge of pole plots.

Z6 : PFs of boundary misorientation axes

1. The misorientation axes parallel to surface normal Z often preserved
2. Only 3 out of 7 axes parallel Z are not preserved at 4680 minutes.
3. Preserved axes parallel to Z have misorientations of $40^\circ, 50^\circ, 60^\circ$ or 90°
4. All axes normal to Z are eliminated.
5. Last pole figure for all misorientation angles gives summary plot

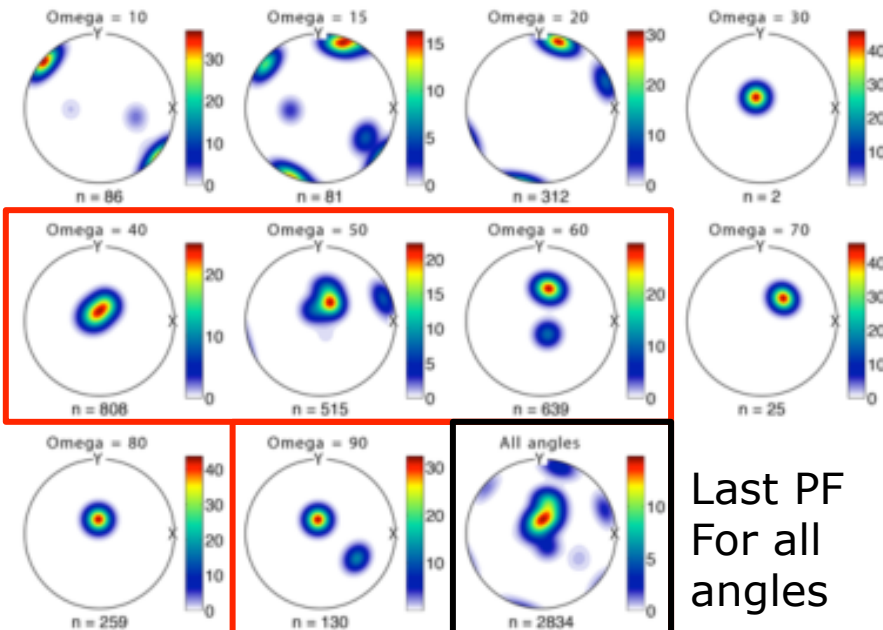
T = 0 minutes

T = 4680 minutes

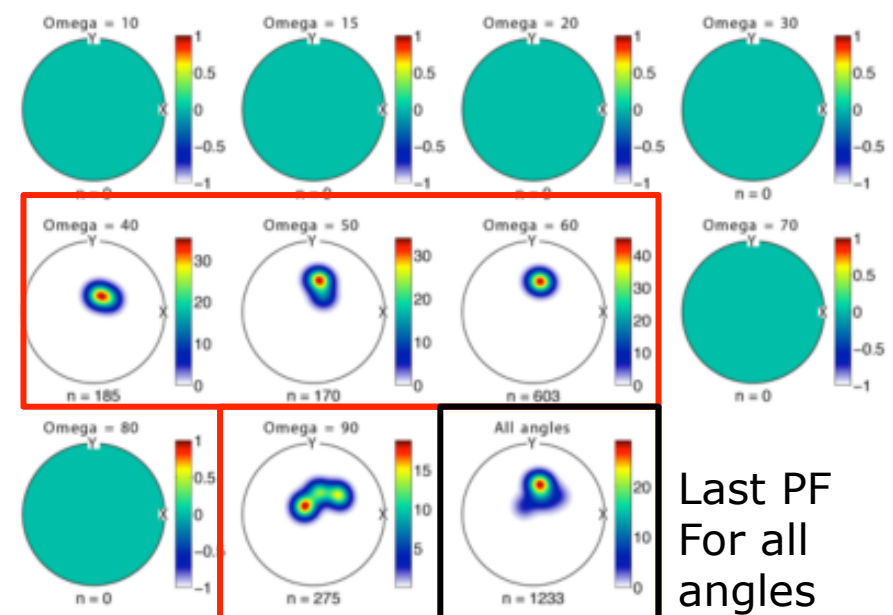
Pole figures misorientation axes in specimen ref

Pole figures misorientation axes in specimen ref

N.B. 'Pole figures' correspond to different misorientation angles



Last PF
For all
angles



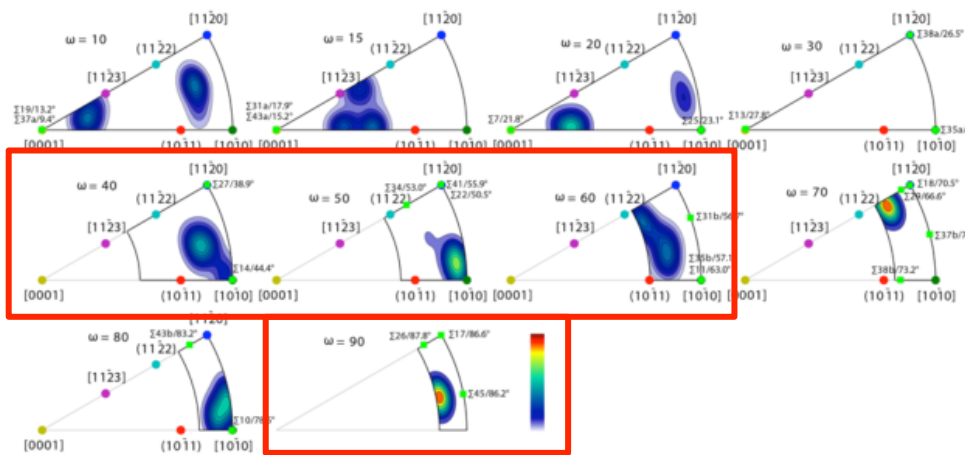
Last PF
For all
angles

Z6 : MDF of boundary misorientation axes

1. At T=0 Misorientation angles are present for all angles except 30°
2. At T=4680 only angles of 40° 50° 60° and 90°
3. At T=4680 misorientation axes m[10-10]/40°; a intermediate direction near m[10-10] and r(10-11) with 50° and 60°, and spread of orientations near the basal plane with 90°.

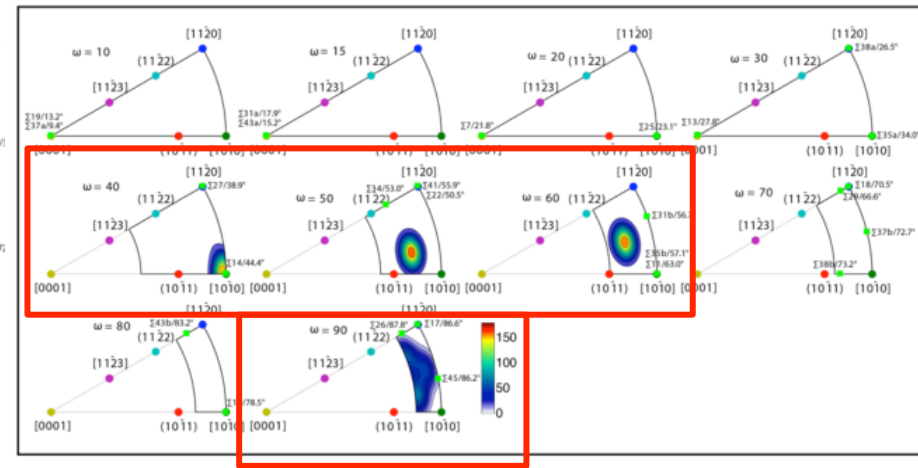
T = 0 minutes

MDF Misorientations of orientations along grain boundaries



T = 4680 minutes

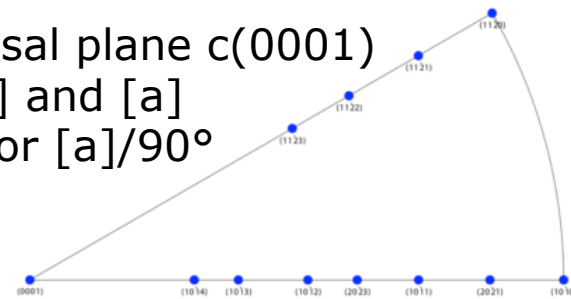
MDF Misorientations of orientations along grain boundaries



Planes with d-spacing greater than 1.5 Angstroms - should be habit planes

Red box misorientations present at T= 4680

4. Preserved misorientation axes are near the basal plane c(0001)
5. So misorientation axes are near directions [m] and [a]
6. Common in hexagonal are [m]/90° & lesser for [a]/90°



Summary of global analysis

- **Specimen coordinates** : Potential grain boundary planes do not evolve significantly with annealing. (c),(m) or (a) are the mostly likely planes.
- **Specimen coordinates** : The misorientation axes preserved at T=4680 minutes is parallel to Z, which is also perpendicular to likely boundary planes (c),(m) or (a). A misorientation axis (vertical) in the boundary plane (normal horizontal) is called a pure tilt boundary geometry.
- **Crystal coordinates** : MDF indicates misorientation axes are near the basal plane [m]- or [a]-axes are likely candidates. A twist boundaries [m]/90° with plane (m), which is very common in hexagonal could be present.
- **A probably global solution** : would be a pure tilt boundaries with a misorientation of [a]/90° and boundary plane of (0001). The (0001) plane is also the plane that displays the most evolution in sample coordinates during annealing.

Burger phase relationships

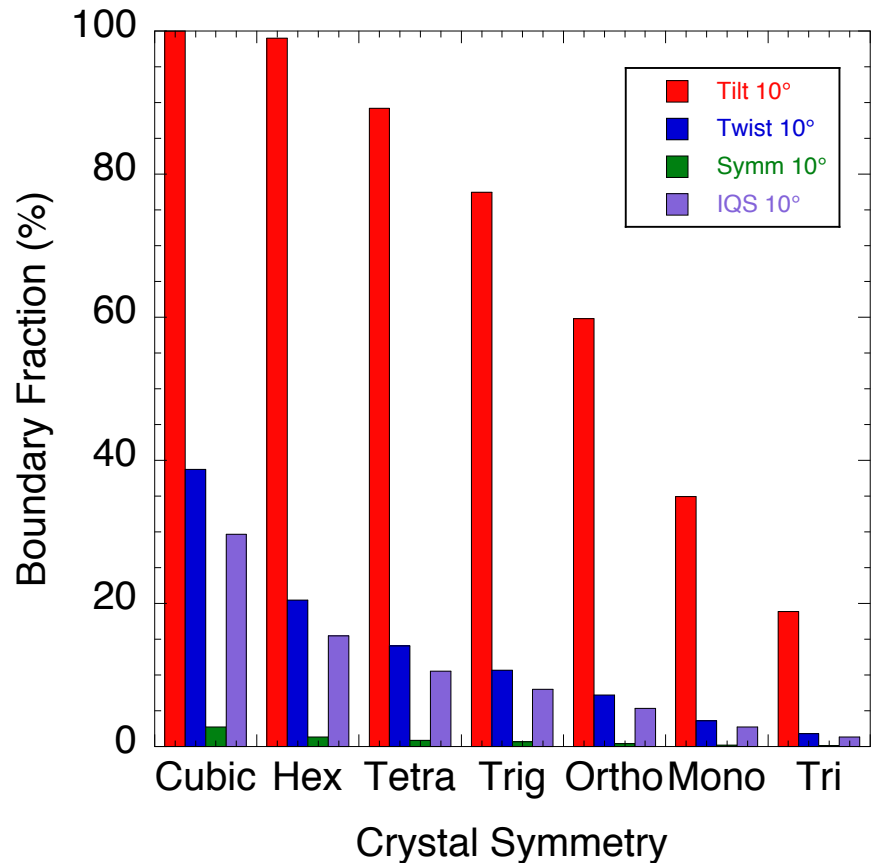
Number	Olivine	Antigorite	axis/angle
• No.1	(100)ol	(001)atg	[12 -6 10]/119.33°
•	[001]ol	[001]atg	* [-12 6 0]/120.67°
• No.2	(010)ol	(001)atg	[-1 0 0]/90.01°
•	[001]ol	[010]atg	*none
• No.3**	(100)ol	(010)atg	[-12 -6 0]/119.33°
•	[001]ol	[010]atg	*[-12 -6 0]/120.67°
• No.4**	(010)ol	{210}atg	[-5 9 0]/93.00°
•	[100]ol	[001]atg	* [5 -9 0]/94.13°

*Equivalent by symmetry for orthorhombic-monoclinic symmetry of olivine to antigorite phase transition.

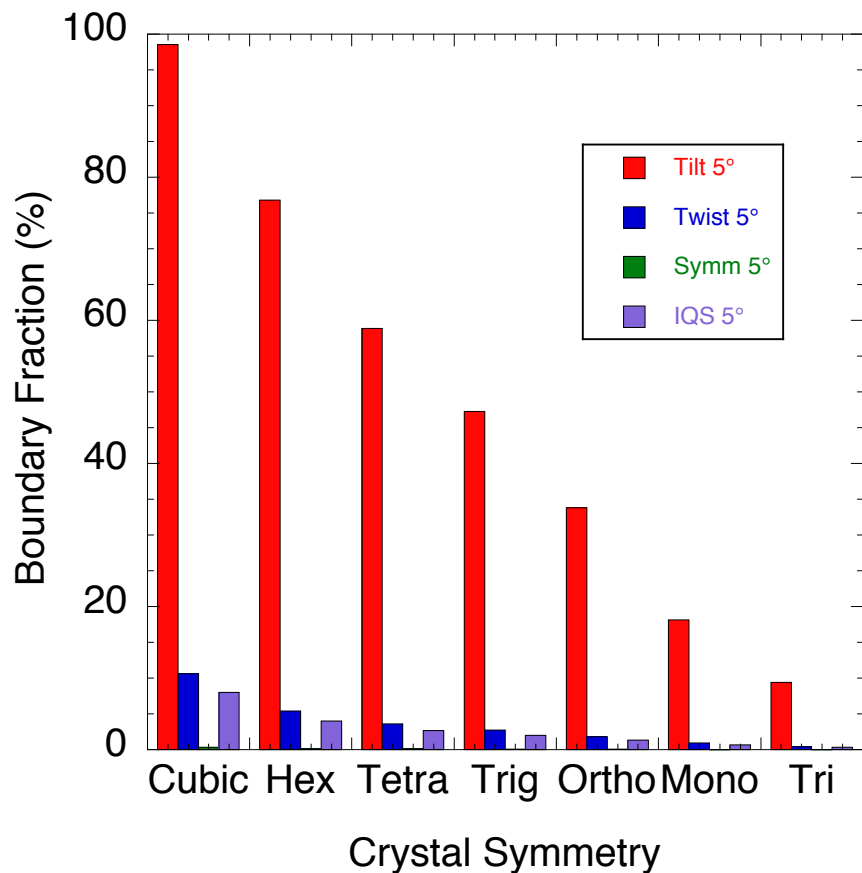
** Not previously reported by Boudier et al. [2009]

Effect of crystal symmetry on geometric characteristics of random grain boundaries

Accurate angles to pure boundaries within tolerance of $\delta=10^\circ$



Accurate angles to pure boundaries within tolerance of $\delta=5^\circ$



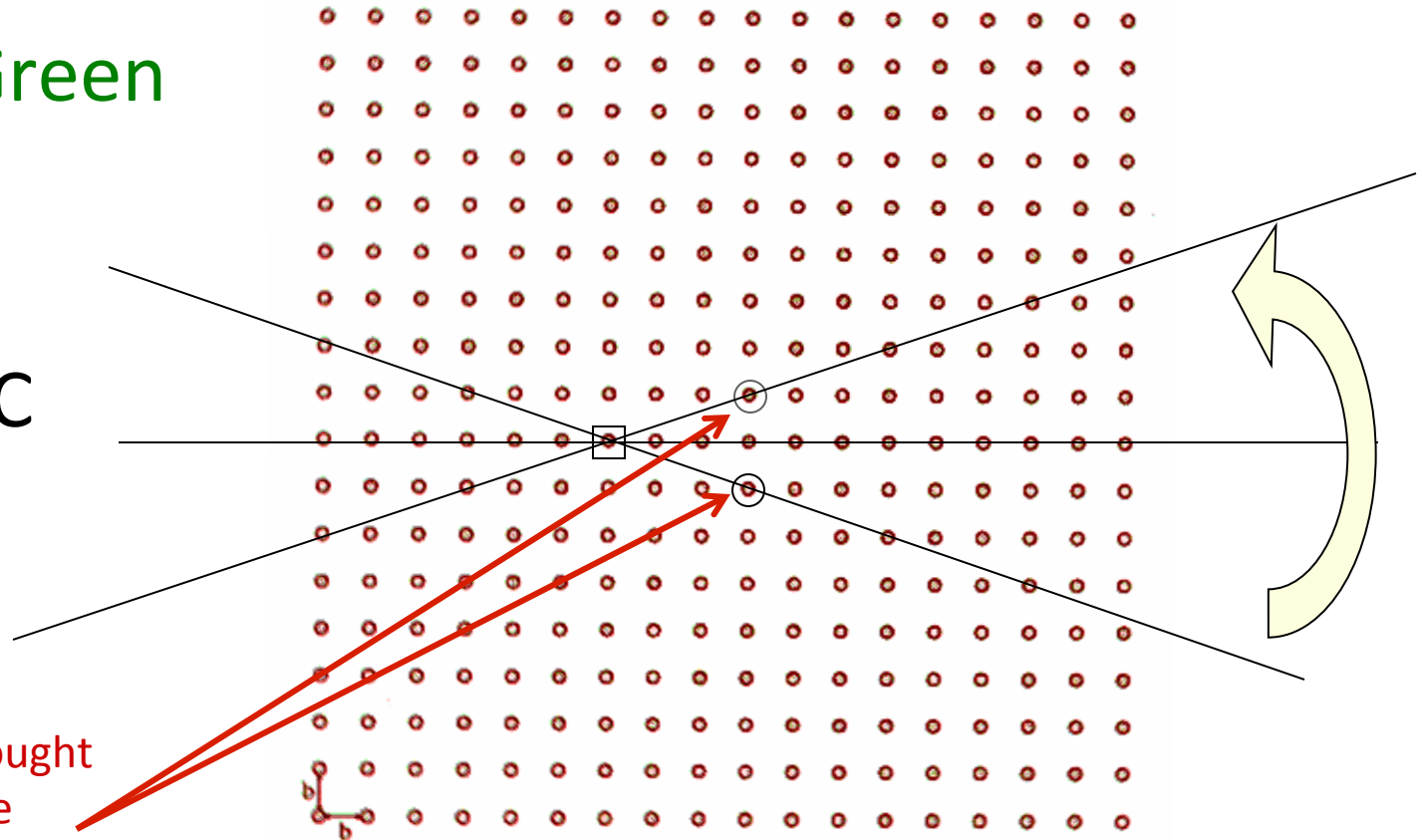
IQS =properly (improperly) quasi-symmetric

Work in progress with Adam Morawiec and Krzysztof Glowinski

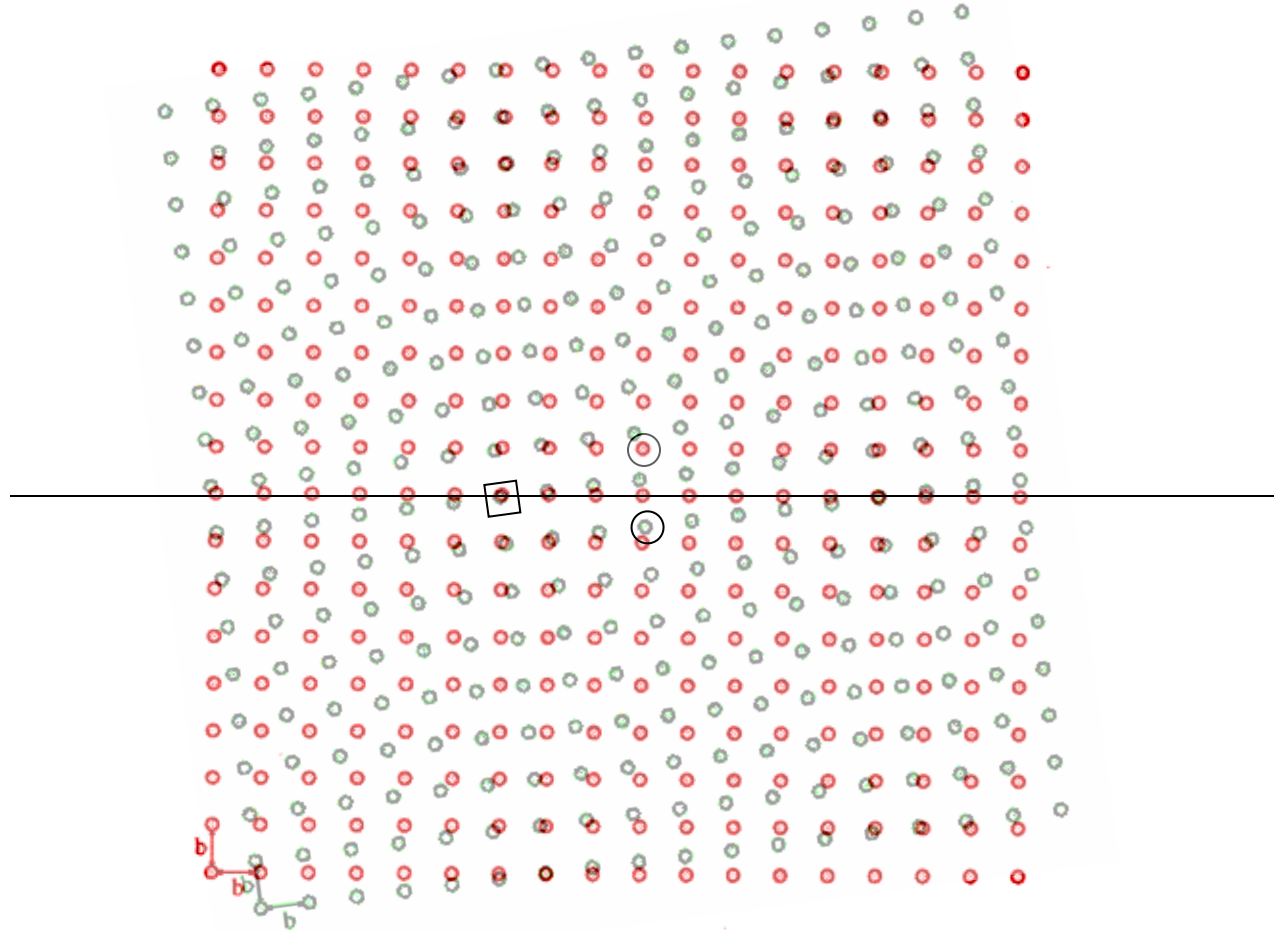
Rotation to Coincidence $\Sigma 5$

Red and Green
lattices
coincide
Cubic : FCC

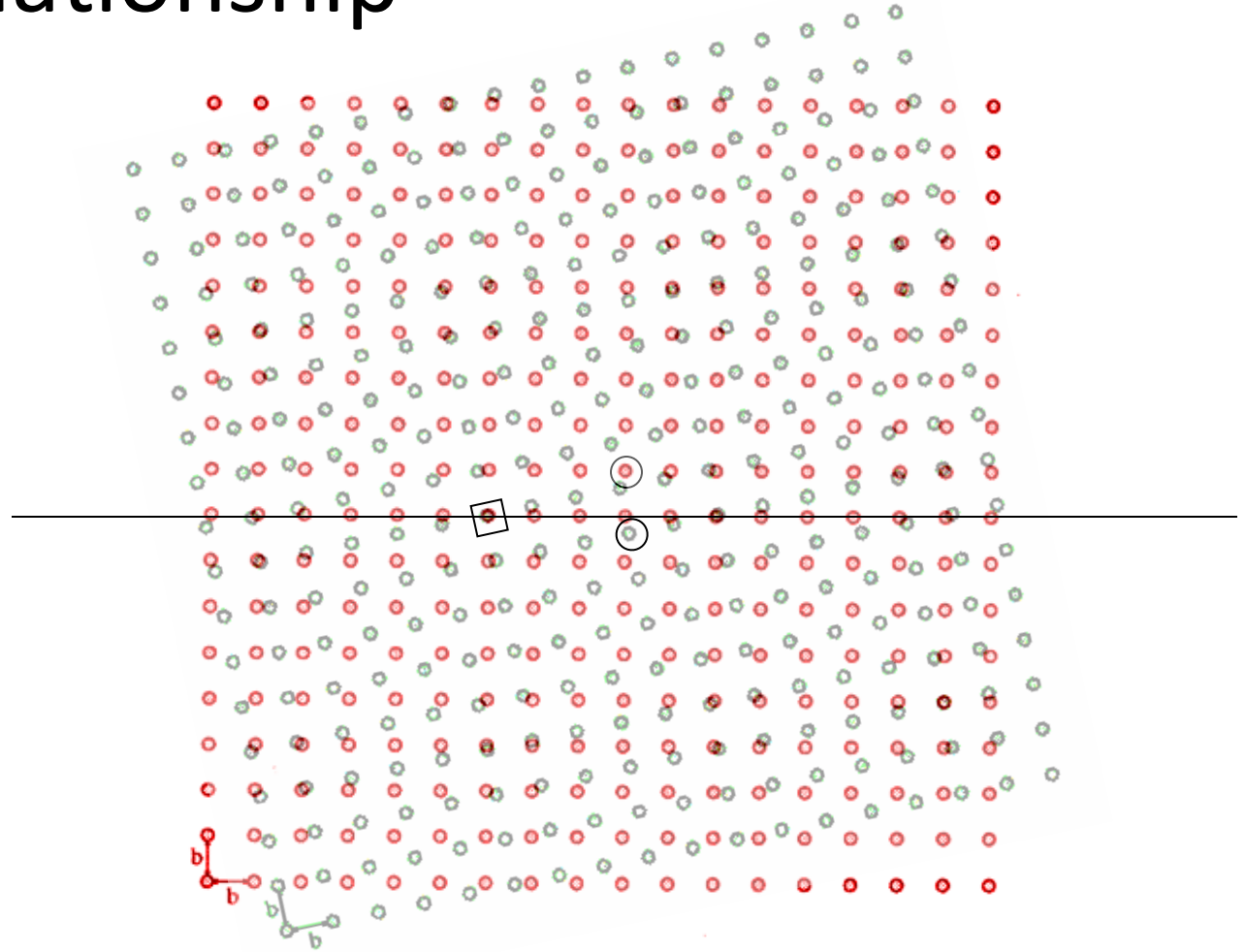
Points to be brought
into coincidence



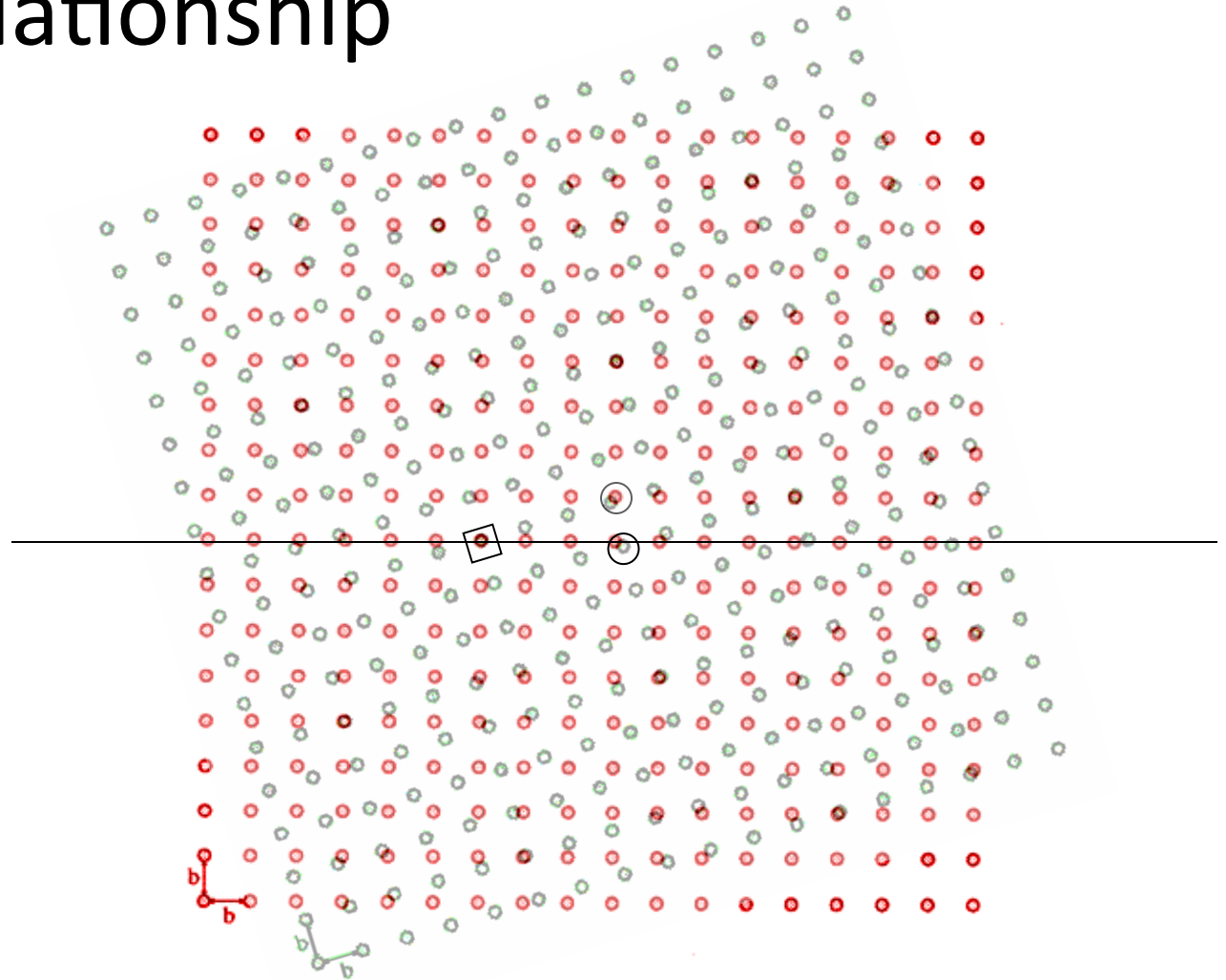
rotating to the $\Sigma 5$ relationship



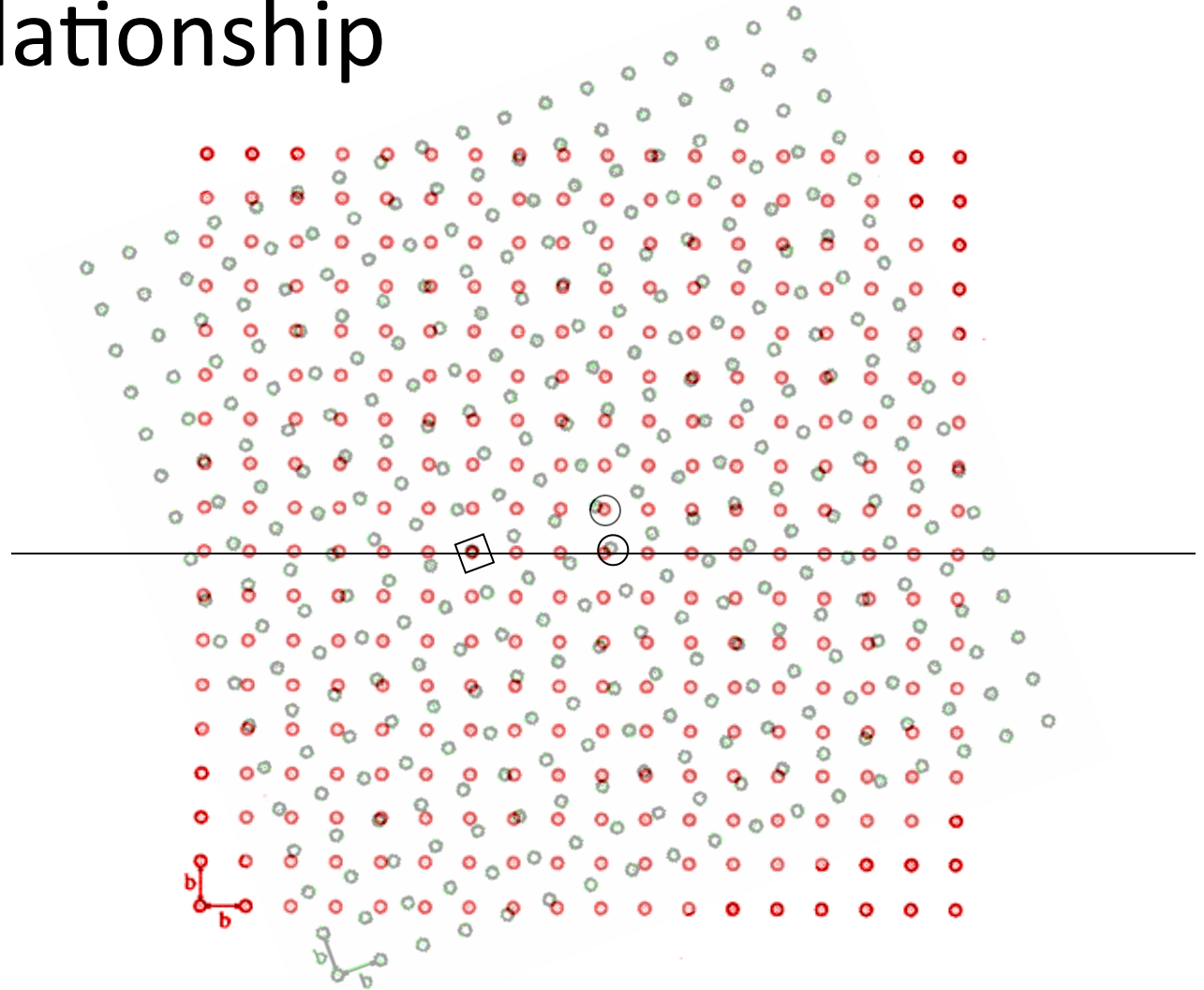
rotating to the $\Sigma 5$ relationship



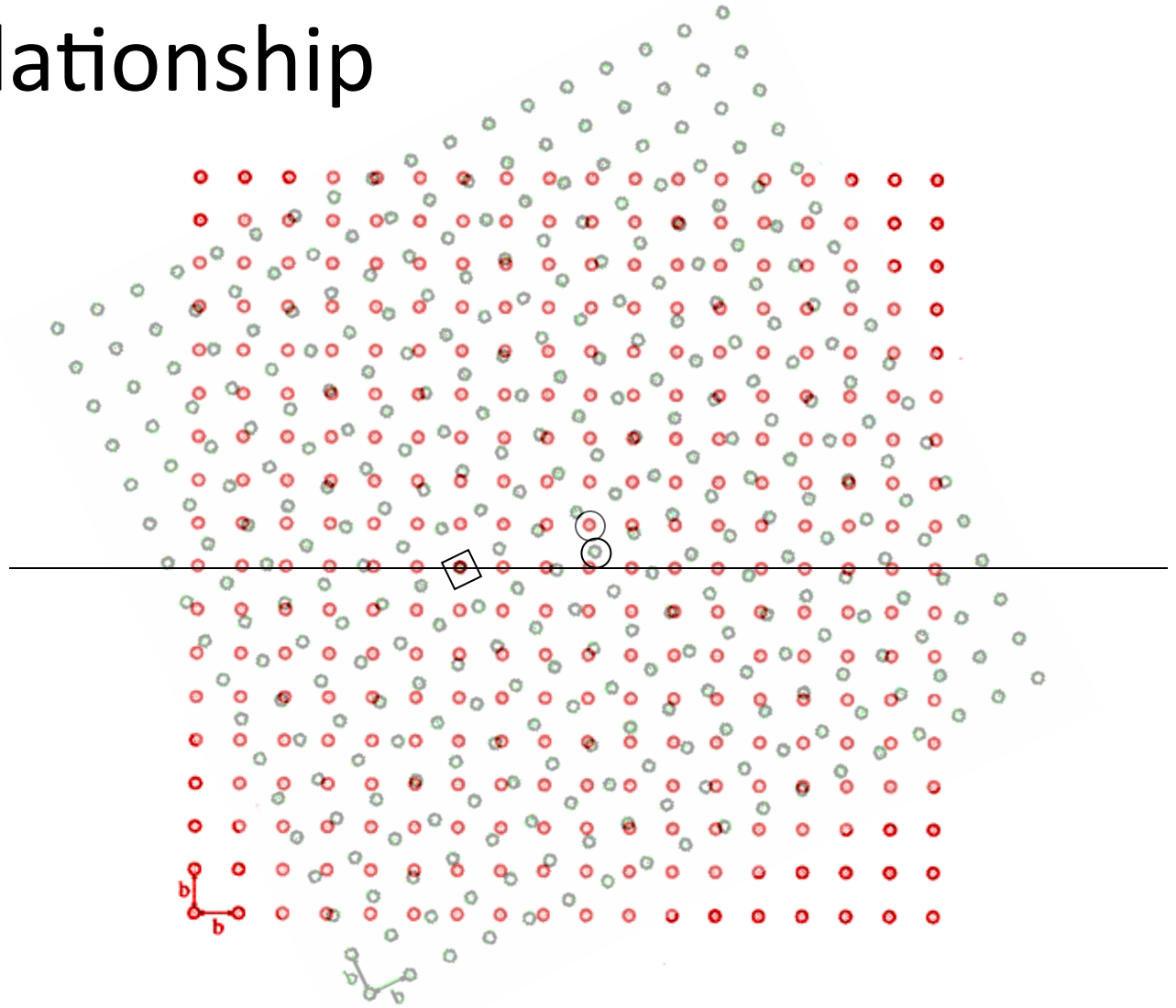
rotating to the $\Sigma 5$ relationship



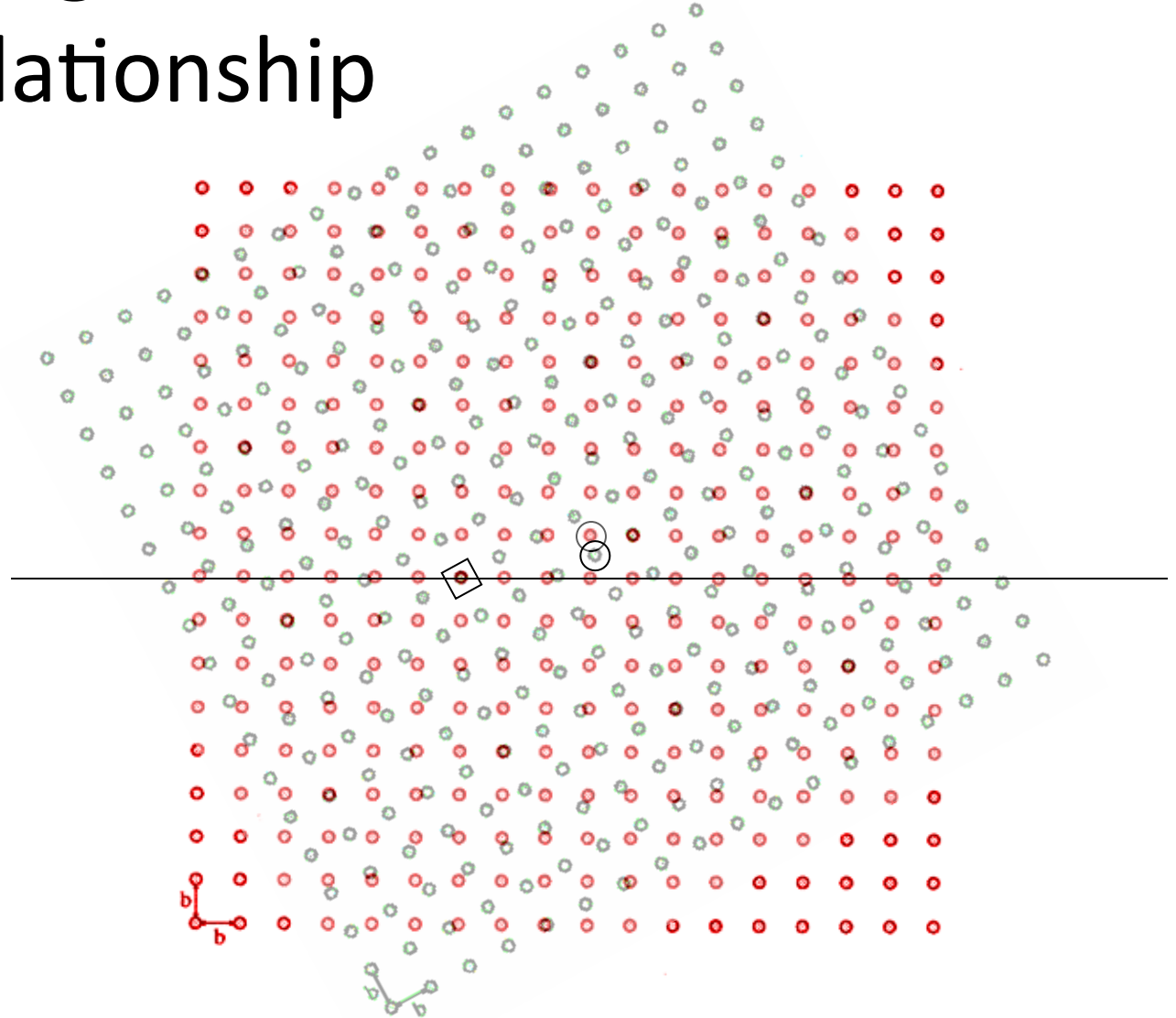
rotating to the $\Sigma 5$ relationship



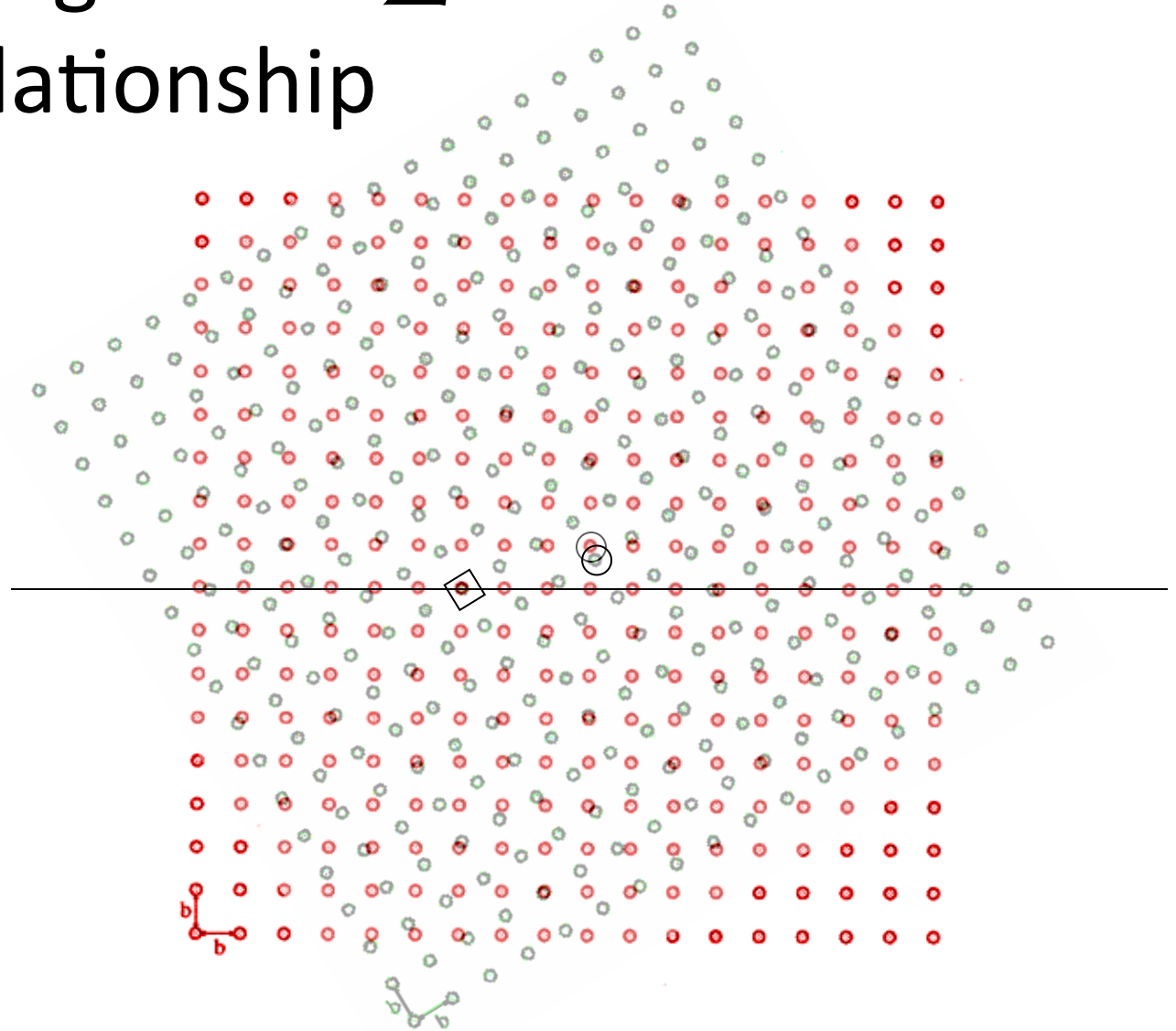
rotating to the $\Sigma 5$ relationship



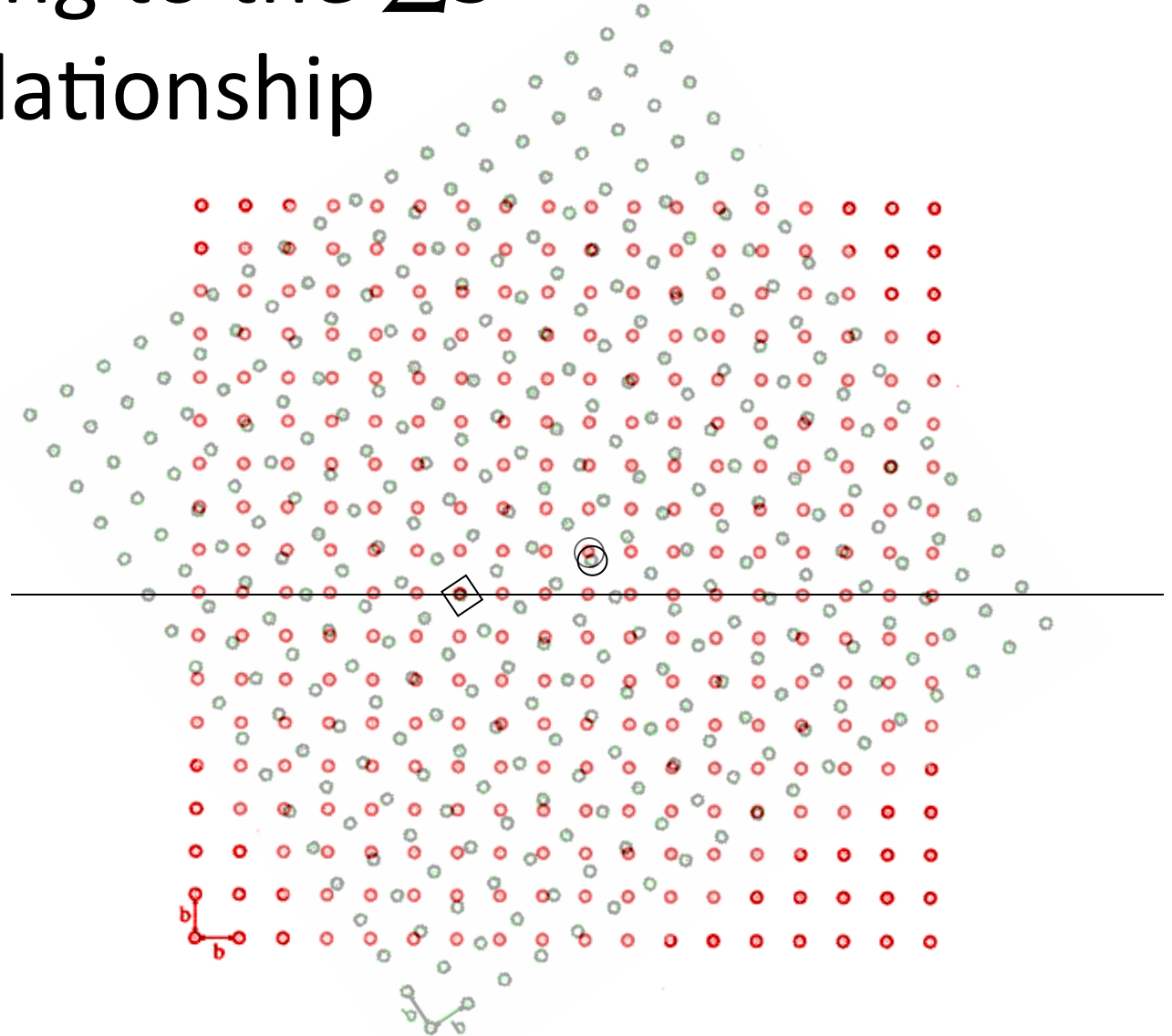
rotating to the $\Sigma 5$ relationship



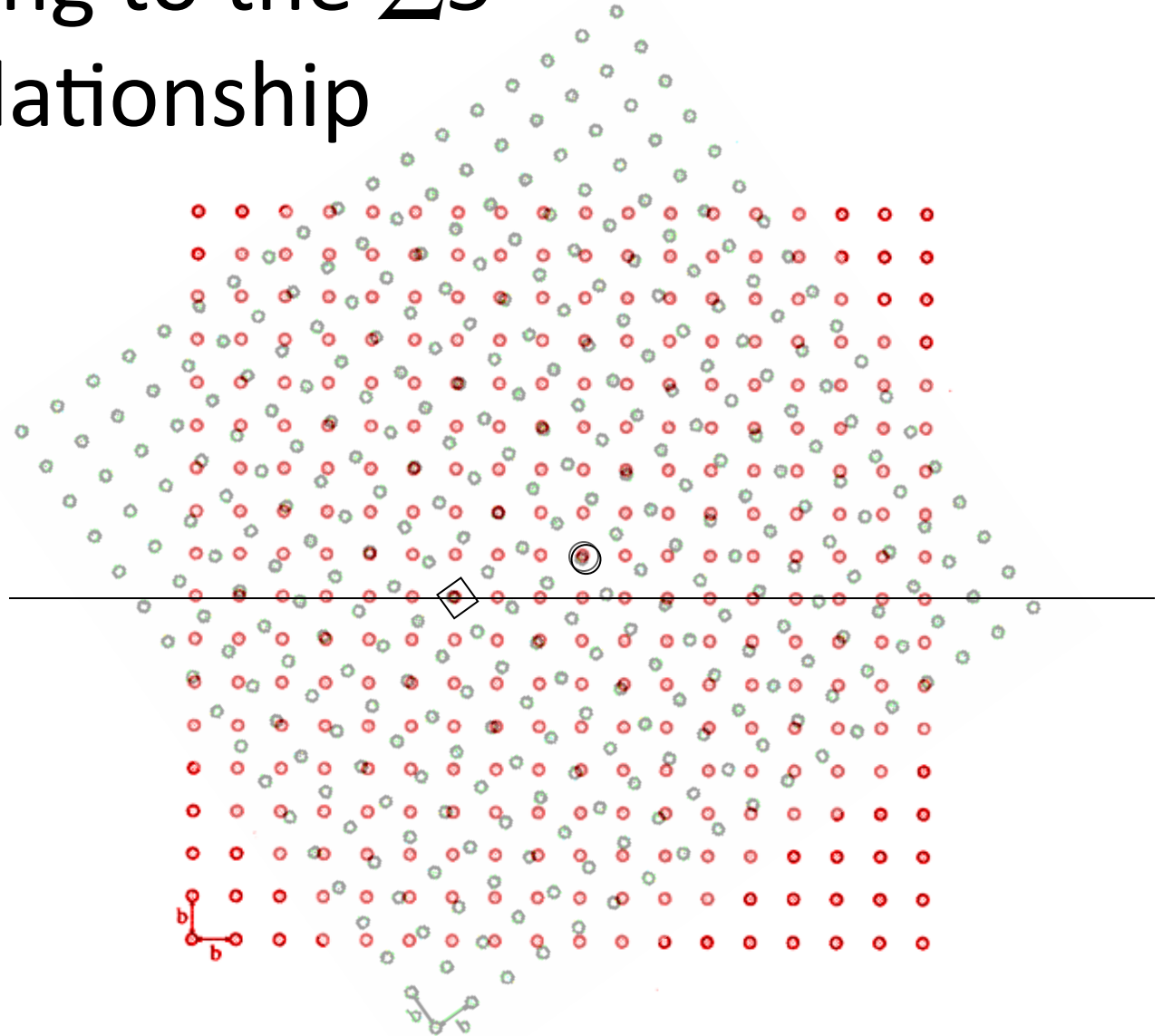
rotating to the $\Sigma 5$ relationship



rotating to the $\Sigma 5$ relationship



rotating to the $\Sigma 5$ relationship



$\Sigma 5$ relationship

STOP!

Red and Green
lattices
coincide
after rotation
of
 $2 \tan^{-1} (1/3)$
 $= 36.9^\circ$

