Analysis of EBSD Data

27-750
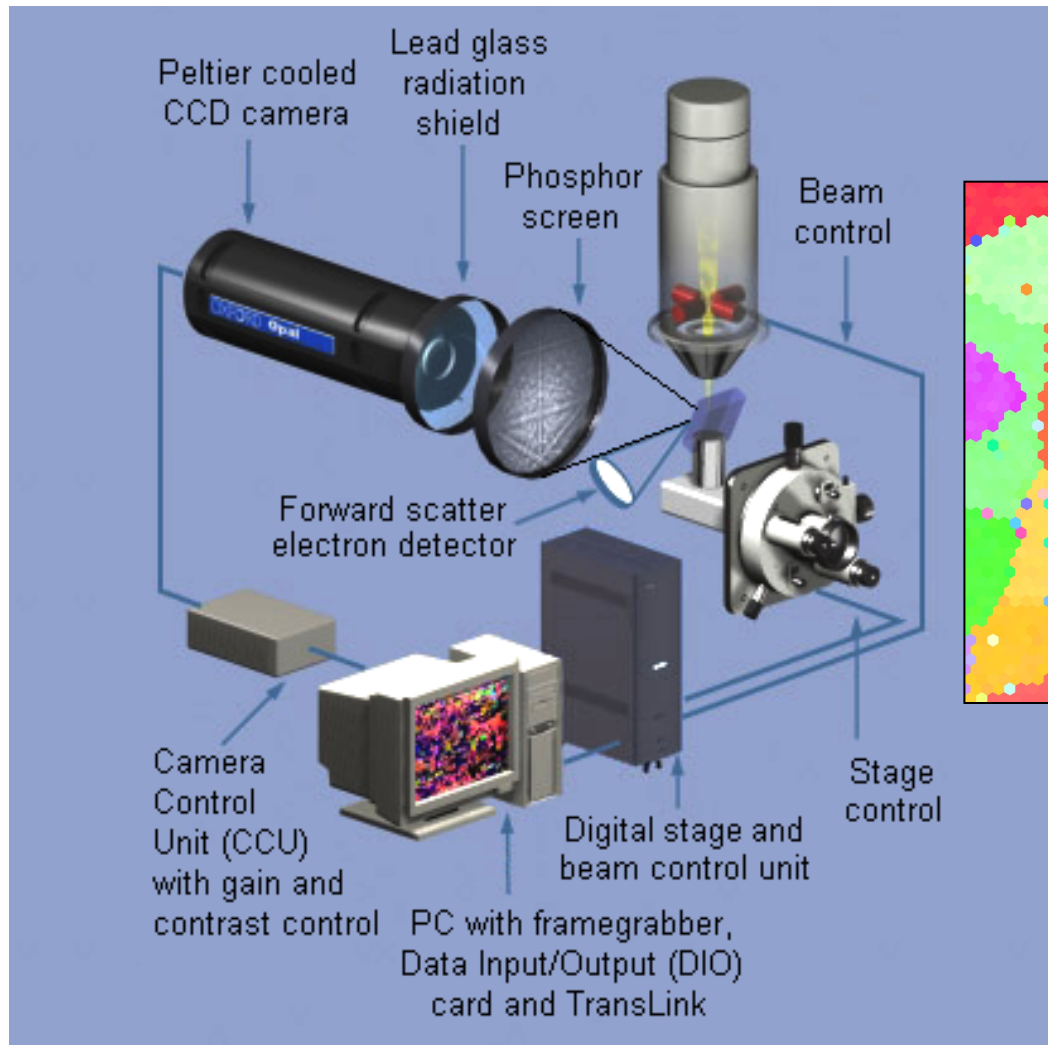
Texture, Microstructure & Anisotropy

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G.S. Rohrer, P.N. Kalu[1], T. Bennett[2],
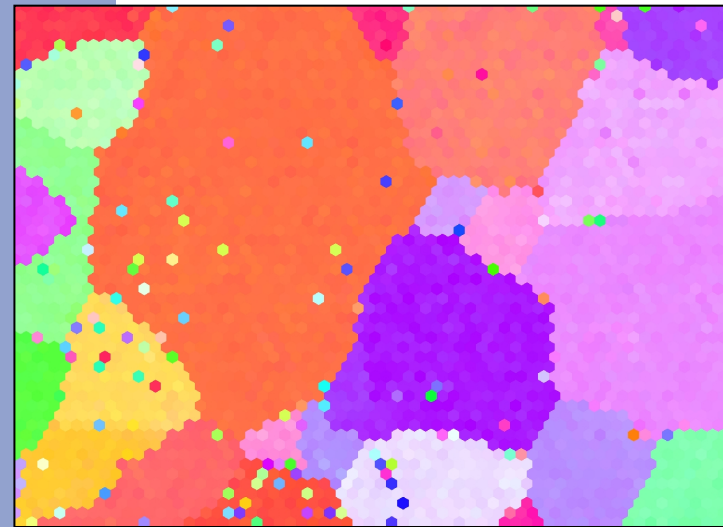N. Bozzolo[3] and F. Wagner[4]

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Electron Back-Scatter Diffraction (EBSD/OIM)

Schematic diagram of a typical EBSD system (Oxford INCA)

Provides (2D regular grid) maps of crystal orientation from polished cross-sections

Adams, B., K. Kunze and S. I. Wright (1993) *Metall. Mater. Trans.* **24A**: 819

Overview

- Understanding the program:
  - Important menus
  - Definition of Grains in OIM
  - Partitioning datasets
- Cleaning up the data:
  - Types
  - Examples of Neighbor correlation
  - *Importance of reporting clean-up in reports*
- Orientation:
  - System Definition
  - Distribution Functions (ODFs)
  - Plotting ODFs

Overview

- Misorientation:
    - Definitions - Orientation vs. Misorientation
    - Distribution Functions (MDFs)
    - Plotting MDFs
- Other tools:
    - Plotting Distributions
    - Interactive tools
- Frames of Reference:
    - Spatial versus Euler frames
    - Different suppliers of software
    - Issues with Hexagonal materials
- Important: the menus change as the software packages are updated. Although this lecture is illustrated from (older versions of) the TSL software, similar functions area available in other EBSD analysis software. Mtex also provides a number of the analysis functions.

Questions & Answers

- How are Orientation Distributions computed?
  - The discrete orientations provide the input data to which the coefficients of the generalized spherical harmonic functions are fitted.

- What is the difference between a discrete plot and a contour plot and when should I use them?
  - The discrete plots provide individual points in pole figures, inverse pole figures, ODs etc. Contour plots are always based on the fitted generalized spherical harmonic functions.

- What is meant by the various different measures of orientation spread within a grain, and what are they useful for?
  - The names given to the functions vary across the packages. There is a pixel-based measure that computes the average of the misorientation between a given point/pixel and its first nearest neighbor points (generally, 8 NN in a square lattice); there is also an average over all points in a given grain (e.g. Grain Average Misorientation). This is sensitive to only local orientation gradients. There is also a pixel-based measure that gives the misorientation between the given point and the average orientation for the grain; likewise there is an average quantity for the whole grain. This pair of measures are sensitive to long range orientation gradients (found, e.g., in shear bands, kink bands etc.).

Questions & Answers

- Why do I have to worry about reference frames?
  - Orientations are given in reference to a frame that is different from the frame in which the coordinates of the image; see the notes for details. Different softwares have different alignments, and hexagonal materials are a particular problem because of different conventions for the alignment of the orthonormal frame used for calculation versus the crystallographic frame of reference.

- What is "clean-up"?
  - "Clean-up" is a generic term for the various steps used to remove unreliable or non-indexed points from the map and replace them with (in general) more reliable orientations from neighboring pixels. Generally speaking, the methods are analogous to "erosion" and "dilation" used in image processing.

- How is the grain structure determined (slide 9)?
  - The procedure that is typically used is known as a "burn algorithm" in percolation analysis. One starts at an arbitrary pixel location and uses it as the starting point of a grain; add any nearest neighbor pixel to the grain that has a misorientation with the first point less than some user-chosen threshold. Repeat until no more points can be added according to the threshold. The largest threshold typically used is 15°, i.e. the limit for low-angle boundaries in cubic materials.

Navigating the menus
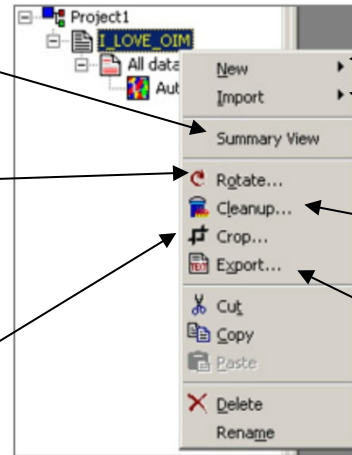
- There are two menus that access virtually everything:

Check the scan stats

Rotate the *orientations* of each point about *sample frame*

Cut out scan sections

Creates new partitions

Imports data as partitions

Access to routines that cleanup the dataset

Use this to export text .ang files

Check the partition stats & definition

Change the partition properties:
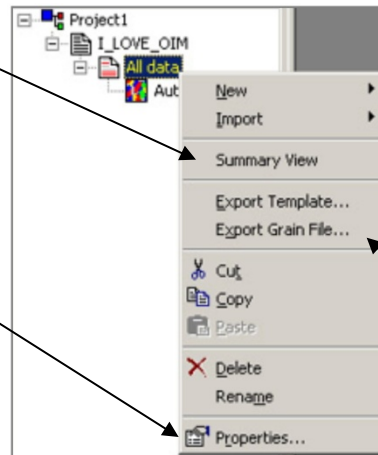- Decide which points to include
- Define a "grain"

Access to menu for:
- Maps
- Texture calculation
- Texture plots

Export grain ID data associated with each point

Grain Definitions

- OIM defines a set of points to constitute a grain if:

- A path exists between any two points (in the set) such that it does not traverse a misorientation angle more than a specified tolerance

- The number of *points* is greater than a specified number

Points with a CI less than specified are excluded from *statistics*

Partition Properties

Formula | Grain Size

Grain Tolerance Angle 5

Minimum Grain Size 2

Minimum Confidence Index 0

Apply partition before calculation ☑

Twin Boundaries
Boundaries listed will be excluded from the grain size calculation.

Plane Normal	Direction	Angle	Toler

Add   Remove
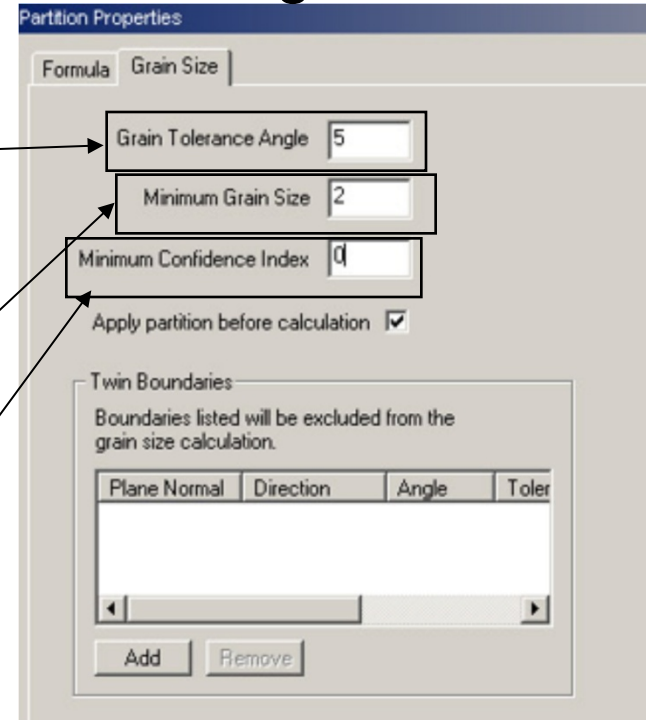
Note: Points that are excluded are given a grain ID of 0 (zero) in exported files

Grain Definitions

Examples of definitions
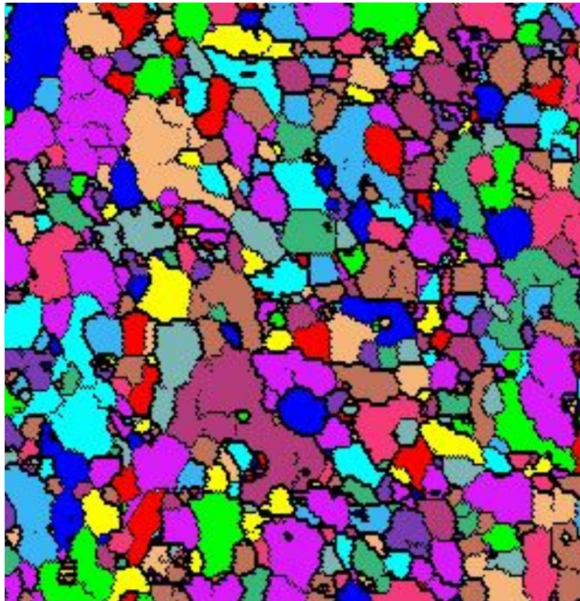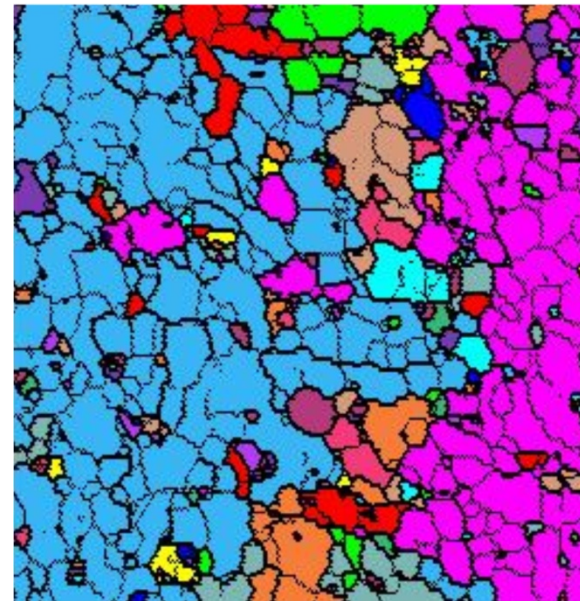
| 3 degrees | 15 degrees |

Note that each color represents 1 grain

Partitioning Datasets

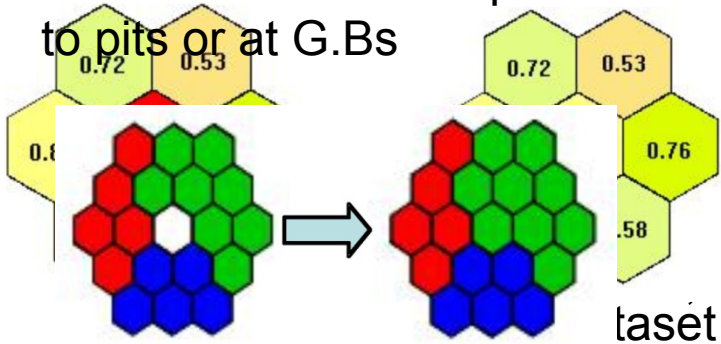- Choose which points to include in analysis by setting up selection formula

Data Cleanup

Grain Dilation:
--Acts only on points that do not belong to any grain as defined
--A point becomes part of the grain with the most number of surrounding points
--Use when majority of points are high CI and only a few bad points exist

Neighbor CI Correlation
--Performed only on points with CI less than a given minimum
--The orientation and CI of the neighbor with highest CI is assigned to these points
--Takes the orientation and CI of the neighboring point with highest CI

- Use to remove bad points due to pits or at G.Bs

Cleanup Dataset

Cleanup Type
- (•) Grain Dilation
- ( ) Grain CI Standardization
- ( ) Neighbor CI Correlation
- ( ) Neighbor Orientation Correlation
- ( ) Neighbor Phase Correlation

Grain Tolerance Angle 5
Minimum Grain Size 2
Minimum Confidence Index 0
Cleanup Level 0
Single Iteration ☐

Operation
- ( ) Cleanup inplace
- (•) Cleanup and add to project as new dataset
- ( ) Cleanup and export as new data file
  - New data file [   ] Browse
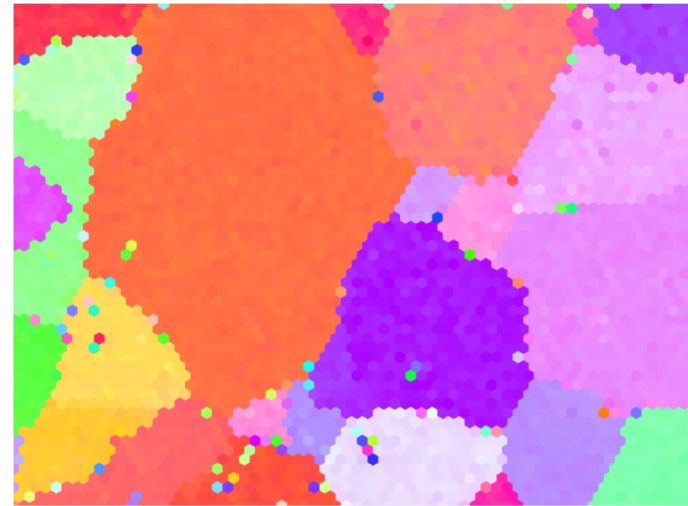
OK   Cancel

...taset
directly to file
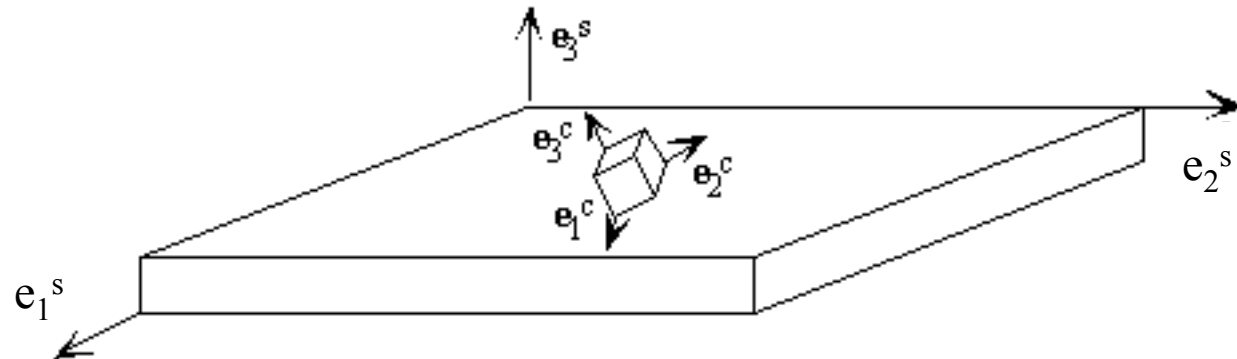
Neighbor Correlation Example
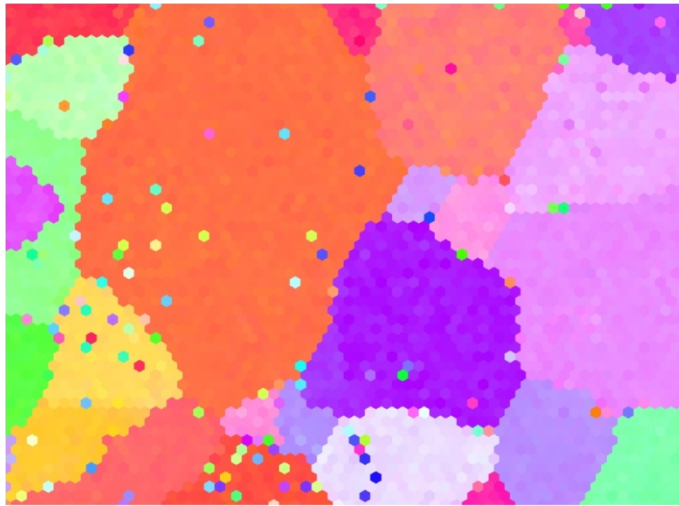
No Cleanup

Level 0

Level 3

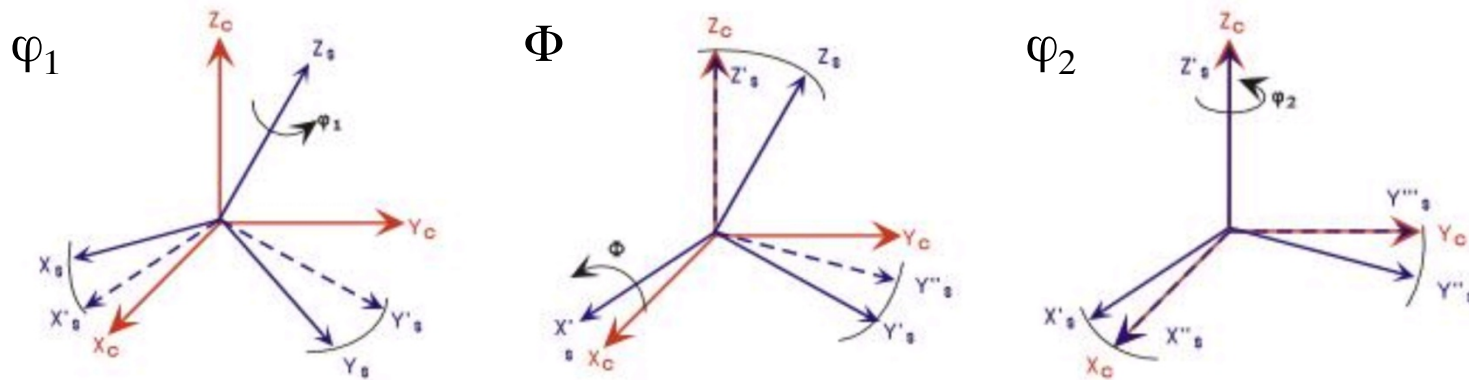Note that Higher cleanup levels are iterative (i.e. Level 3= Levels 0,1,2,3)

Definition of Orientation

- By definition an orientation is always relative. The OIM uses the sample surface to define the orthogonal reference frame.

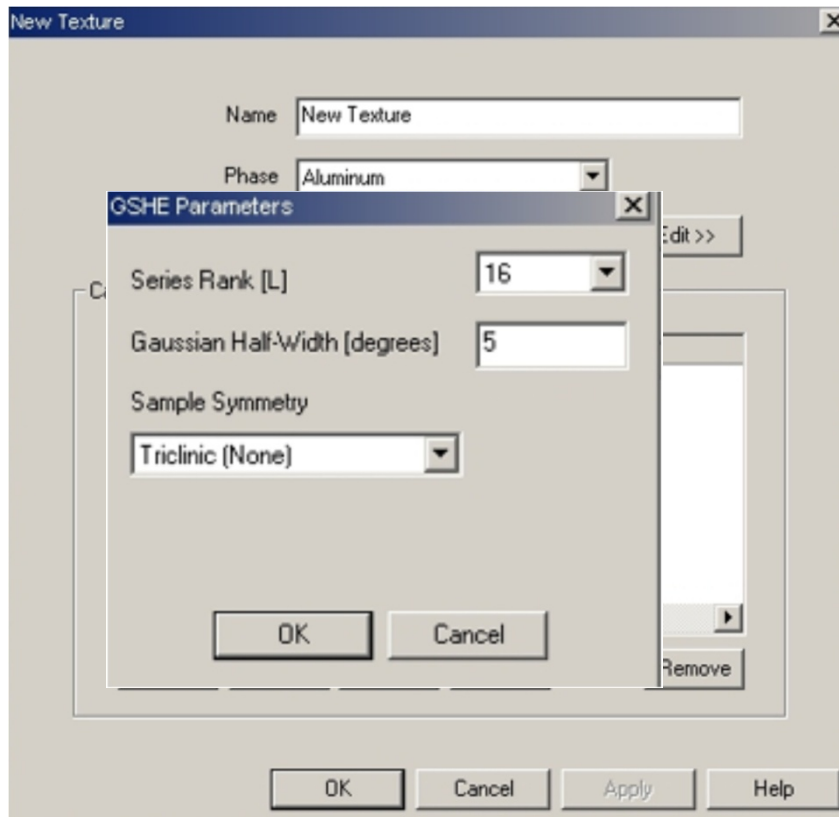- Quantities are transformed **from** sample frame to **crystal** frame

NB: a more comprehensive discussion of reference frames is given later

Orientation Distribution Functions

- The ODF displays how the measured orientations are distributed in orientation space

- Two types of distributions can be calculated:

Continuous ODF:
- Generalized Spherical Harmonic Functions: Rank defines the "resolution" of the function
- Equivalent to a Fourier transform
- Calculation time rises steeply with rank number (32 is an effective maximum)
- Time intensive
- Mostly appropriate for weaker textures
- Some smoothing is inherent

Plotting Orientation Distributions

- One must select the types of data visualization desired
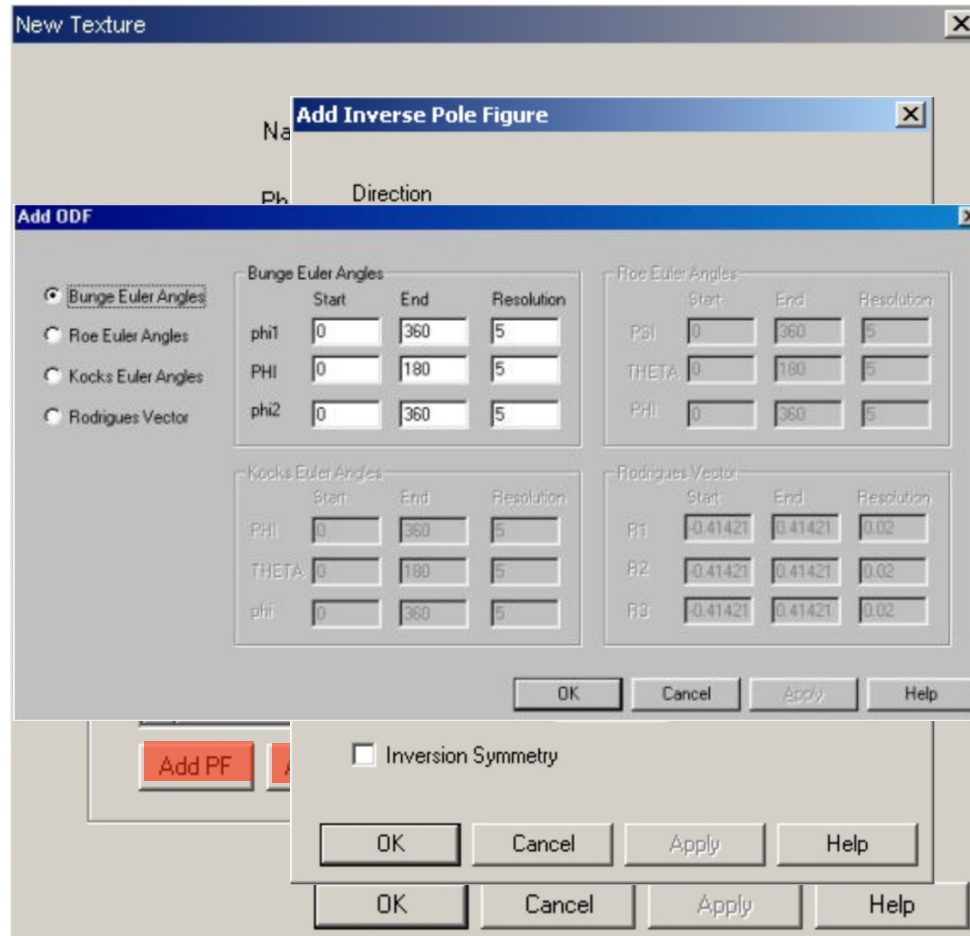
- Euler space plot shows the distribution of intensity as a function of the Euler angles
- Used to visualize pockets of texture as well as "fiber" textures
- Resolution defines how many slices are possible in the plot to be entered one at a time

Types of ODF/Pole Figure/ Inverse PF Plots
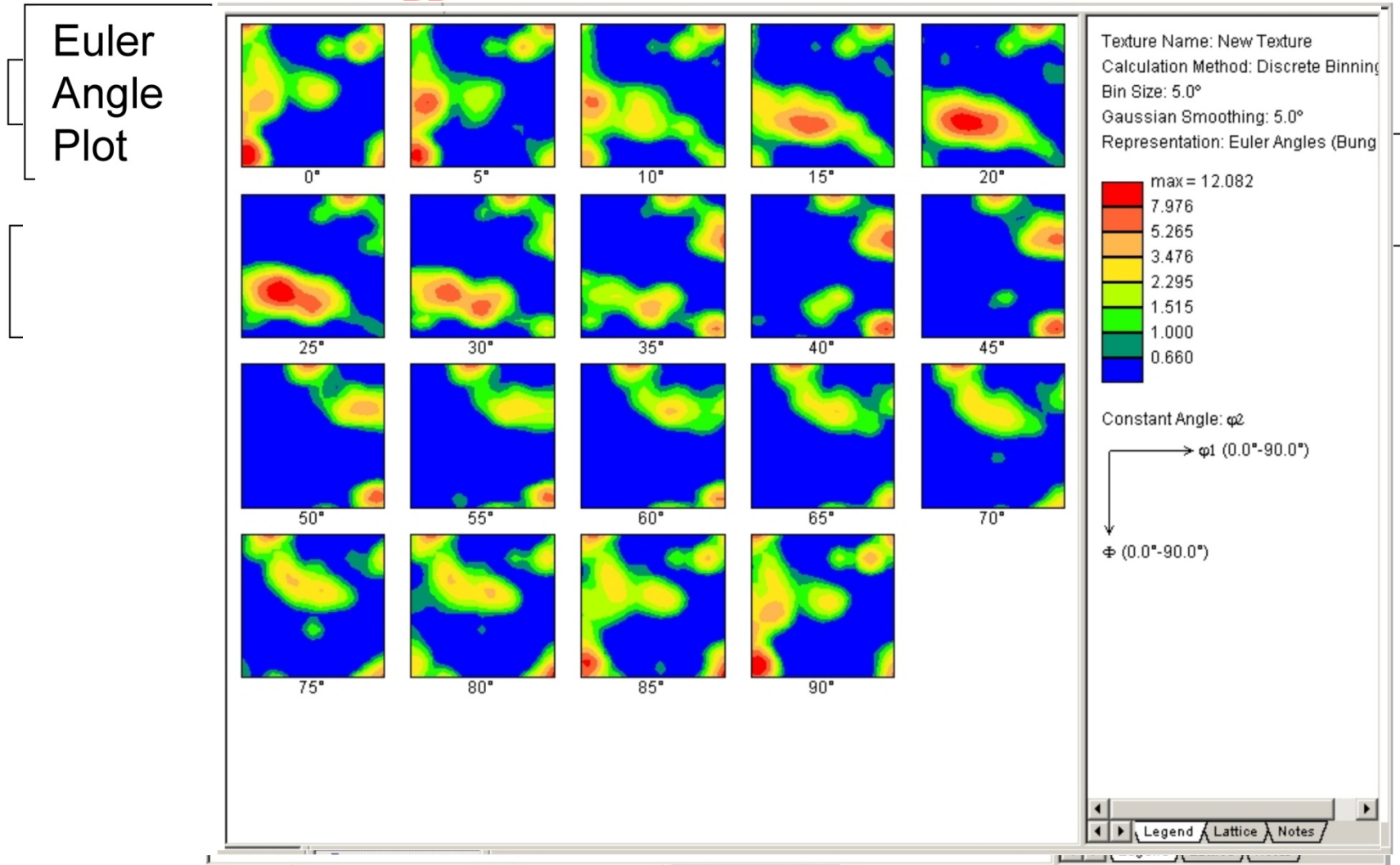
NB: a more comprehensive discussion of reference frames is given later

Preparation of the data for analysis

The *Average Orientation* of the pixels in a grain
is given by this equation:

$$\overline{q} = (q^1 + q^2 + ... + q^N)/\left\| q^1 + q^2 + ... + q^N \right\|.$$
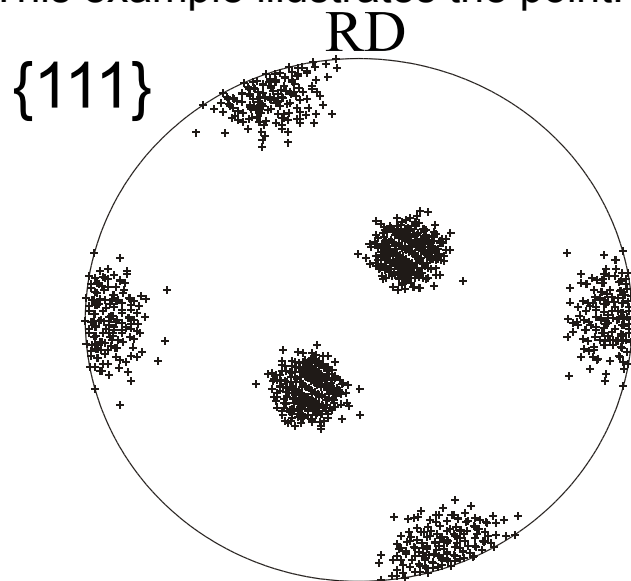
Very simple, n'est-ce pas?
However, there is a problem...
As a consequence of the crystal symmetry, there are several equivalent orientations.   *i=1,24*
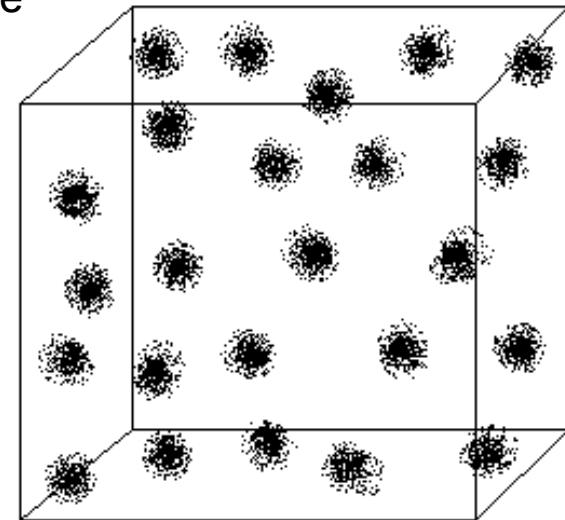This example illustrates the point:

$$M(g)_{\text{équivalent}} = M(g)_{\text{mesuré}} \left[S_i \right]_{\text{cristal}}$$
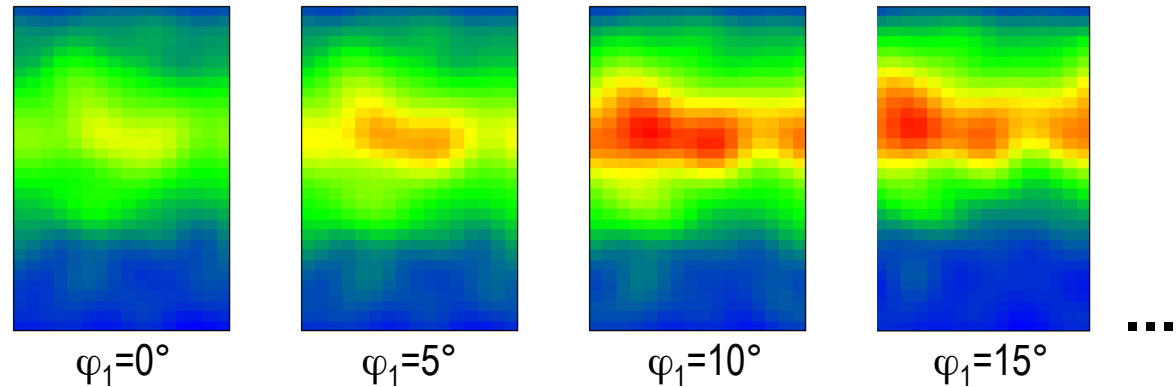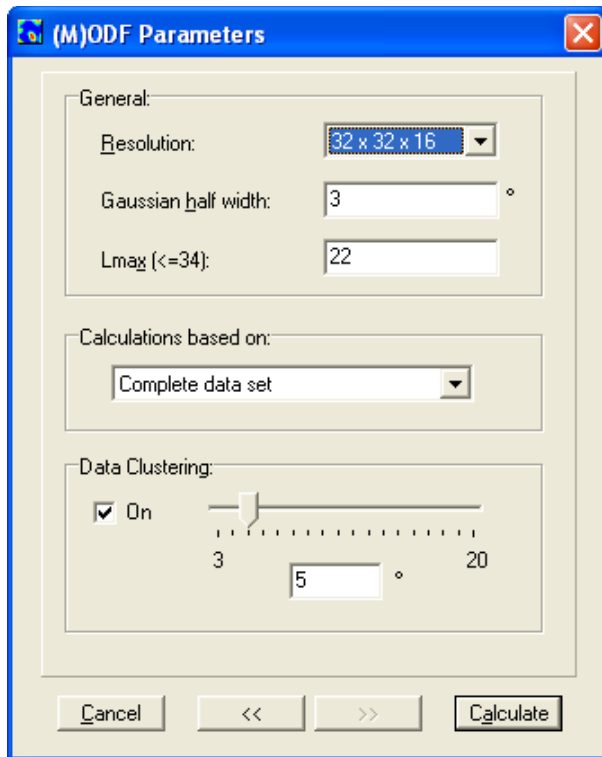
RD

{111}

10 000 orientations near to the
Brass component:

represented
• by a {111} pole figure
• and, in the complete Euler
space to show the 24
equivalents resulting from
application of cubic crystal
symmetry

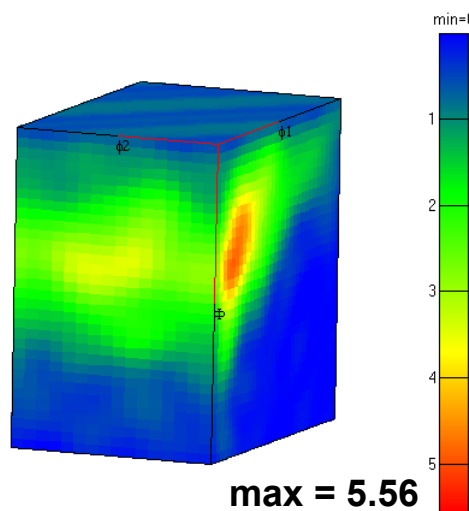Cho J H, Rollett A D and Oh K H (2005) Determination of a mean orientation in electron backscatter diffraction measurements, *Metall. Mater. Trans*. **36A** 3427-38

Parameters for texture analysis: example of Zr alloy
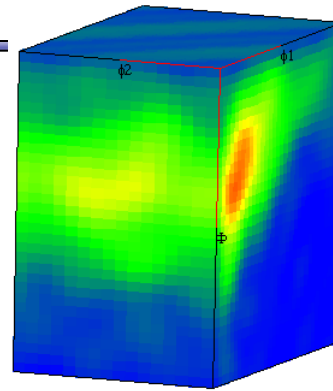

Courtesy of N. Bozzolo, CEMEF

Parameters for texture analysis

Courtesy of N. Bozzolo

Resolution   32x32x16
Gaussian   3°
L_{max} 22
Bin Size   5°

max = 5.56

Effect of the binning resolution

16x16x8
3°
22
5°
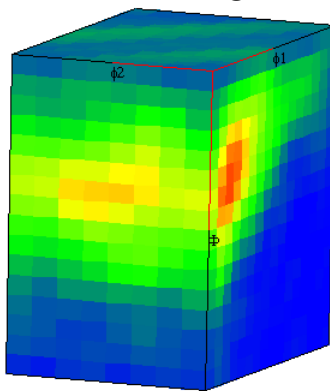
max = 5.37

Effect of the width of the Gaussian

32x32x16
8°
22
5°
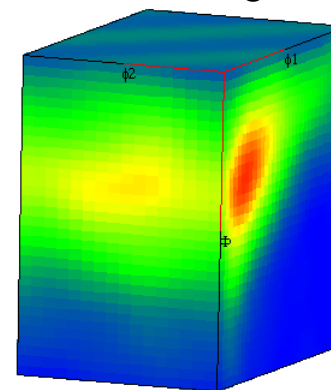
max = 4.44

Effect of the maximum rank in the series expansion, L_{max}

Resolution	32x32x16
Gaussian	3°
L_{max}	22
Bin Size	5°

L_{max} = 34

L_{max} = 22

L_{max} = 16

L_{max} = 8

L_{max} = 5

max = 6.36

max = 5.56

max = 5.17

max = 4.04

max = 2.43
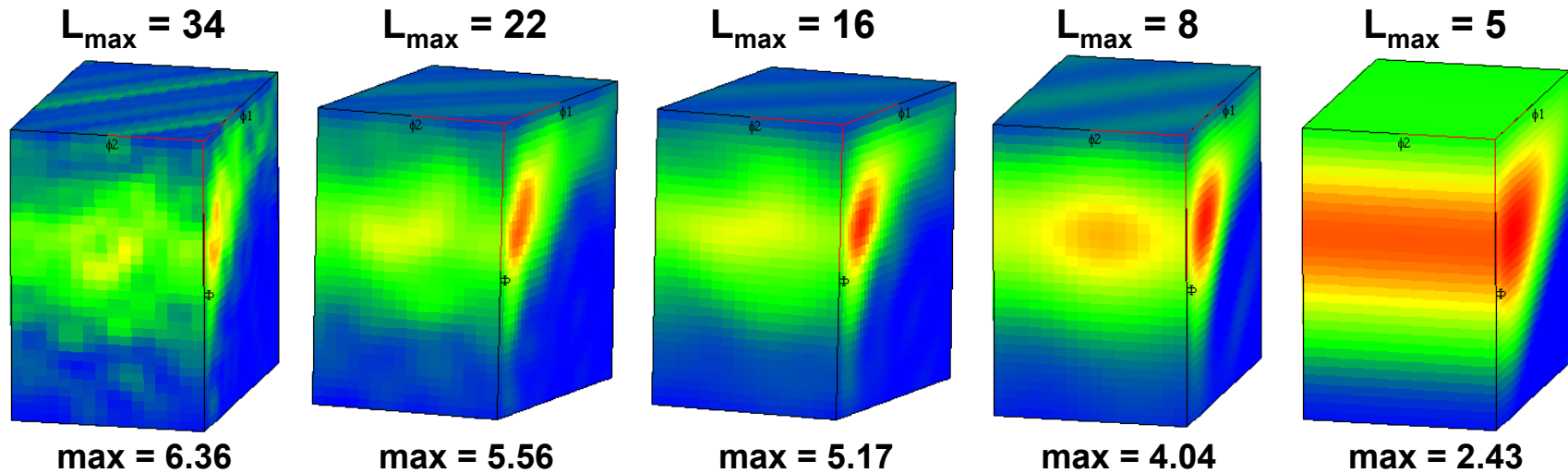
Clearly, taking the fitting to higher order (angular frequency) provides better resolution of the texture

Direct Method
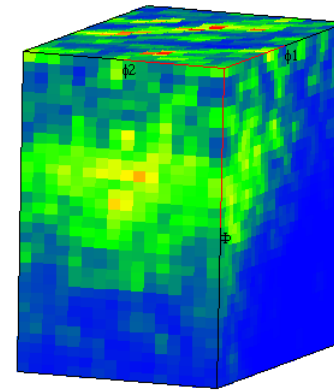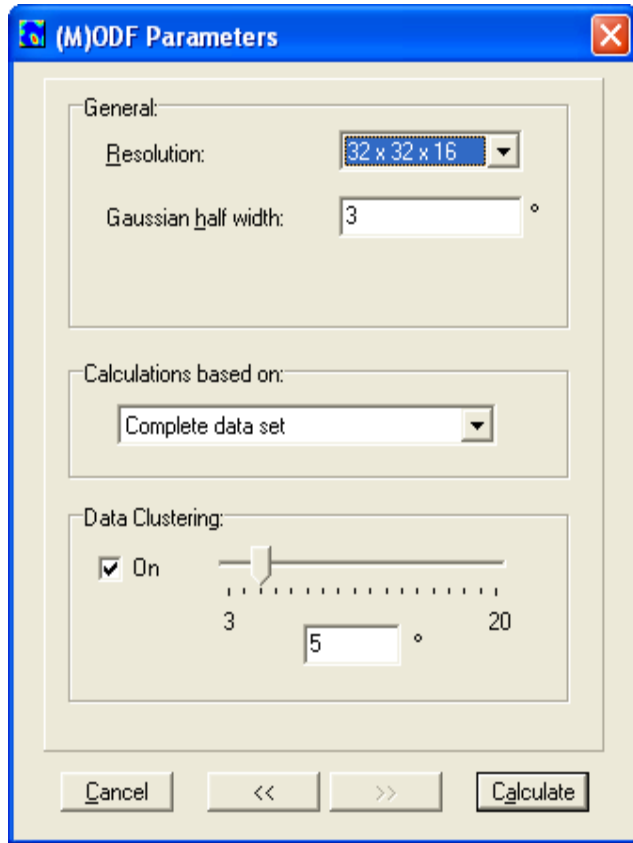
max = 5.56

In effect the harmonic method gives some "smoothing". Without this, a coarse binning of, say, 10°, produces a very "lumpy" result because the Gaussian applied around each point is not sufficiently wide to give a continuous distribution.

Same, with **10° binning** :

max = 31 !

$\varphi_1 = 5°$
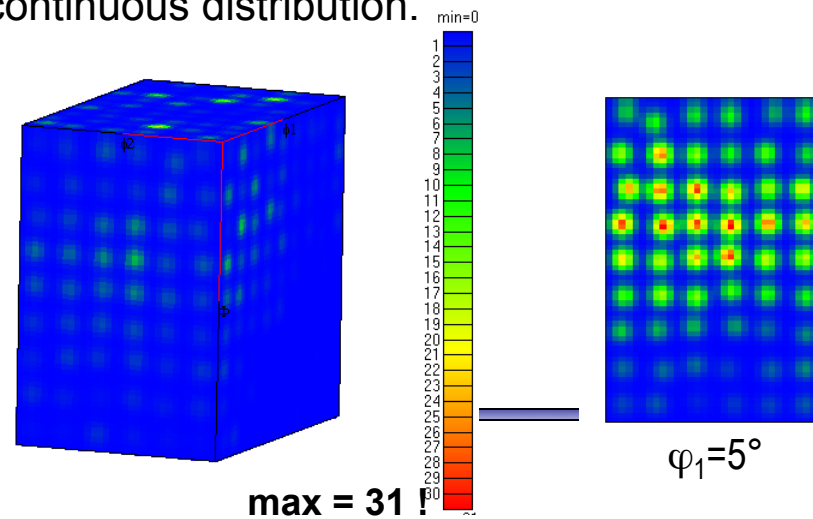
Statistical Aspects

Texture = distribution of orientations
→ Problem of sampling!

Triclinic sample symmetry

- Number of grains measured
- Width of the Gaussian (and/or L_{max})
- Influence of the sample symmetry

Orthorhombic sample symmetry

Zirconium, equiaxed
Sections thru the OD at constant φ_1 (L_{max} = 34)

Courtesy of N. Bozzolo

$\varphi_0 = 4°$

8.2 at {0 30 25}   9.0 at {-5 30 40}   15.5 at {-5 35 50}

$\varphi_0 = 8°$

7.1 at {0 35 25}   6.9 at {-5 35 35}   7.3 at {345 35 50}

80000 grains   **16000 grains**   **2000 grains**

$\varphi_0 = 8°$

6.6 at {0 35 30}   6.7 at {0 35 30}   5.8 at {5 30 15}

Gaussienne de $\varphi_0 = 4°$

7.6 at {0 35 30}   7.9 at {0 35 30}   8.3 at {15 30 30}

0.7	
1.4	
2.0	
2.8	
4.0	
5.6	
8.0	
11.3	
16.0	
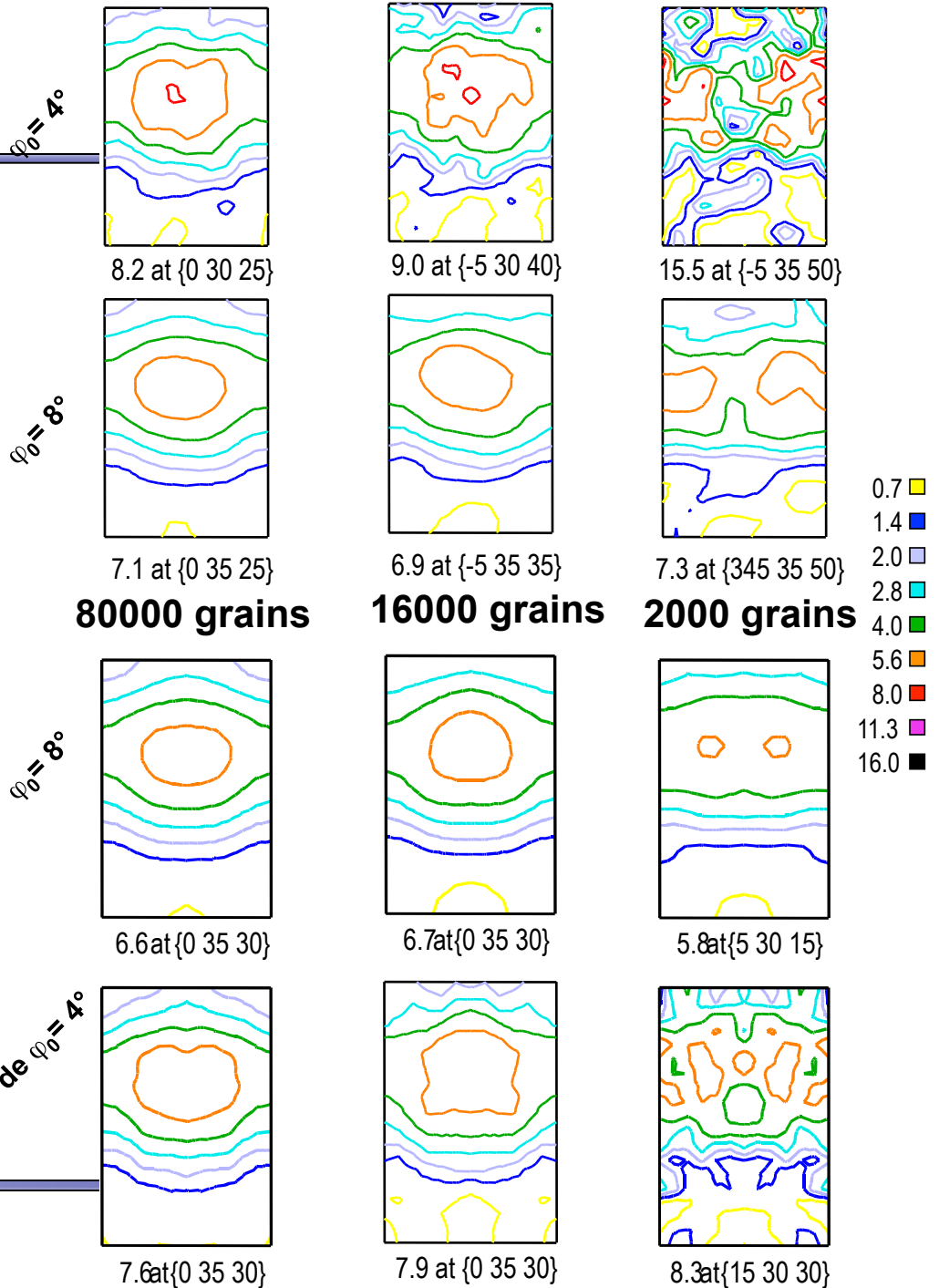
Courtesy of N. Bozzolo

Statistical Aspects Homogeneity/heterogeneity of the specimen...

Not just the number of grains must be considered but also their spatial distribution:

Single EBSD map (1 mm²)

Multiple maps, different locations (total =1 mm²)

equiaxed Ti
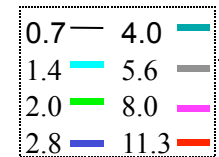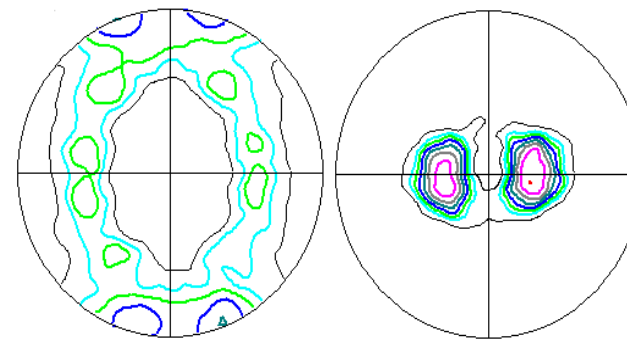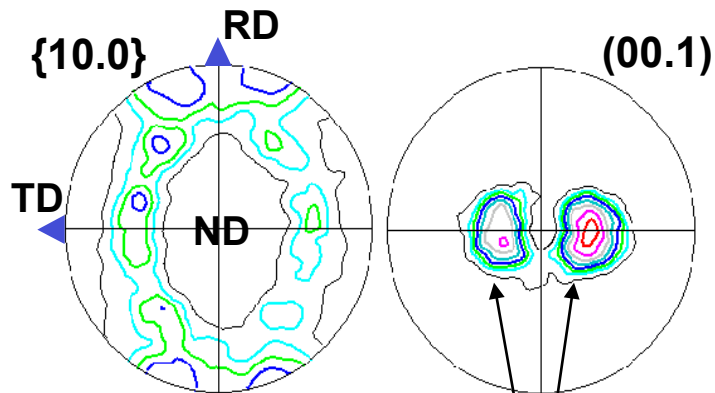
asymmetry of intensity

Texture – Microstructure Coupling

Example : partial texture of populations of grains identified by a grain size criterion
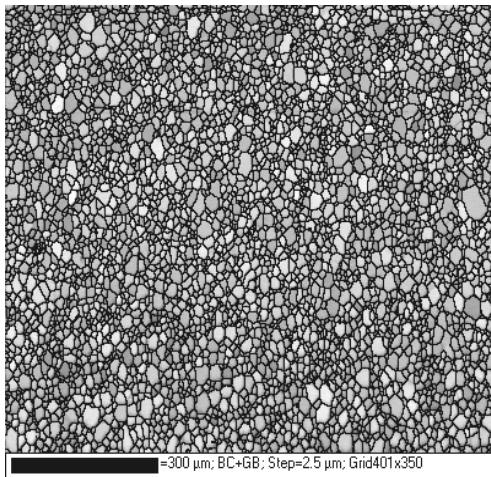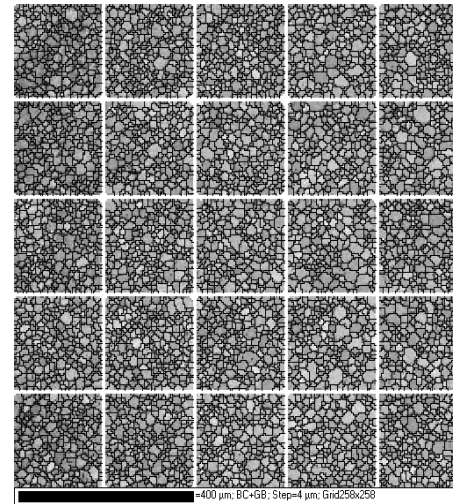(zirconium at the end of recrystallization)

$\varphi_1 = 0°$

Φ

φ_2

0.7	🟨
1.4	🟦
2.0	⬜
2.8	🟦
4.0	🟩
5.6	🟧
8.0	🟥
11.3	🟪
16.0	⬛

7.41
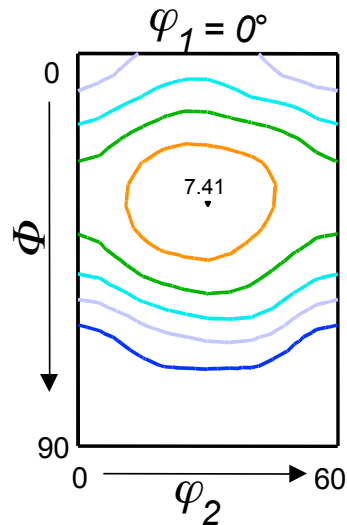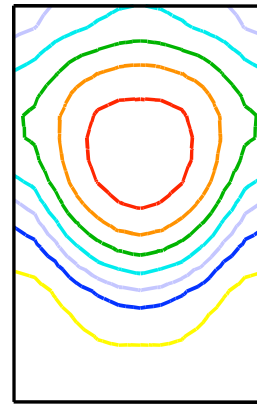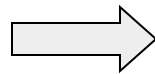
Global texture

$D > \bar{2}D$ (=11 µm)
3496 grains
17.9% surf.

partial texture of the
largest grains
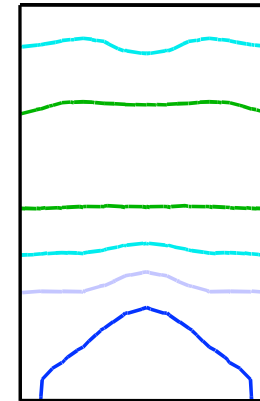
$D \leq D/2$ (=2.75 µm)
14255 grains
1.7% surf.

Partial texture of the
smallest grains

Important for texture evolution during grain growth: the large grains grow at the expense of the small grains. Since the large grains have a different texture, the overall texture also changes during growth.
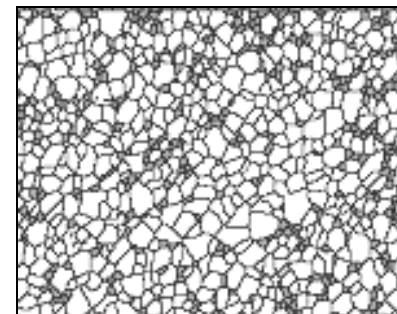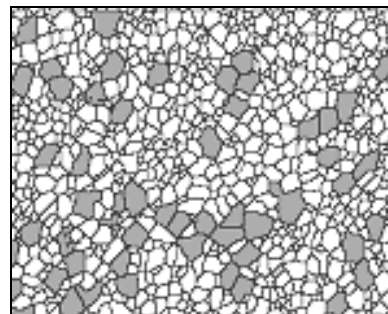
Definition of Misorientation
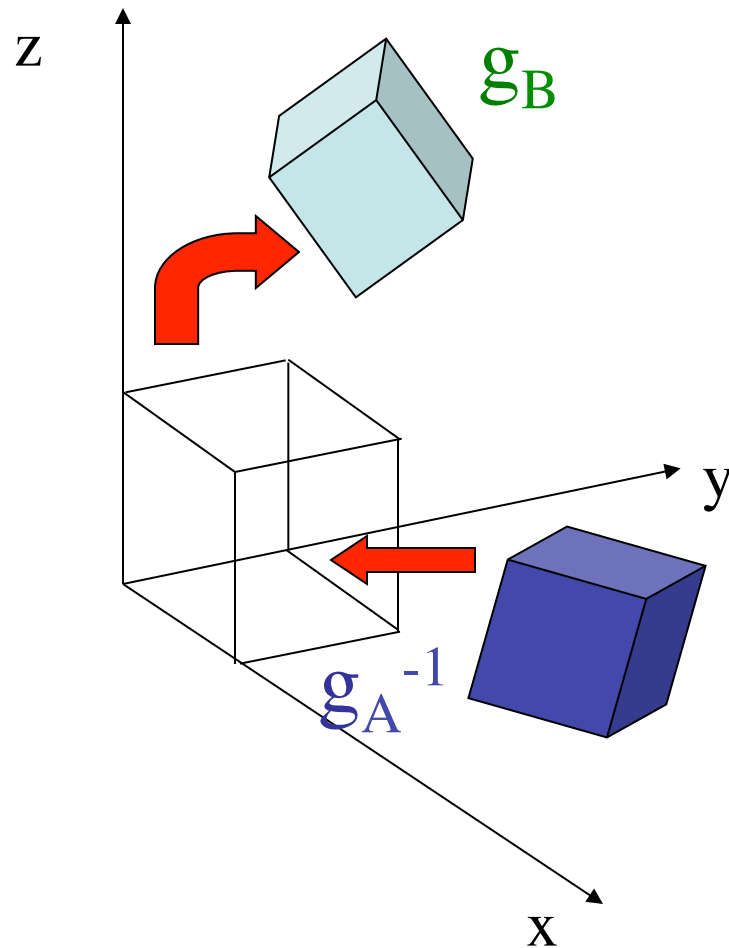
- Misorientation is an orientation defined with another crystal orientation frame as reference instead of the sample reference frame

- Thus a misorientation is the axis transformation from one point (crystal orientation) in the dataset to another point

  x,y,z are sample reference axes

  g_A is **orientation** of data point A (reference orientation) w.r.t sample reference

  g_B is **orientation** of data point B w.r.t. sample reference

$$\text{Misorientation} = g_B g_A^{-1}$$

g_B

g_A^{-1}

z

y

x

Misorientation Distribution Functions

- Calculating MDFs is very similar to calculating ODFs

Texture Reduced:
- Requires both Correlated and Uncorrelated MDFs to be calculated **for the same plot type**
- This MDF is simply the Correlated / Uncorrelated values
- May be used to amplify any features in the correlated MDF texture points across a G.B.
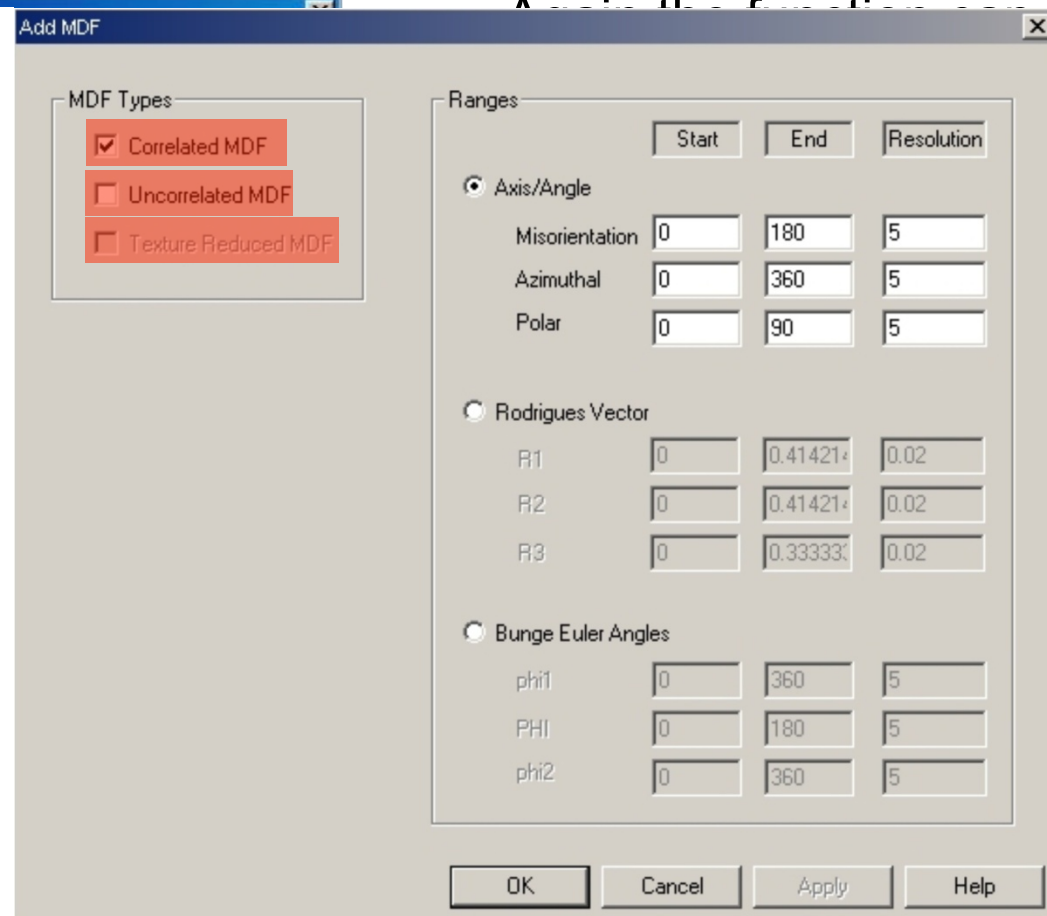
Plotting MDFs

Select plot type (previously calculated)

Set the discretization of the plots

If different types calculated, choose

These only apply to Euler angle plots

Sections through Misorientation Space
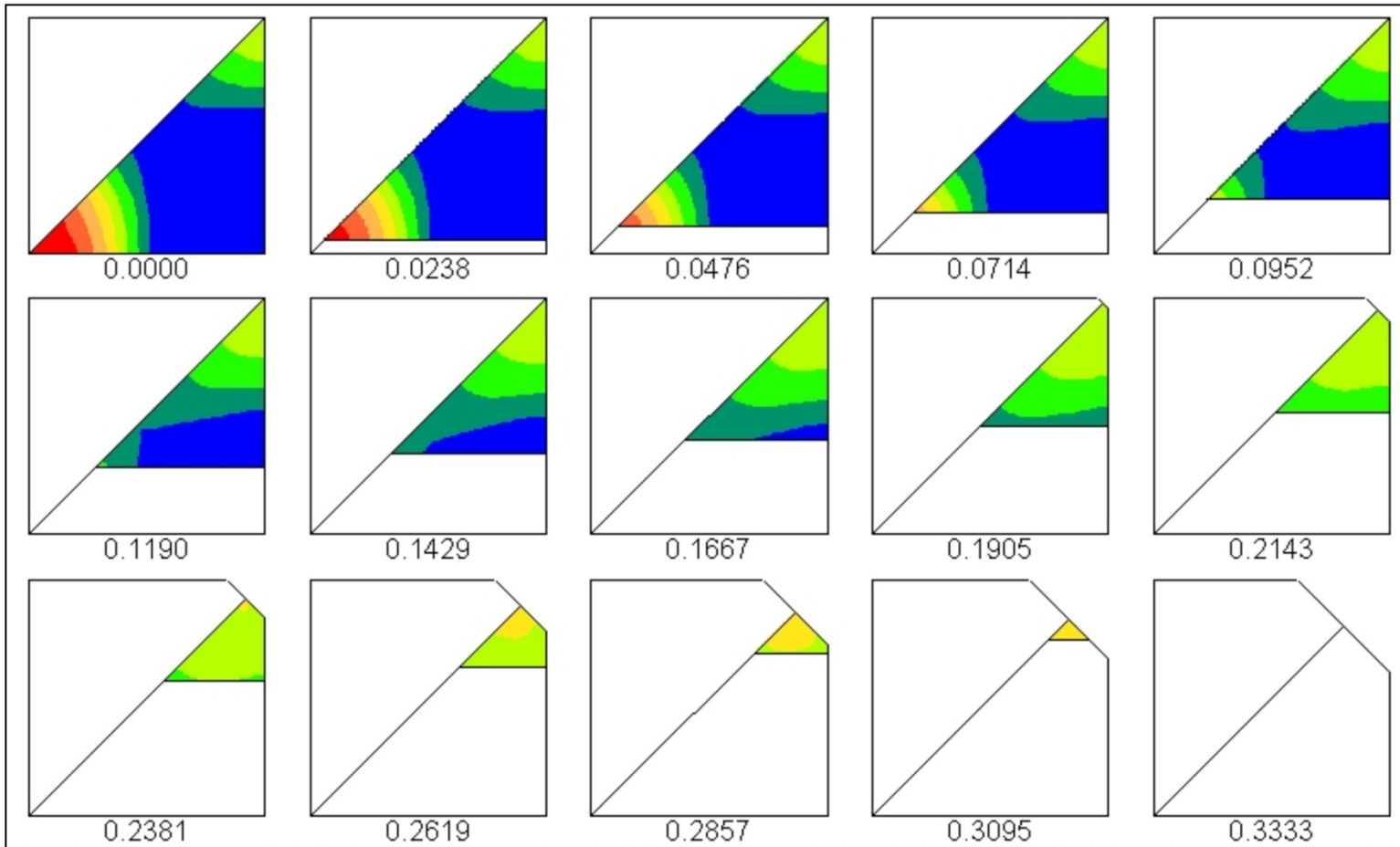
Rodrigues vector plots are shown as sections through an R-vector, usually R3

Charts

Charts are easy to use in order to obtain s

Project1

Grain Size (diameter)

ant

Image Quality

Range | Parameters

Method

○ Percentage

● Absolute

Minimum: 0

Maximum: 100

Minimum	Maximum	Average	
11.5	67	40.7673	Calculate

OK | Cancel | Apply | Help

Choose plot values and range

Displays data range. You can calculate the range

Use to select partition if you have any (e.g. by grain size)

Fraction

0.07
0.06
0.05
0.04

0.20

Image Quality

0.02
0.00

0   10   20   30   40   50

Grain Size (Diameter) [microns]

Image Quality

10   20   30   40   50   60

Misorientation Angle [degrees]

40

40
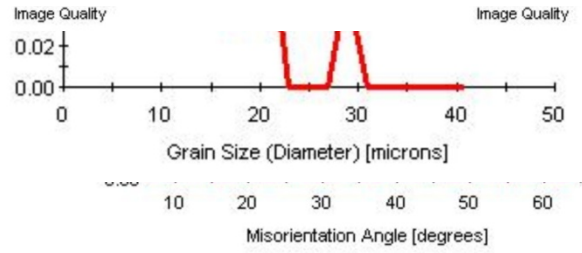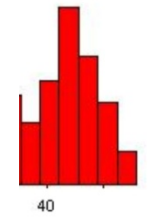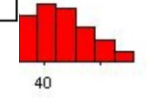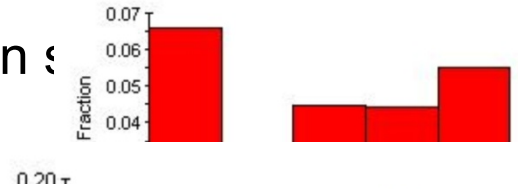
Kernel Average Misorientation (KAM)

$$\Delta g = \{O_c\} g_B g_A^{-1} \{O_c\}$$

• For each point (orange box), compute the misorientation (θ, angle only, purple arrows) for each nearest neighbor (26 in 3D).

• For all values < chosen threshold (ψ, say, = 5°) compute an average value.

• Use of a threshold eliminates any contribution from high angle boundaries.
High values indicate orientation gradients, obviously, which are closely related to GND.

• Averaged over a grain gives Grain Ave. Misorientation (GAM)

$$KAM = \left\langle \theta\left(g_{\text{point}}, g_{\text{neighbor}}\right) \middle| \theta < \psi \right\rangle$$
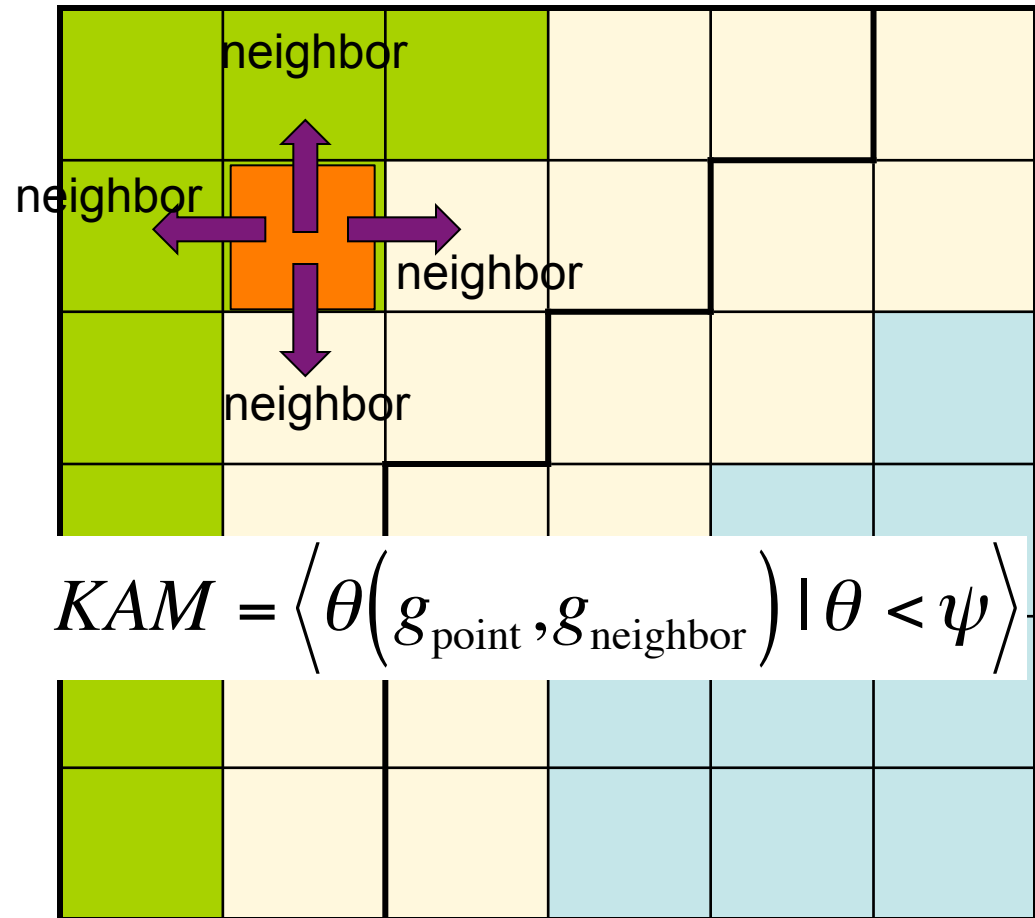
Why is KAM important? Nucleation of recrystallization, e.g.

Intra-Granular Misorientation (IGM)

$$\Delta g = \{O_c\} g_B g_A^{-1} \{O_c\}$$

- For all points in a given grain compute an average value, $g_{GrainAverage}$.
- For each point, compute the misorientation (θ, angle only) with the average orientation.
- High values indicate large differences from the grain averaged orientation.
- Variation from dark (large IGM) to light (small IGM) shows the idea.
- Sometimes called the Grain Reference Deviation (GRD).
- When averaged over the grain, one obtains the Grain Orientation Spread (GOS).

$$IGM(\mathbf{x}) = \theta\left(g(\mathbf{x}), g_{GrainAverage}\right)$$
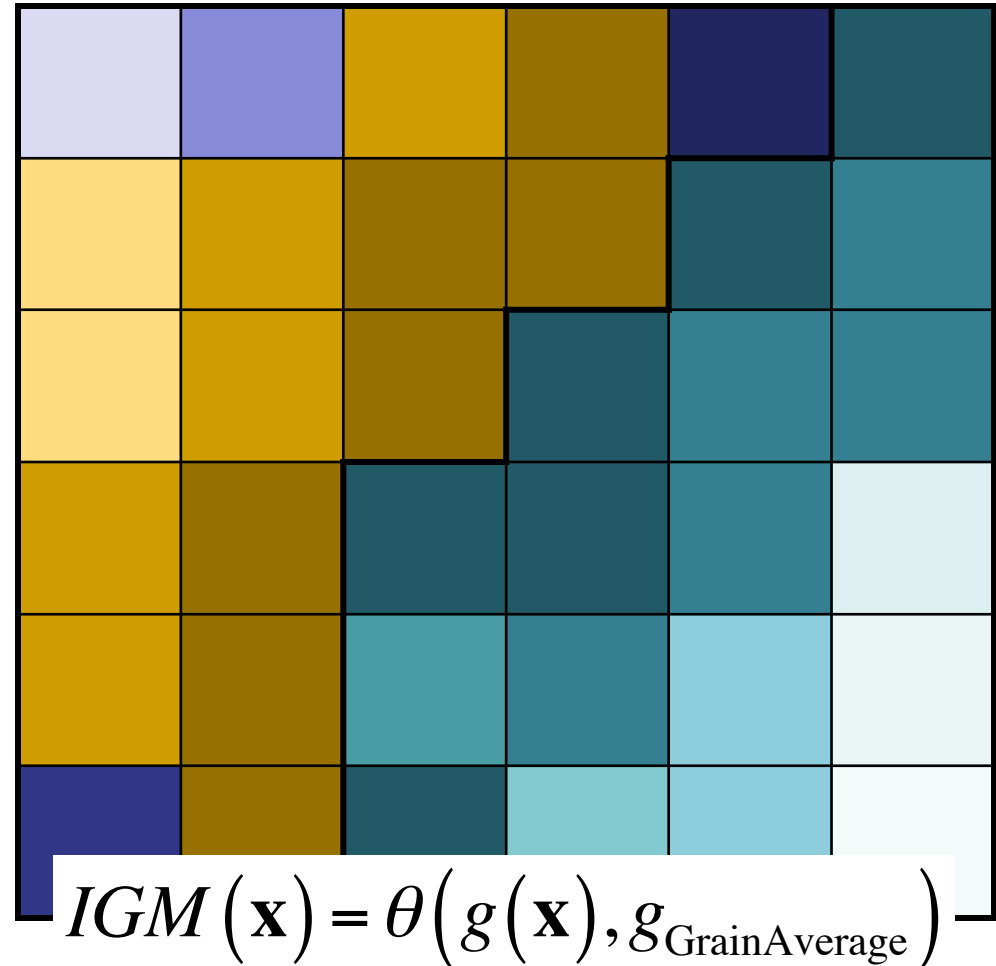
Why is IGM important? Long range orientation gradients, for example

GOS and GAM

n = no. nearest neighbors
N = number of pixels

$$GAM = \frac{1}{N}\frac{1}{n}\sum_{j=1}^{N}\sum_{i=1}^{n}\Delta g_{ij}\left(g_i,g_j\right)$$

$$GOS = \frac{1}{N-1}\frac{1}{N}\sum_{j=1}^{N}\sum_{i=1}^{N}\Delta g_{ij}\left(g_i,g_j\right), \quad j\neq i$$

200 µm
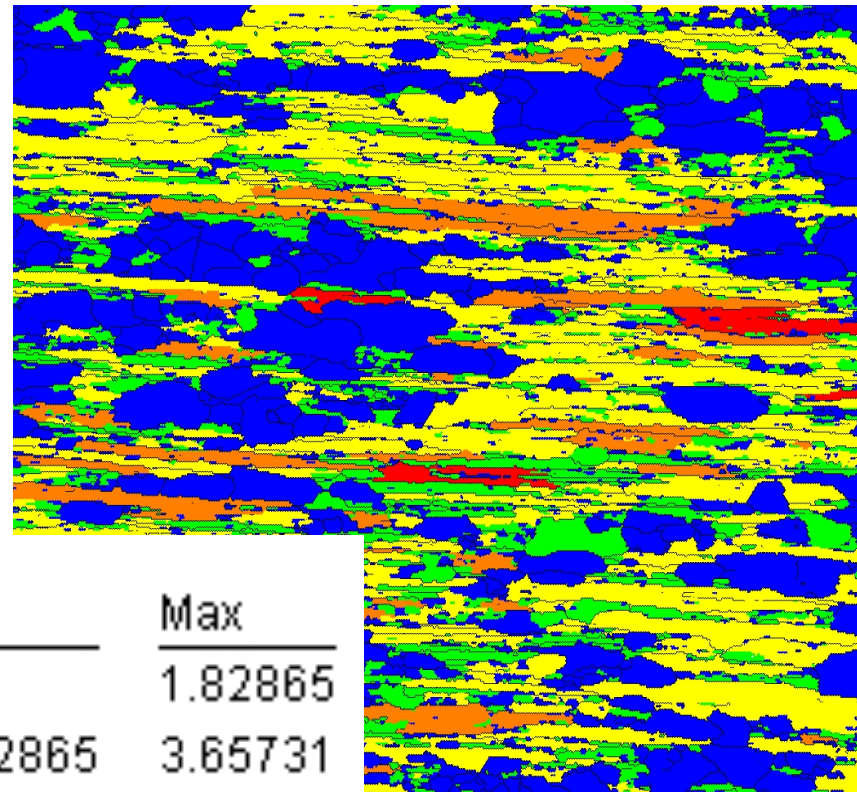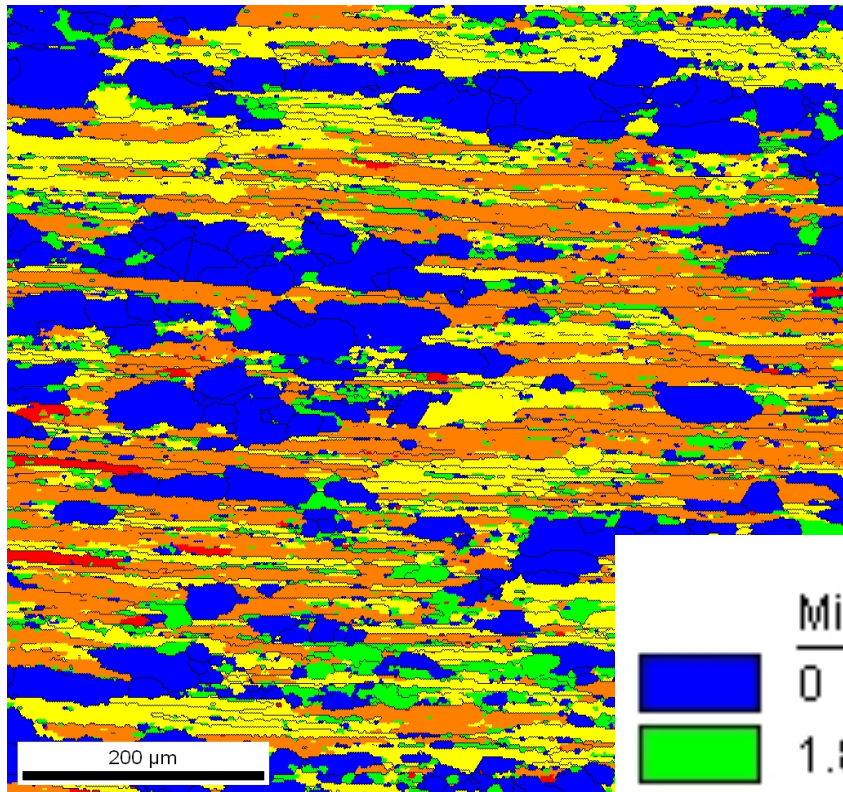
	Min	Max
(blue)	0	1.82865
(green)	1.82865	3.65731
(yellow)	3.65731	5.48596
(orange)	5.48596	7.31461
(red)	7.31461	9.14327

GAM
Nearest neighbor pixel pai   irs   ▪
⇒ short range orientation   ge orientation gradients

M.H. Alvi

GOS and GAM

Recrystallized

Recrystallized

Unrecrystallized

Unrecrystallized

GAM

GOS
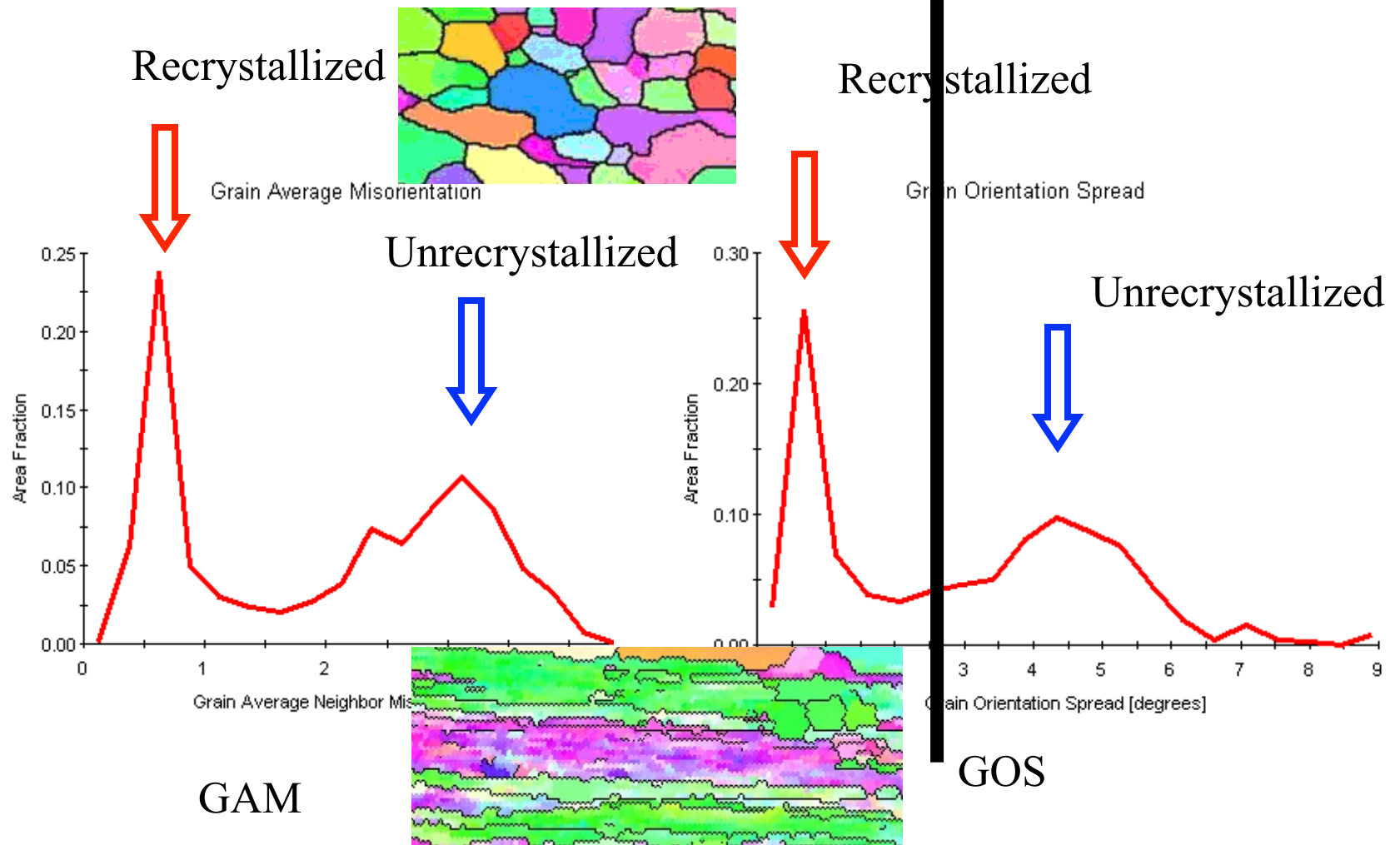
Overlapping peaks for deformed and recrystallized regions.

M.H. Alvi

Partitioned scan: threshold GOS = 3°

Deformed Grains
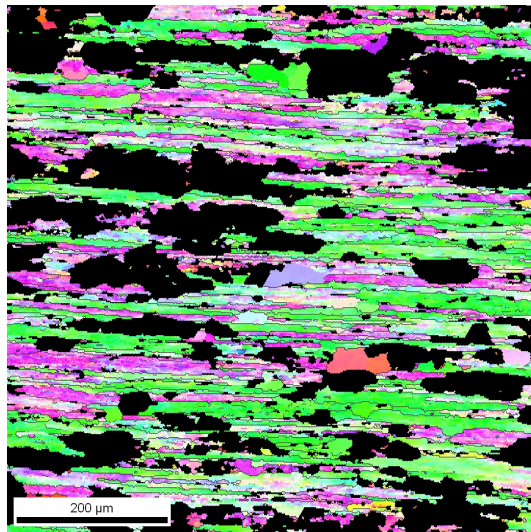
Recrystallized Grains

M.H. Alvi
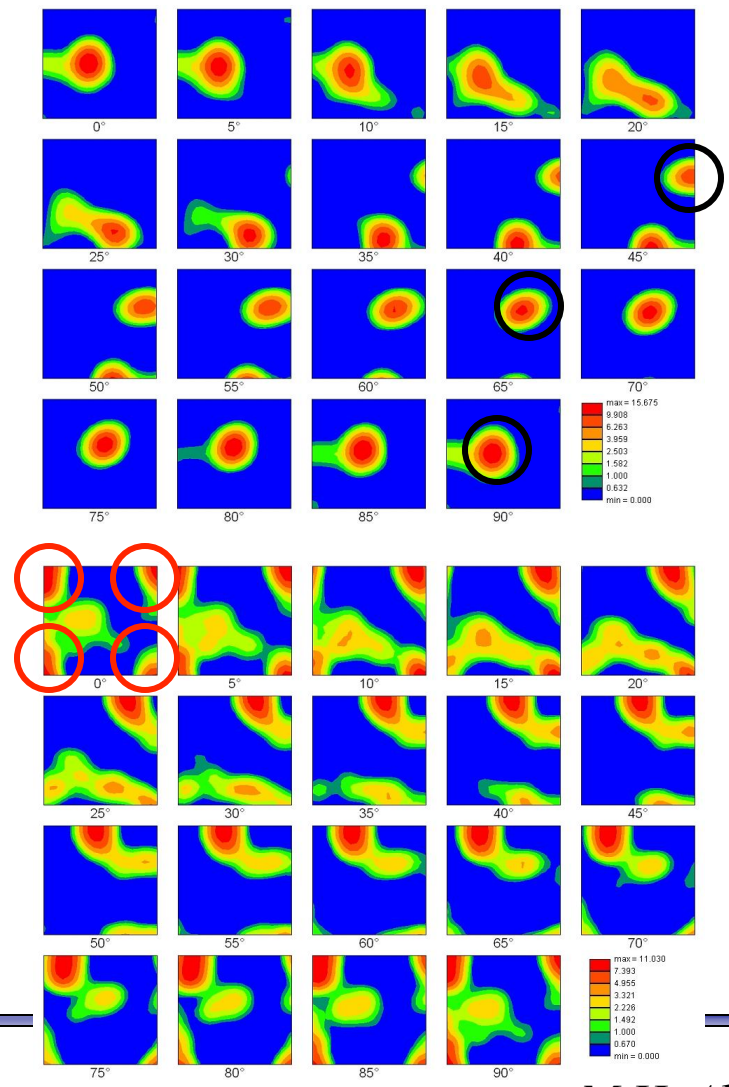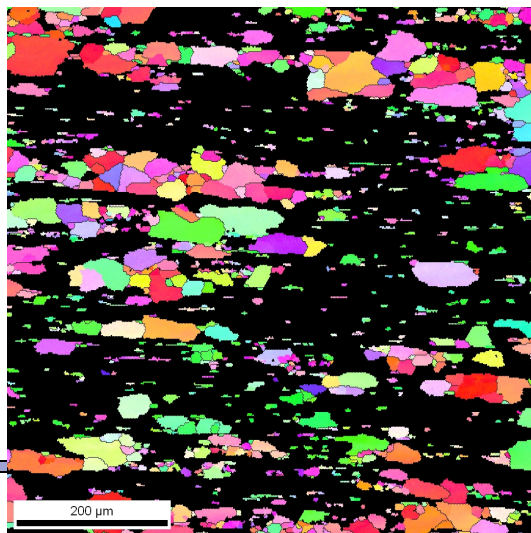
As-deformed Fe-1%Si

T.A. Bennett

As 1.5% temper-rolled

As 8% temper-rolled
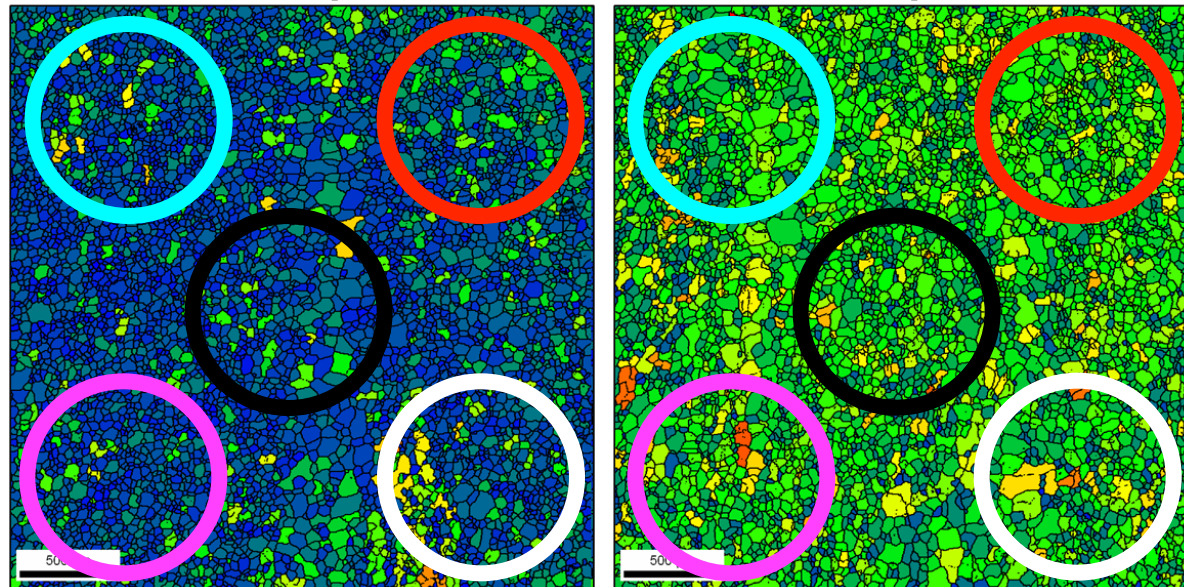
Intergranular variations in GOS greater in 8% temper-rolled material.

Maps shaded according to GOS.

AGG is a local phenomenon.

AGG occurs more readily in 8% material because of greater <u>local</u> intergranular orientation gradients.

	Min	Max
	0.229345	7.85205

Density of abnormally large grains will be higher in the 8% material.

Presence of several <u>same-stored-energy</u> regions in 1.5% material leads to lower density of abnormally large grains.

Grains that grow abnormally <u>already exist</u> in the as-deformed material.

Orientation Spread, Fe-1%Si

15 min   **0.5 min**

30 min   **5 min**

60 min   **15 min**
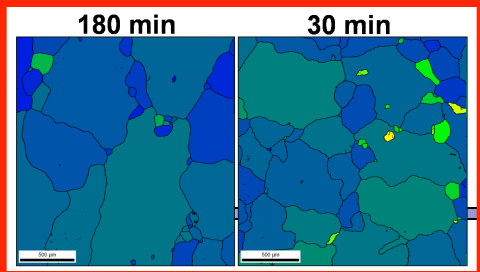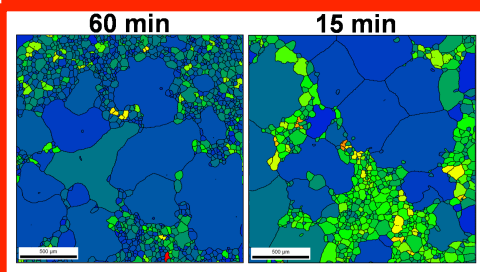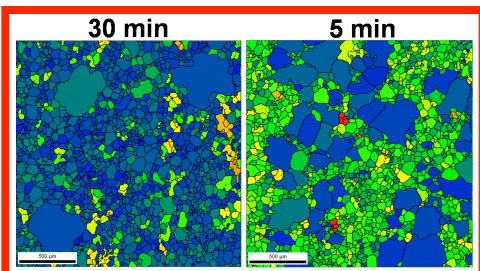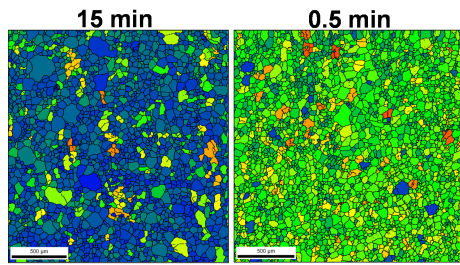
180 min   **30 min**

1.5% and 8% temper-rolled Fe-1%Si, annealed in air at 787°C for various times.

1.5% temper-rolled

8% temper-rolled

180 min.

30 min.

	Min	Max
	0.0337706	6.65443
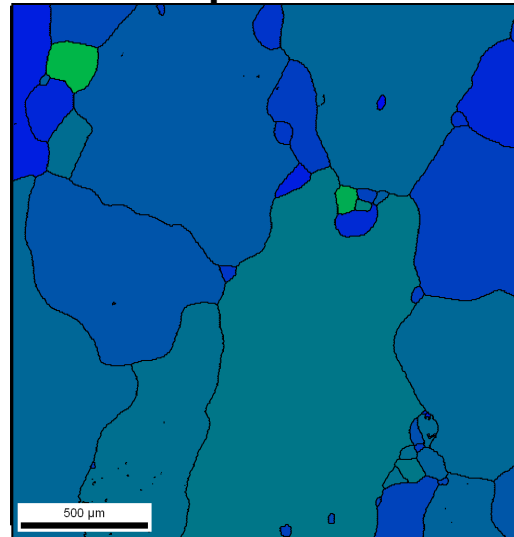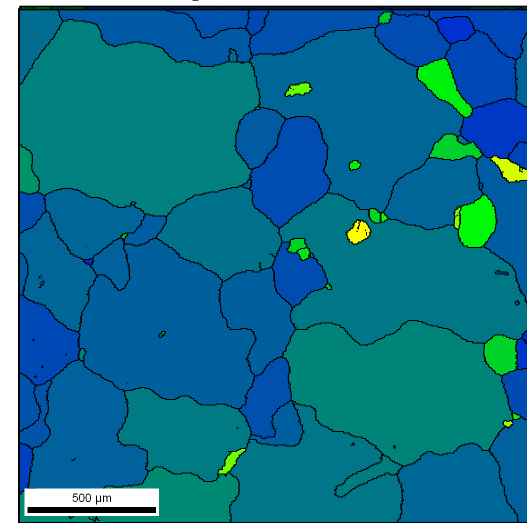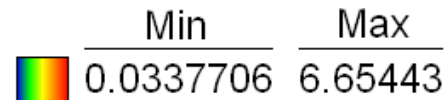
T.A. Bennett

Overall, GOS decreases with annealing time.

Pure Nb: Longitudinal Section Etched

3mm from top of cavity
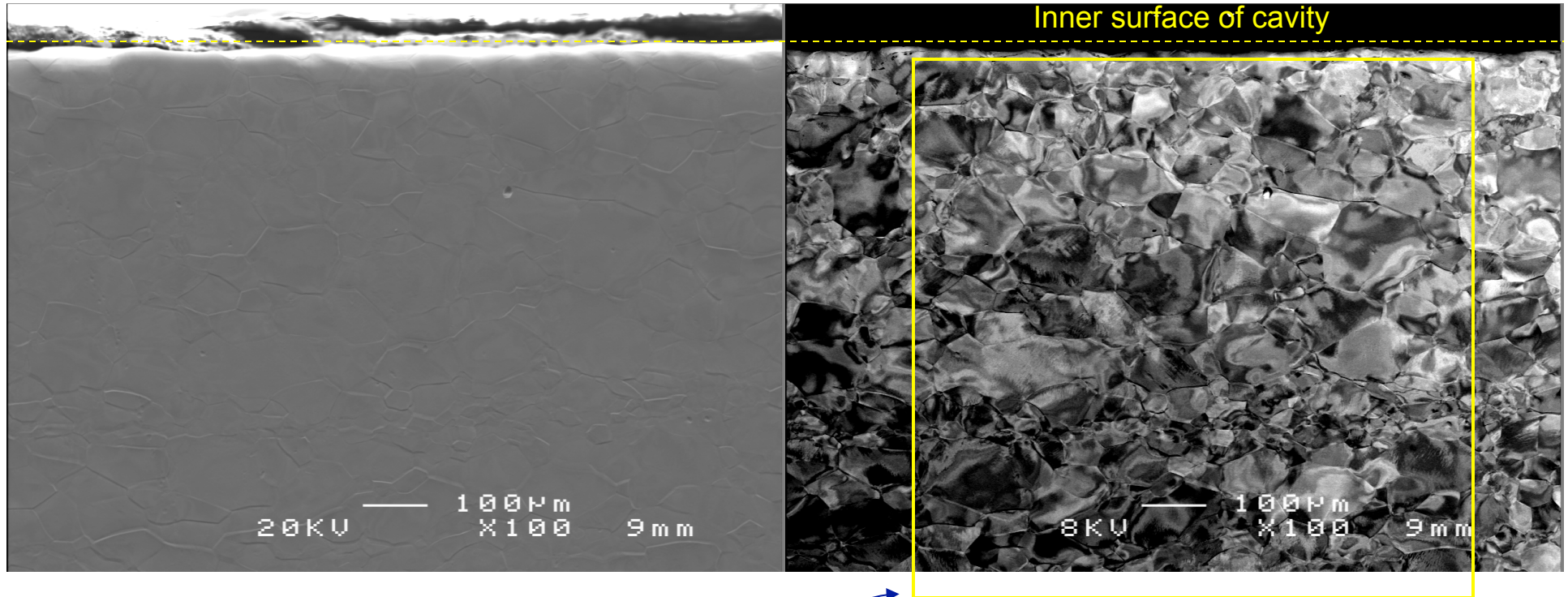
Secondary electron image

EBSD Grid

Backscattered electron image

R. Crooks

Nb: EBSD IPF Map

R. Crooks
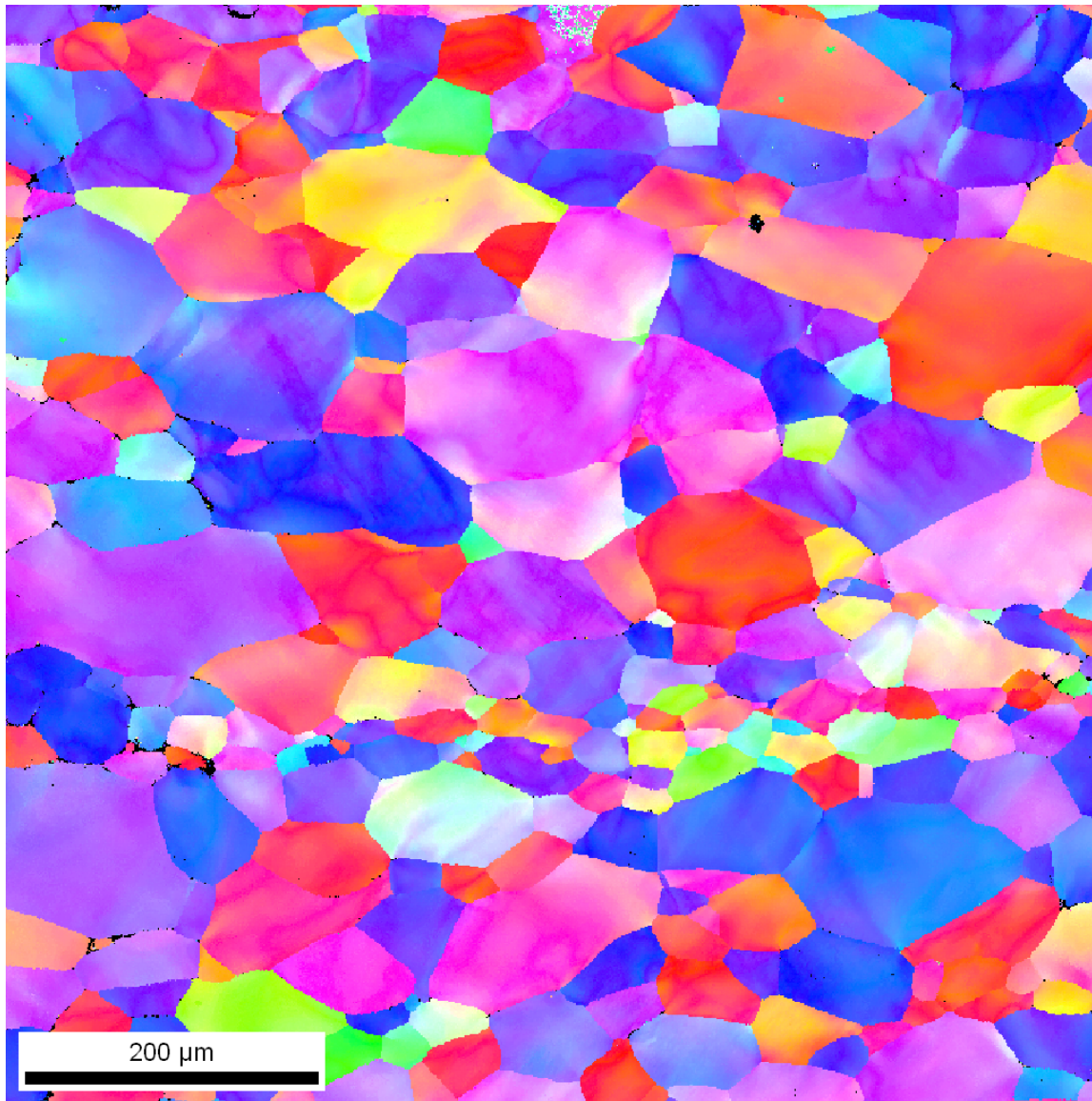
Crystal directions normal to sheet surface

Color Coded Map Type: Inverse Pole Figure [001]

Nb

1 1 1

0 0 1   1 0 1
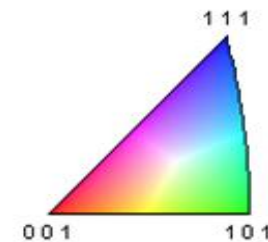
Boundaries: <none>

Color changes within grain show distortion of crystal

95% hit rate, 560,200 data points, 1 μm spatial resolution

Nb: EBSD GOS Map

Strain in isolated grains
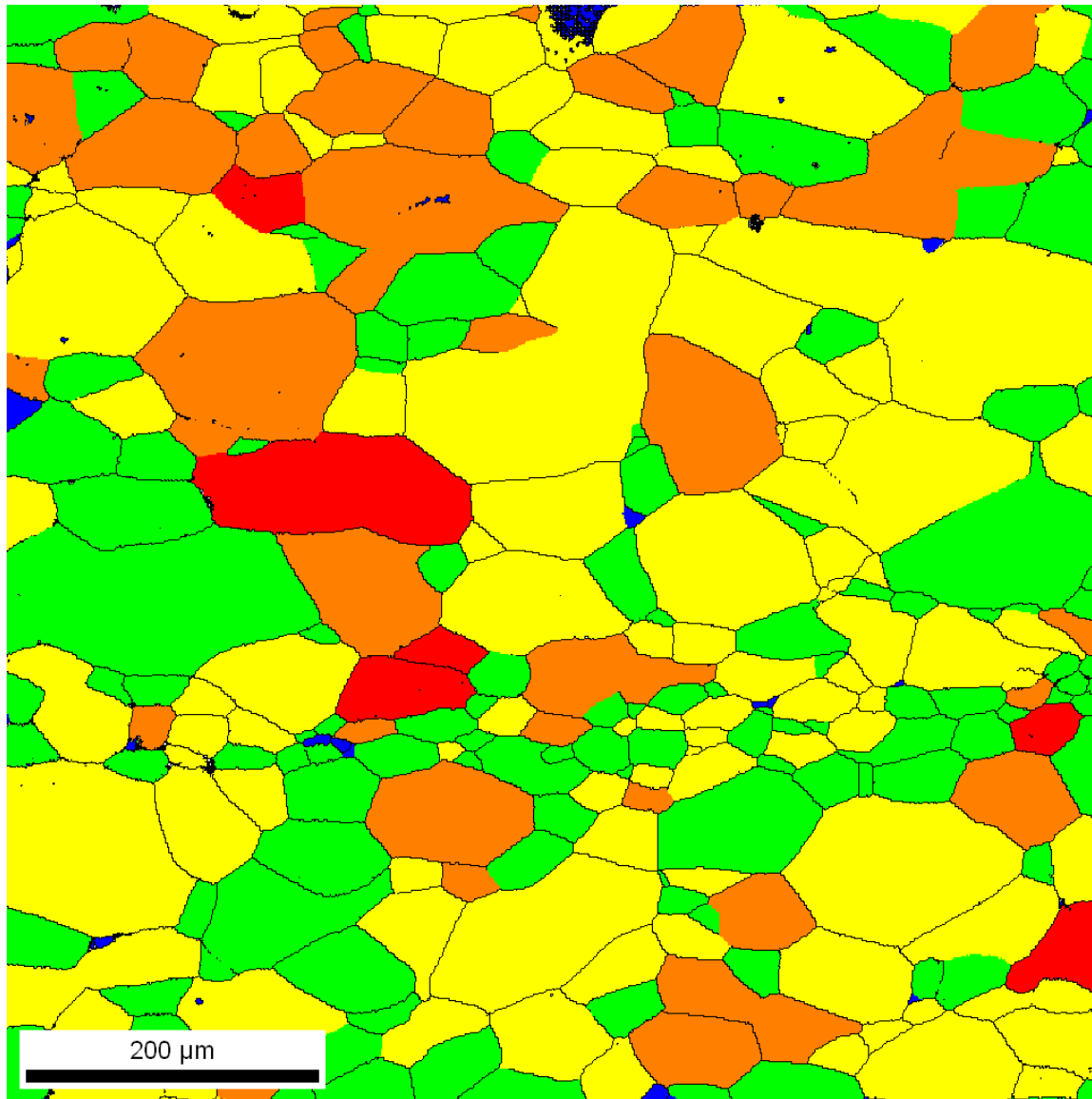
GOS: The average orientation is first calculated for each grain. The spread is then the average deviation between the orientation of each point in the grain and the grain average.

Color Coded Map Type: Grain Orientation Spread

Min	Max	Total Fraction	Partition Fraction
0	1.22203	0.004	0.004
1.22203	2.44406	0.275	0.275
2.44406	3.66609	0.478	0.478
3.66609	4.88812	0.202	0.202
4.88812	6.11016	0.038	0.038

Boundaries: Rotation Angle

Min	Max	Fraction	Number	Length
15°	180°	0.024	26493	2.65 cm

200 μm
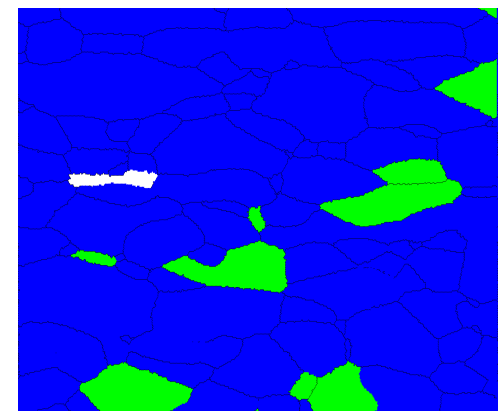
R. Crooks

1 μm spatial resolution

As-received sheet

39

Nb: EBSD KAM Map

Color Coded Map Type: Kernel Average Misorientation

	Min	Max	Total Fraction	Partition Fraction
(blue)	0	0.7	0.735	0.735
(green)	0.7	1.4	0.248	0.248
(yellow)	1.4	2.1	0.013	0.013
(orange)	2.1	2.8	0.001	0.001
(red)	2.8	3.5	0.001	0.001

Boundaries: Rotation Angle

	Min	Max	Fraction	Number	Length
—	15°	180°	0.024	26493	2.65 cm

*For statistics - any point pair with misorientation exceeding 0° is considered a boundary total number = 1117135, total length = 1.12 m)

0
250
500
750

200 µm

Stored Strain Energy very high at 500 µm from inner surface
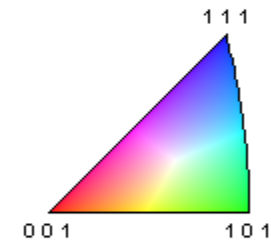
R. Crooks

1 µm spatial resolution

40

Nb: EBSD IPF Map 500 μm deep

Color Coded Map Type: Inverse Pole Figure [001]

Nb

Boundaries: Rotation Angle

	Min	Max	Fraction	Number	Length
──	15°	180°	0.011	8093	2.43 mm

*For statistics - any point pair with misorientation exceeding 0° is considered a boundary
total number = 743433, total length = 22.30 cm)

750 x 500, 0.3 μm spatial resolution

R. Crooks

41

Nb: EBSD GOS Map 500 µm deep

Color Coded Map Type: Grain Orientation Spread

	Min	Max	Total Fraction	Partition Fraction
(blue)	0	1.14192	0.010	0.010
(green)	1.14192	2.28385	0.343	0.343
(yellow)	2.28385	3.42577	0.341	0.341
(orange)	3.42577	4.5677	0.149	0.149
(red)	4.5677	5.70962	0.153	0.153

Boundaries: Rotation Angle

	Min	Max	Fraction	Number	Length
—	15°	180°	0.011	8093	2.43 mm

*For statistics - any point pair with misorientation exceeding 0° is considered a boundary total number = 743433, total length = 22.30 cm)

80 µm

0.3 µm spatial resolution

R. Crooks

42

Nb: EBSD KAM Map 500 μm deep

Color Coded Map Type: Kernel Average Misorientation

	Min	Max	Total Fraction	Partition Fraction
🟦	0	0.7	0.669	0.669
🟩	0.7	1.4	0.311	0.311
🟨	1.4	2.1	0.013	0.013
🟧	2.1	2.8	0.001	0.001
🟥	2.8	3.5	0.002	0.002

Boundaries: Rotation Angle

	Min	Max	Fraction	Number	Length
—	15°	180°	0.011	8093	2.43 mm

*For statistics - any point pair with misorientation exceeding 0° is considered a boundary total number = 743433, total length = 22.30 cm)

80 µm

Stored Strain Energy

KAM 3rd neighbor x 0.3 μm spatial resolution

R. Crooks

Nb: EBSD GROD Map 500 μm deep

Severely deformed, >15° in 50 μm
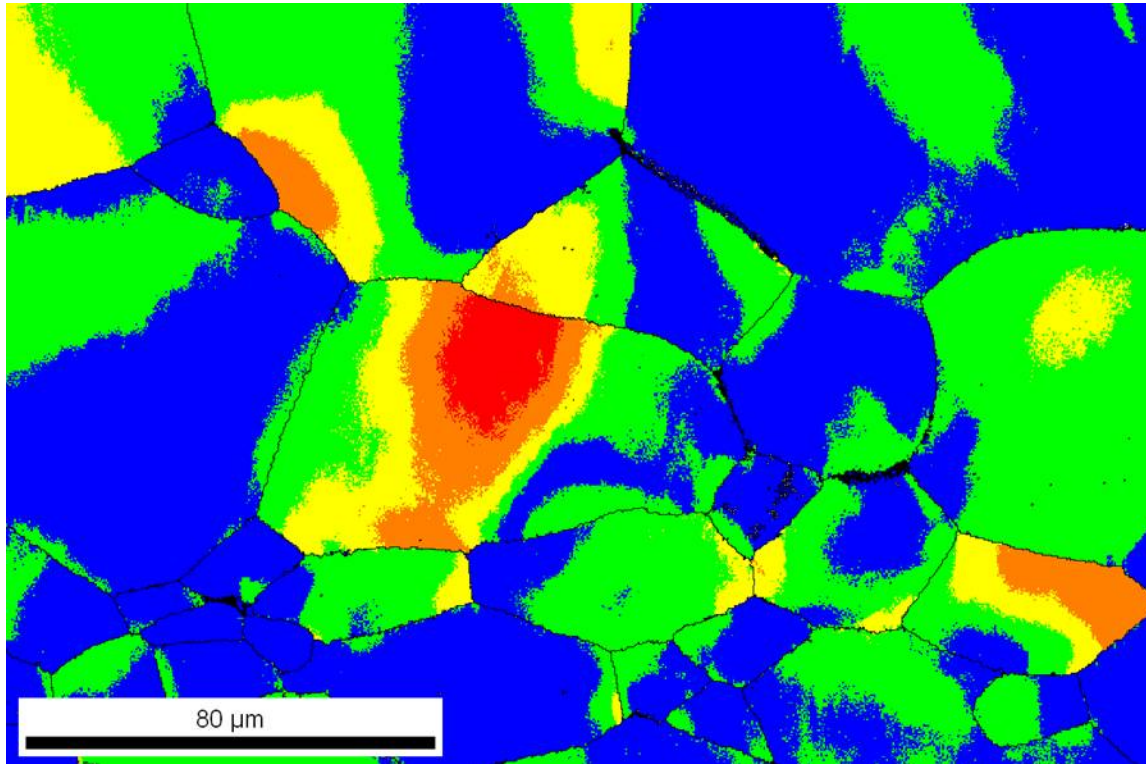
Color Coded Map Type: Grain Reference Orientation Deviation

	Min	Max	Total Fraction	Partition Fraction
(blue)	0	3.87436	0.488	0.488
(green)	3.87436	7.74872	0.369	0.369
(yellow)	7.74872	11.6231	0.088	0.088
(orange)	11.6231	15.4974	0.038	0.038
(red)	15.4974	19.3718	0.013	0.013

Boundaries: Rotation Angle

	Min	Max	Fraction	Number	Length
—	15°	180°	0.011	8093	2.43 mm

*For statistics - any point pair with misorientation exceeding 0° is considered a boundary
total number = 743433, total length = 22.30 cm)

80 μm

Deviation from grain minimum KAM

Nb: Backscattered electron image
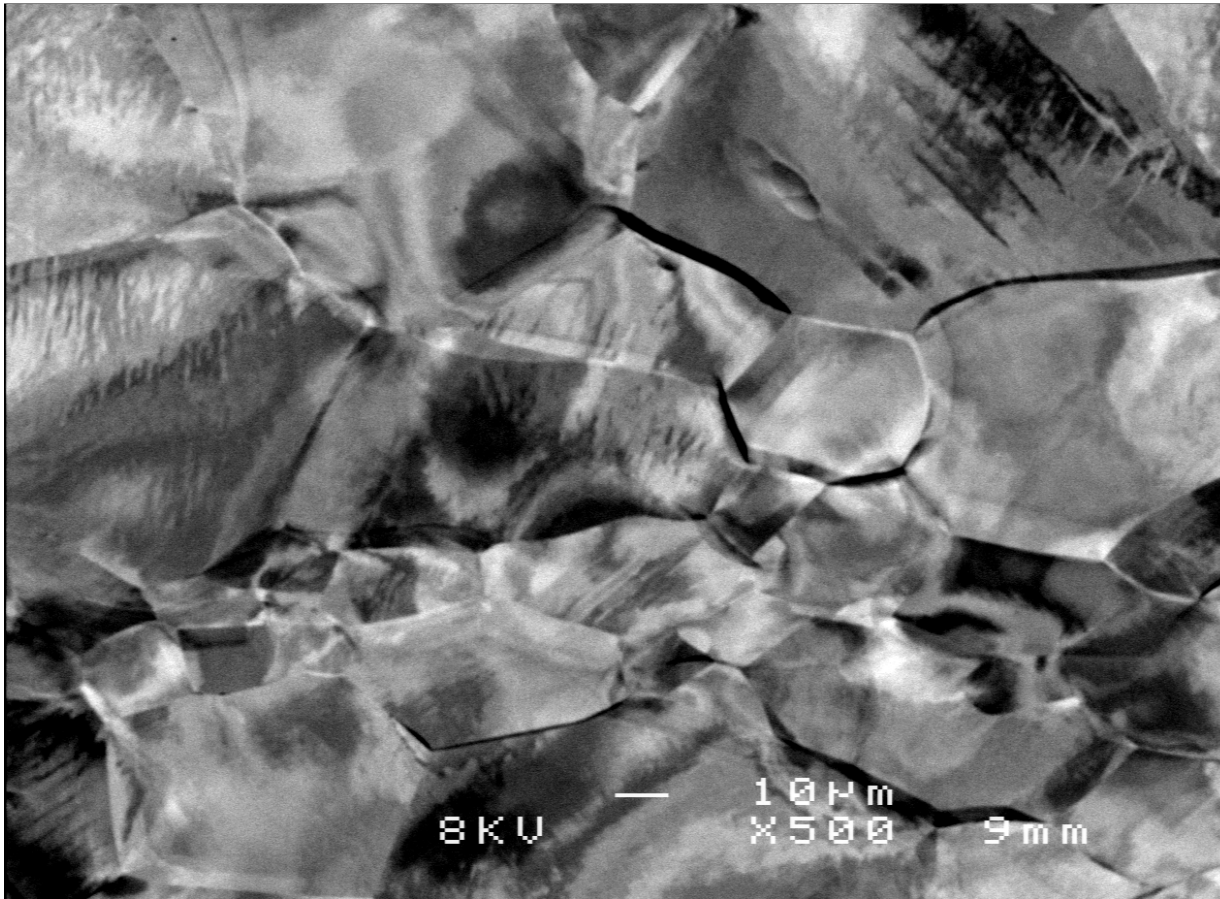
Channeling contrast of
Polished and etched
surface resembles
EBSD map

In as-deep-drawn
condition, severe
strain
located in pockets
through-thickness.

Greater strain at 300
and 500 μm
than at surface.

R. Crooks

Reconstructed Boundaries

• The software includes an analysis of grain boundaries that
• Data MUST be on
outputs the information as a (long) list of line segment data.
hexagonal grid
• use of the GB segment analysis is an essential preliminary step
• Clean up the data to
before performing the stereological 5-parameter analysis of GBCD.
desired level
• The data must be on a hexagonal/triangular grid. If you have a
map on a square grid, you must convert it to a hexagonal grid. Use
the software called OIMTools to do this (freely available fortran
program).

• This type of data is
required for stereological
analysis of 5-parameter
grain boundary character
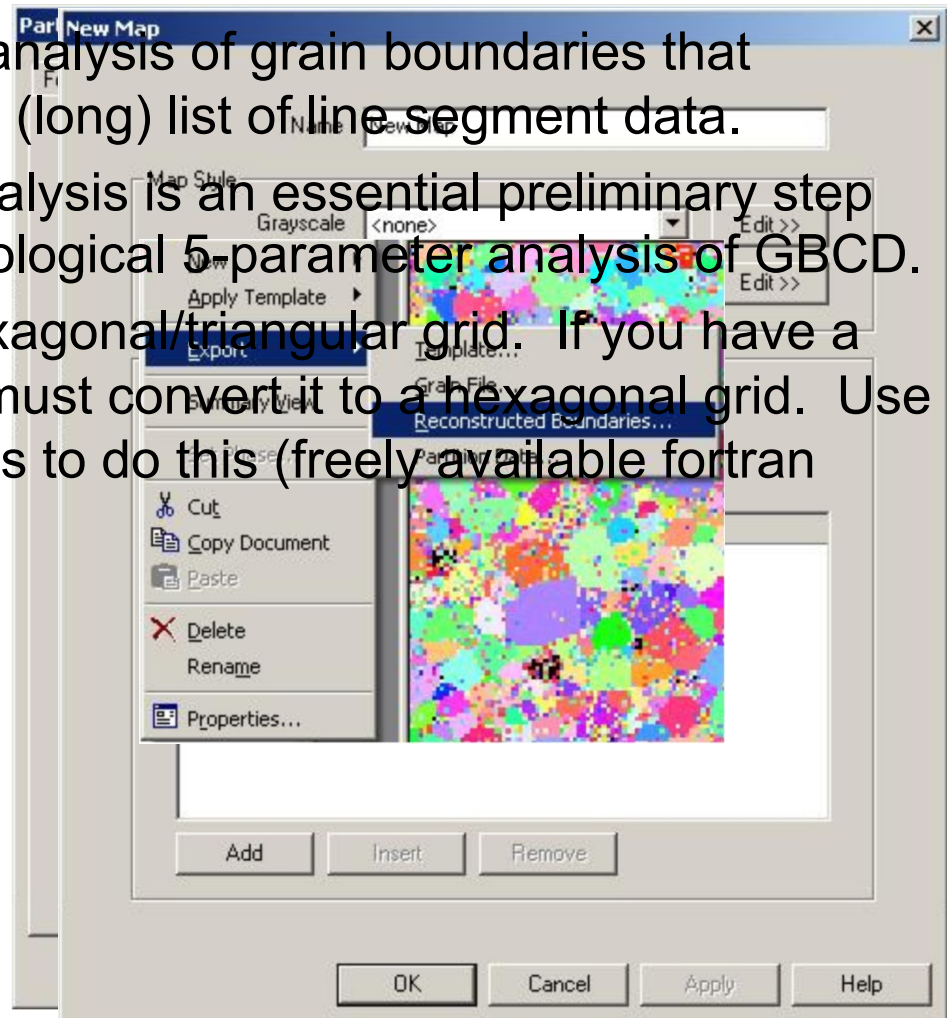
Reference Frames

- This next set of slides is devoted to explaining, as best we can, how to relate features observed in EBSD images/maps to the Euler angles.

- In general, the Euler frame is not aligned with the x-y axes used to measure locations in the maps.

- The TSL (OIM™) and Channel (HKL) softwares both rotate the image 180° relative to the original physical sample.

- Both TSL (OIM™) and Channel (HKL) softwares use different reference frames for measuring spatial location versus the the Euler angles, which is, of course, extremely confusing.

TSL / OIM Reference Frames

$Z_{spatial}$ points *in* to the plane
Z_{Euler} points *out* of the plane

$TD = y_{Euler} = 010_{sample}$ $x_{spatial}$

The purple line indicates a direction, associated with, say, a scratch, or trace of a grain boundary on the specimen.

$RD = x_{Euler}$
$= 100_{sample}$

111

$y_{spatial}$

Physical specimen:
Mounted in the SEM, the tilt axis is parallel to "$x_{spatial}$"

001   101
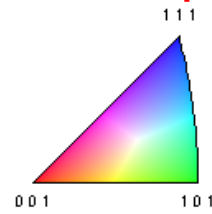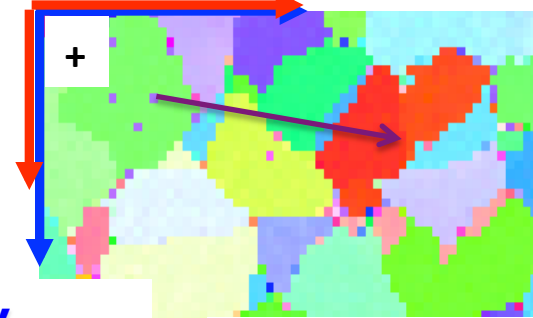
Image:
Note the 180° rotation.

ND
$= z_{Euler}$

Sample Reference Frame for Orientations/Euler Angles

-RD
$= -x_{Euler}$

-TD
$= -y_{Euler}$

"+" denotes the Origin

$y_{spatial}$
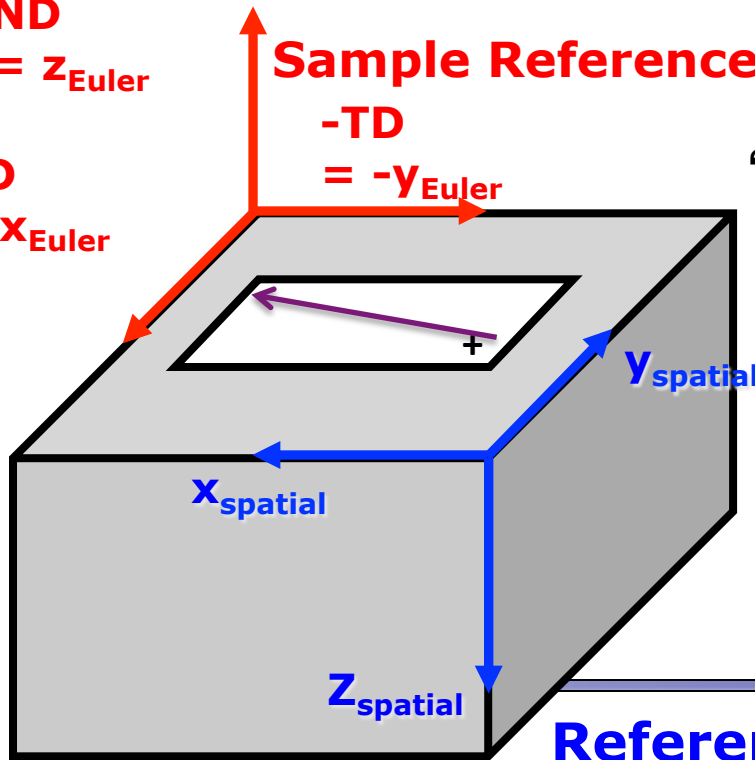
Crystal Reference Frame:
Remember that, to obtain directions and tensor quantities in the crystal frame for each grain (starting from coordinates expressed in the Euler frame), one must use the Euler angles to obtain a transformation matrix (or equivalent).

$x_{spatial}$

$Z_{spatial}$

Reference Frame for Spatial Coordinates

TSL / OIM Reference Frames for Images

Conversion from spatial to Euler and vice versa (TSL only)

From Herb Miller's notes:

The axes for the TSL Euler frame **are** consistent with the RD-TD-ND system in the TSL Technical Manual, but only with respect to maps/images, not the physical specimens.

The axes for the HKL system **are** consistent with the information provided by users in Metz. Here, x is in common, but the two y-axes point in opposite directions.

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Note that the transformation is a 180° rotation about the line *x=y*
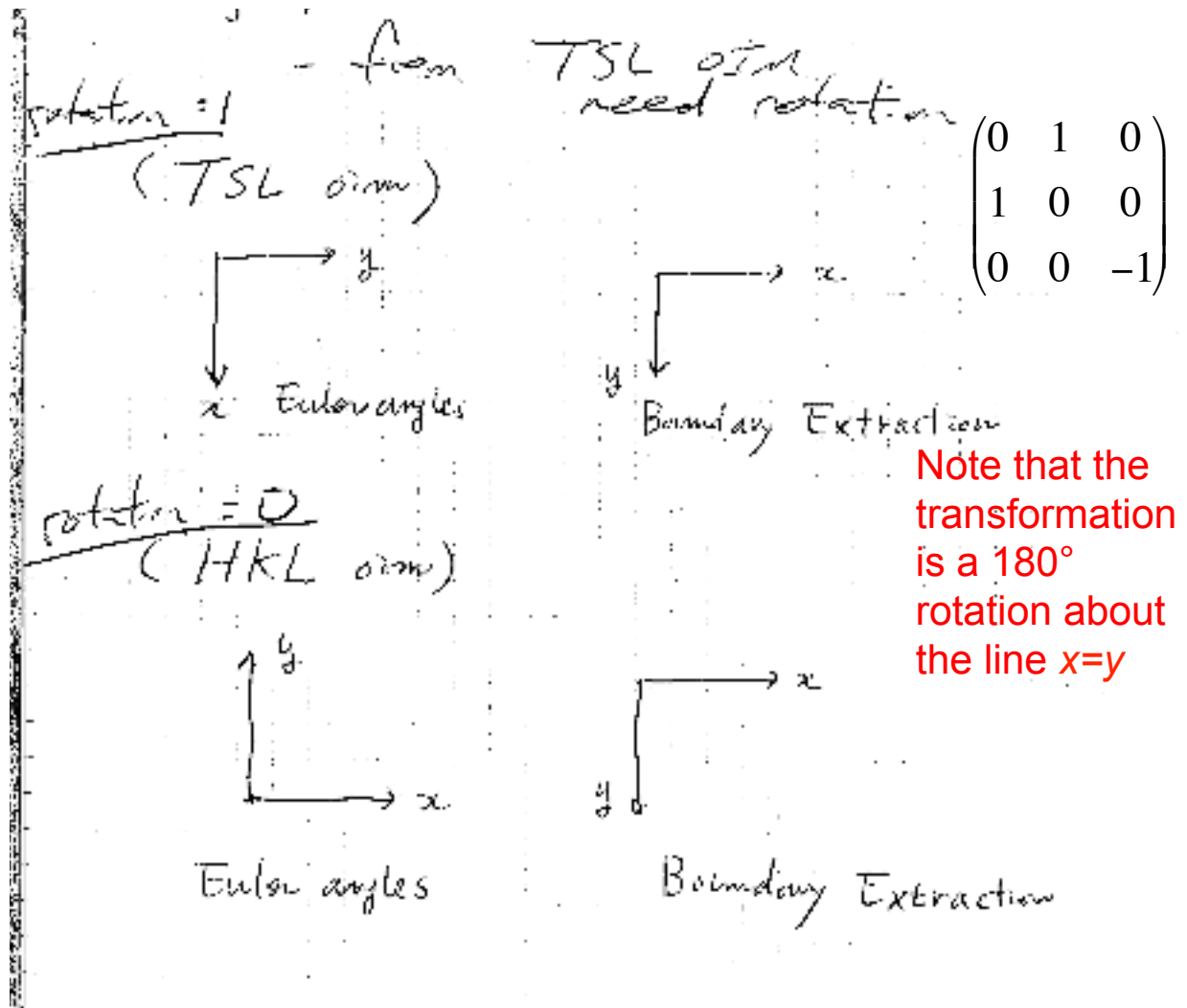
Notes: the image, as presented by the TSL software, has the vertical axis inverted in relation to the physical sample, i.e. a 180° rotation.

TSL / OIM Reference Frames:
Coordinates in Physical Frame, Conversion to Image

• The previous slides make the point that a transformation is required to align spatial coordinates with the Euler frame.

• However, there is also a 180° rotation between the physical specimen and the image. Therefore to align physical markings on a specimen with traces and crystals in an image, it is necessary to take either the physical data and rotate it by 180°, or to rotate the crystallographic information.

ND
$= z_{Euler}$

-TD
$= -y_{sample}$

-RD
$= -x_{Euler}$

Sample Reference Frame for Orientations

$y_{spatial}$

$x_{spatial}$

$z_{spatial}$

+
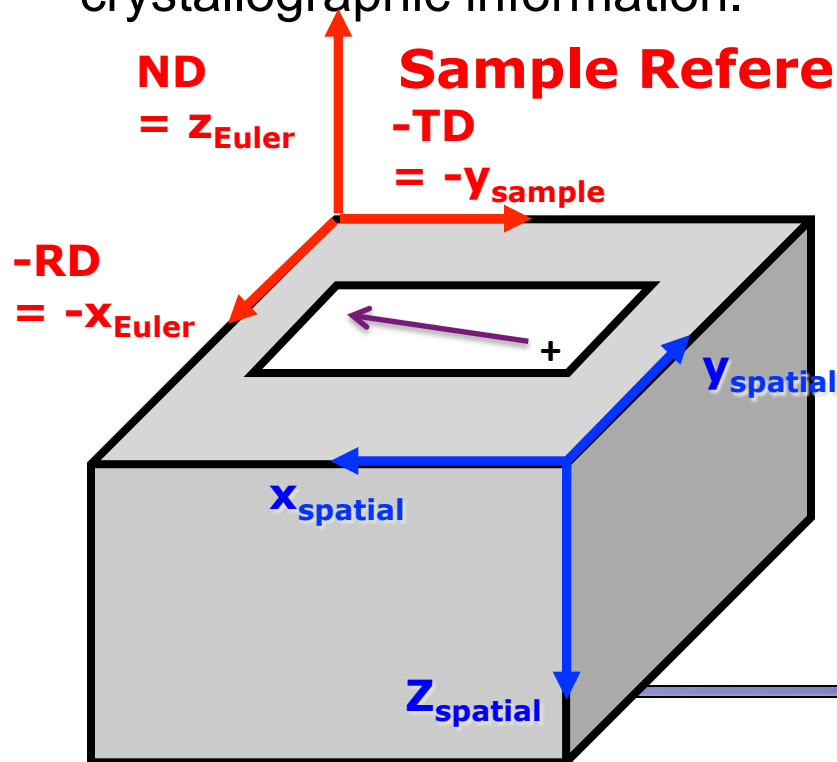
• How to measure lines etc. on a physical specimen?

• Answer: use the spatial frame as shown on the diagram to the left (which is NOT the normal, mathematical arrangement of axes) and your measured coordinates will be correct in the images, provided you plot them according to the IMAGE spatial frame. The purple line, for example, will appear on the image (e.g. an IPF map) as turned by 180° in the x-y plane.

Cartesian Reference Frame for Physical Measurement

$$\mathbf{x}_{Euler} \quad \mathbf{y}_{Cartesian}$$

$$\mathbf{y}_{Euler}$$
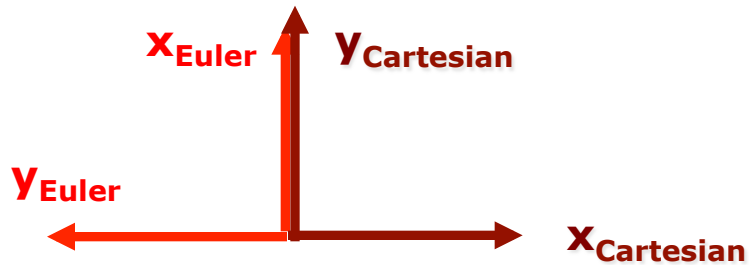
$$\mathbf{x}_{Cartesian}$$

$$\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

• How to measure lines etc. on a physical specimen using the standard Cartesian frame with x pointing right, and y pointing up?
• Answer: use the Cartesian frame as shown on the diagram to the left (which IS the normal, mathematical arrangement of axes and is NOT the frame used for point coordinates that you find in a .ANG file). Apply the transformation of axes (passive rotation) as specified by the transformation matrix shown and then your measured coordinates will be in the same frame as your Euler angles. This transformation is a +90° rotation about $\mathbf{z}_{sample}$. In this case, the z-axis points out of the plane of the page.

TSL / OIM Reference Frames: Labels in the TSL system

$= x_{spatial}$
$= y_{Euler}$

$= y_{spatial}$
$= x_{Euler}$
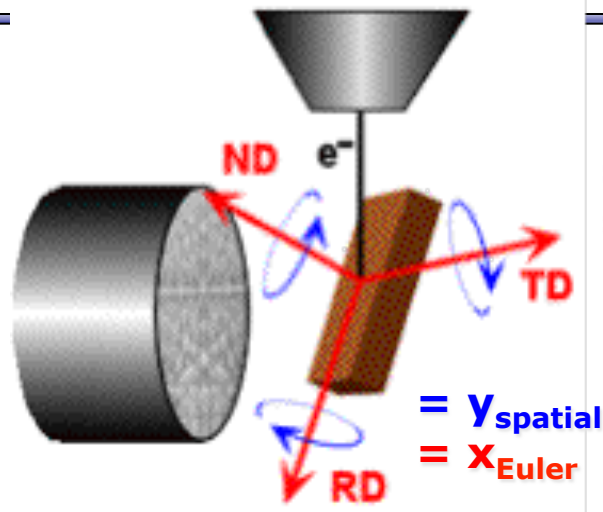
The diagram is reproduced from the TSL Technical Manual (v5 and older); the designation of RD, TD and ND is only correct for Euler angles in reference to the plotted maps/images, *not* the physical specimen

- What do the labels "RD", "TD" and "ND" mean in the TSL literature?
- The labels should be understood to mean that RD is the x-axis, TD is the y-axis and ND the z-axis, all for Euler angles (but *not* spatial coordinates).
- The labels on the Pole Figures are consistent with the maps/images (but NOT the physical specimen).
- The labels on the diagram are consistent with the maps/images, but NOT the physical specimen, as drawn.
- The frame in which the spatial coordinates are specified in the datasets is different from the Euler frame (RD-TD-ND) – see the preceding diagrams for information and for how to transform your spatial coordinates into the same frame as the Euler angles, using a 180° rotation about the line *x=y*.

TSL versus HKL Reference Frames

- The two spatial frames are the same, exactly as noted by Changsoo Kim and Herb Miller previously. The figures show *images* (as opposed to physical specimen).

- The Euler angle references frames differ by a rotation of +90° (add 90° to the first Euler angle) going from the TSL to the HKL frames (in terms of an axis transformation, or passive rotation). Vice versa, to pass from the HKL to the TSL frame, one needs a rotation of -90° (subtract 90° from the first Euler angle).

- The position of the "sample" axes is critical. The names "RD" and "TD" do not necessarily correspond to the physical "rolling direction" and "transverse direction" because these depend on how the sample was mounted in the microscope.

HKL

TD $=010_{sample}$ $= y_{Euler}$

RD $=100_{sample} = x_{Euler}$

$x_{spatial}$

Z (x)   +

$y_{spatial}$

111   001   101

TSL

TD $=010_{sample} = y_{Euler}$

$x_{spatial}$

Z (x)   +

RD $=100_{sample} = x_{Euler}$

111   001   101

$y_{spatial}$
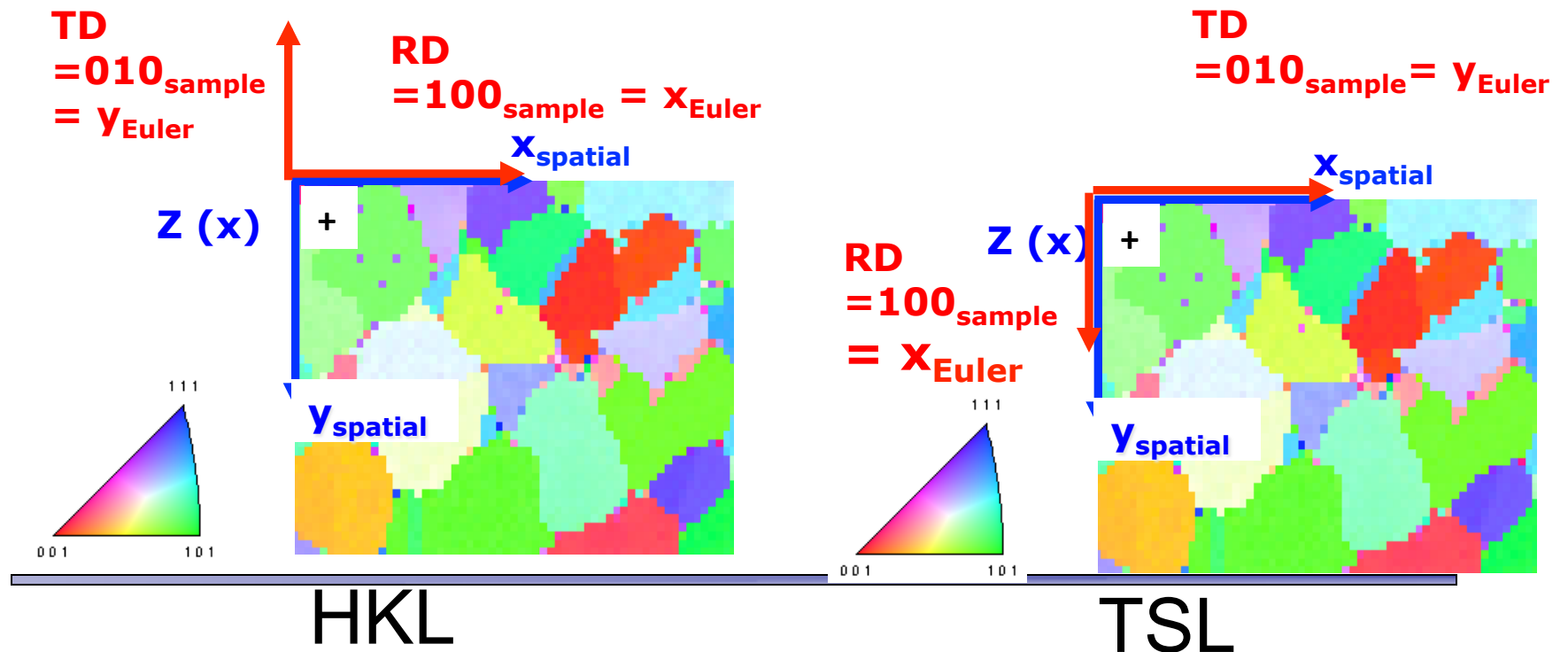
Test of Euler Angle Reference Frames
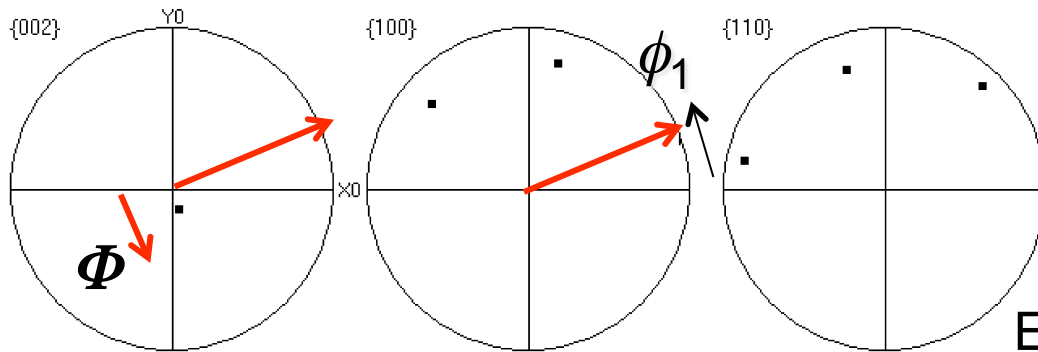
Pole Figures

[HEX_test_map_HKL_In
Zirc-alloy4 (6/mmm)
Complete data set
16 data points
Stereographic projection
Upper hemispheres

Hexagonal crystal symmetry (no sample symmetry)

Euler angles: 17.2°, 14.3°, 0.57°

HKL

A simple test of the frames used for the Euler angles is to have the softwares plot pole figures for a single orientation with small positive values of the 3 angles. This reveals the position of the crystal x-axis via the sense of rotation imposed by the second Euler angle, Φ.

Clearly, one has to add 90° to ϕ_1 to pass from HKL coordinates to TSL coordinates. Note that the CMU TSL is using the x//1120 convention ("X convention"), whereas the Metz Channel/HKL software is using the y//1120 convention ("Y convention").
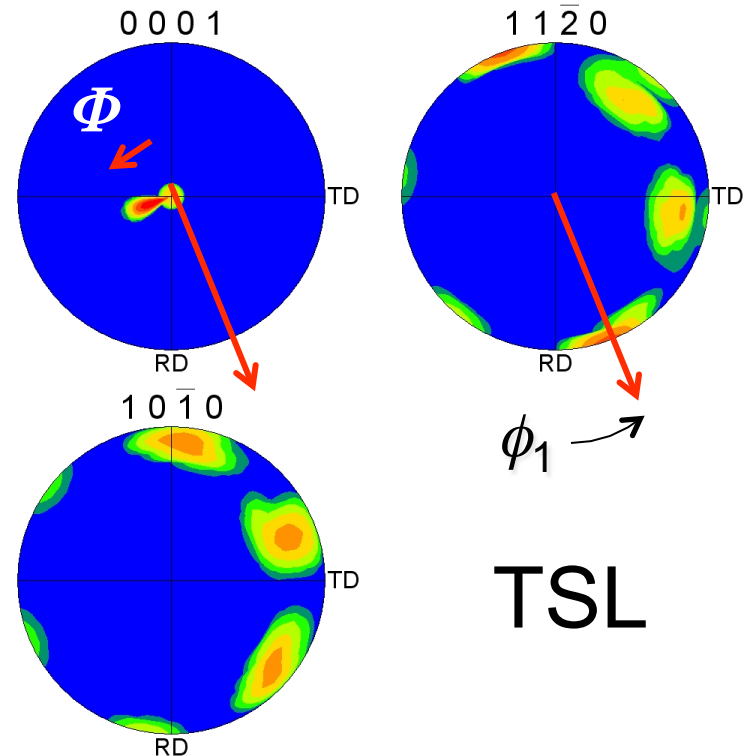
TSL

The Axis Alignment Issue for Hexagonal

- The issue with hexagonal materials is the alignment of the Cartesian coordinate system used for calculations with the crystal coordinate system (the Bravais lattice).

- In one convention (e.g. popLA, TSL), the x-axis, i.e. [1,0,0], is aligned with the crystal a_1 axis, i.e. the [2,-1,-1,0] direction. In this case, the y-axis is aligned with the [0,1,-1,0] direction.

- In the other convention, (e.g. HKL, Univ. Metz software), the x-axis, i.e. [1,0,0], is aligned with the crystal [1,0,-1,0] direction. In this case, the y-axis is aligned with the [-1,2,-1,0] direction.

- See next page for diagrams.

- This is important because texture analysis can lead to an ambiguity as to the alignment of [2,-1,-1,0] versus [1,0,-1,0], with apparent 30° shifts in the data.

- Caution: it appears that the axis alignment is a choice that must be made when installing TSL software so determination of which convention is in use must be made on a case-by-case basis. It is fixed to the y-convention in the HKL software.

- The main clue that something is wrong in a conversion is that either the 2110 & 1010 pole figures are transposed, or that a peak in the inverse pole figure that should be present at 2110 has shifted over to 1010.

Hexagonal Materials: Diagram of Axes

a_3 // $[\bar{1}\,\bar{1}20]$

y // $[010]_{Cartesian}$

a_2 // $[\bar{1}2\bar{1}0]$

x // $[100]_{Cartesian}$

y // $[010]_{Cartesian}$

$[01\bar{1}0]$

x // $[100]_{Cartesian}$

a_1 // $[2\bar{1}\,\bar{1}0]$
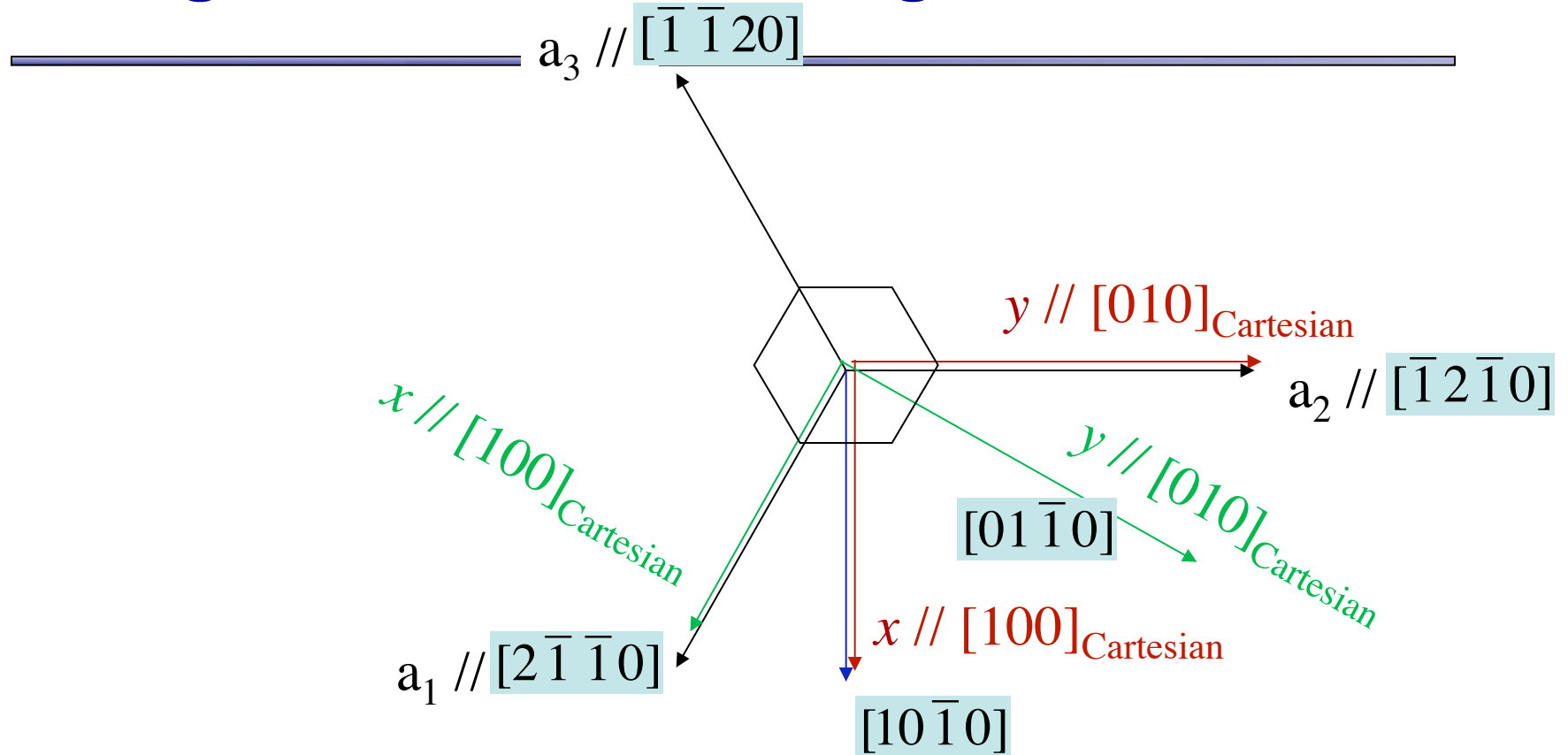
$[10\bar{1}0]$

[uvwx] Direction	Cartesian/ x-convention	Cartesian/ y-convention
$[2\bar{1}\,\bar{1}0]$	+1, 0, 0	+√3, -1, 0
$[\bar{1}2\bar{1}0]$	-1, +√3, 0	0, 1, 0
$[\bar{1}\,\bar{1}20]$	-1, -√3, 0	-√3, -1, 0
$[10\bar{1}0]$	+√3, +1, 0	1, 0, 0
$[01\bar{1}0]$	0, +1, 0	+1, +√3, 0
$[1\bar{1}00]$	+√3, -1, 0	+1, -√3, 0

Euler Angles

- To add to the confusion, all of the different Euler angle conventions can, and are used for hexagonal materials.

- Recall that Bunge Euler angles make the second rotation about the x-axis, whereas Roe, Matthies and Kocks angles rotate about the y-axis.

- Generally speaking there is no problem provided that one stays within a single software analysis system for which the indexing is self-consistent. There are, however, known issues with calculation of inverse pole figures in the popLA package.

HKL frames

Euler angle reference frame

first acquired pixel
(Xpix=1,Ypix=1)

section reference

possible Euler angle reference frames

z pointing out   z pointing in

CS1 = raw data format

CS0 is modified by the user to align axes however they please. The CTF format always exports in CS0 arrangement.

"Virtual chamber" of HKL software, which is used to define the specimen orientation in the microscope chamber (= how to align frame_0 with frame_1); picture is drawn as if the observer was the camera. Note that the maps are turned by 180° with respect to this picture.

- original Euler angles are given in frame_1 (also called CS1)

The ctf format is designed to export Euler angle into frame_0 (CS0), which is correct, provided that the specimen orientation is correctly defined.

58

HKL software
keeping CS0 (sample frame) aligned with CS1(microscope frame)

- relying on what the virtual chamber is showing :
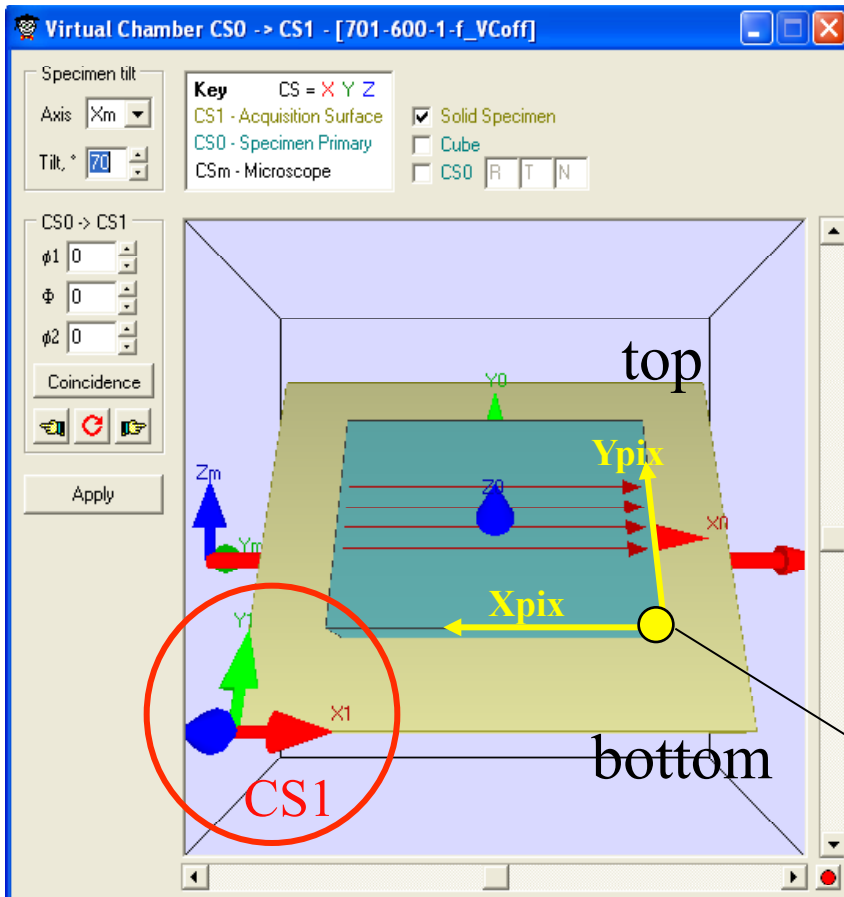
section reference
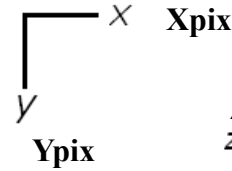
possible Euler angle reference frames
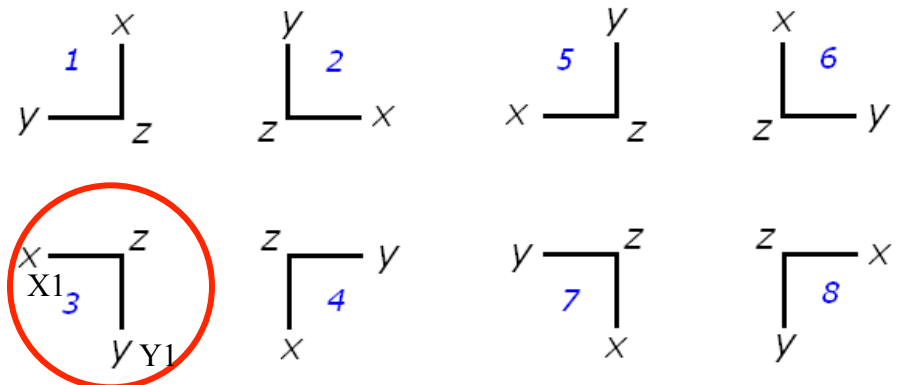
CS1 as shown in the virtual chamber

first acquired pixel ($X_{spatial}$=1,$Y_{spatial}$=1)
= top left pixel of the resulting map

- but this alignment is not consistent with the axes of the PF plots…
or with previous experience with data sets from the HKL software

Beta-transformed Ti (from Nathalie Gey, LETAM – now LEM3)
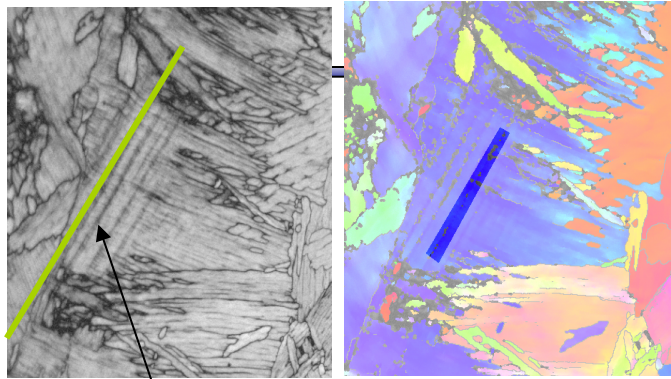
Traces of {10-10} planes

(Z0 pointing out)
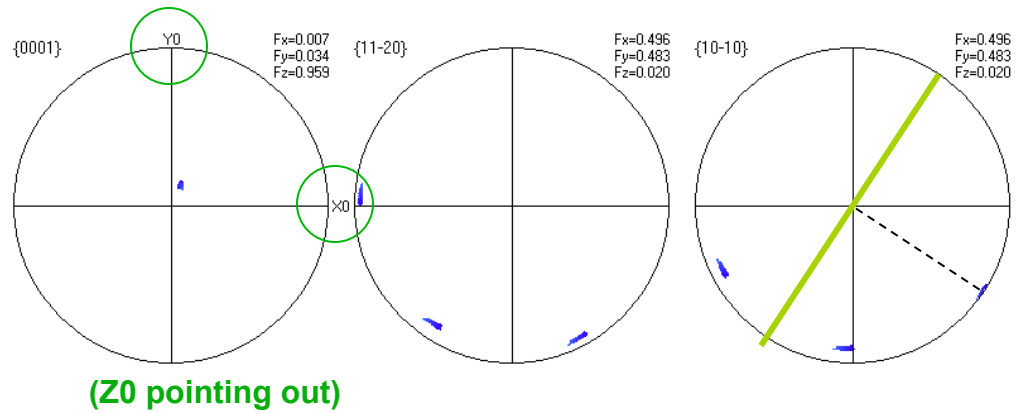
Pole Figures

[HF1_P28cut1_FA.cpr]
Ti-Hex (6/mmm)
Subset3
3608 data points
Equal Area projection
Upper hemispheres

{0001} Y0 Fx=0.007 Fy=0.034 Fz=0.959
{11-20} Fx=0.496 Fy=0.483 Fz=0.020
{10-10} Fx=0.496 Fy=0.483 Fz=0.020

$X_{spatial}$

$Y_{spatial}$ EBSD map
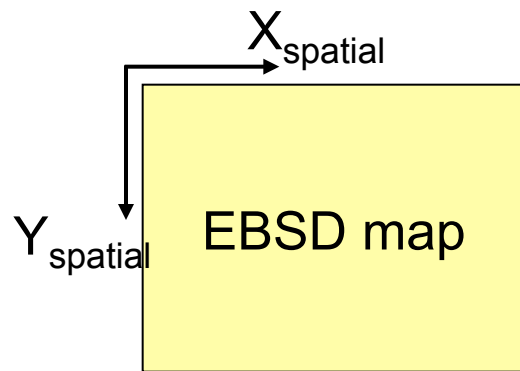
Xpix, Ypix = spatial frame
X0,Y0,Z0 = euler angle frame, supposed
to be aligned with X1,Y1,Z1 (µscope
frame)

section reference

X

y

possible Euler angle reference frames

z pointing out   z pointing in

Euler frame

x   1   y   z   y   2   z   x   y   5   x   z   x   6   z   y

x   3   z   y   z   4   y   x   y   7   z   x   z   8   x   y

Spatial frame
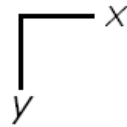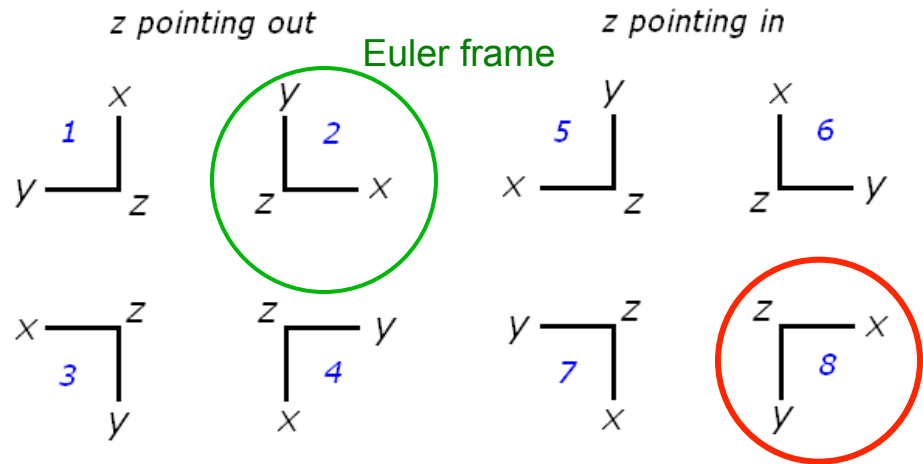
Note that a rotation of the PF axes by 180° around Z to recover the frame numbered 3 on the PF plots, would also be consistent with the trace being perpendicular to <10-10>…

Notes on HKL Frames

There is a discrepancy in the HKL software between how the frame CS1 (and CS0) is represented in the virtual chamber and how the PF axes are placed

The difference is a rotation by 180° around the Z direction (frame numbered 2 versus frame 3)

It is not possible to determine which one is correct from the two previous slides

Nevertheless, the test maps acquired with LETAM's HKL system and with MRSEC's TSL one did show that the frame number 2 was the correct one

Geometrically Necessary Dislocations (GND)

- Orientation gradients in (crystalline) metals and ceramics can be accommodated in various ways.
  1. Elastic distortions of the lattice
  2. Arrays of dislocations
  3. Grain boundaries (high angle)
  4. Disclinations

- Ceramics rarely exhibit orientation gradients because they are difficult to deform plastically (high Peierls stress).

- Elastic distortions are likely to be extremely small in metals because of the low resistance to dislocation motion, generally speaking.

- Dislocation arrays are how orientation gradients are produced within grains. This dislocation content is known as the Geometrically Necessary Dislocation density (GND) and represents a lower bound on the dislocation density. Statistically stored dislocations are considered to be unobservable at the scale of EBSD. GND is created during the plastic deformation of metals.

- High angle grain boundaries with atomically disordered interface structures also accommodate orientation gradients (in the sense of a sharp interface limit).

- Disclinations are an alternative approach to accommodating orientation gradients. They are more controversial because there are very few direct observations of disclinations, by contrast to lattice dislocations.

GND, contd.

- We now address the analysis of GND.

- There is a tensor known as the dislocation tensor or Nye's tensor, α.

$$\alpha_{ij} = e_{ikl}\left(\varepsilon^e_{jl,k} + g_{jl,k}\right)$$

- Here, ε^e is the elastic strain tensor and g is the lattice orientation expressed as an orientation matrix in the usual fashion. In the absence of long-range elastic stress fields, Nye's original formulation of the dislocation tensor is obtained:

$$\alpha_{ij} = e_{ikl}g_{jl,k}$$

- The dislocation tensor can thus be directly calculated from the observable, i.e. the gradient of the orientation field. We can also write: $\alpha = \text{curl}(\boldsymbol{g})$

J.F. Nye, "Some geometrical relations in dislocated crystals" *Acta Metall.*, **1**, 153 (1953).
El-Dasher *et al.*, 2003. "Viewpoint: experimental recovery of geometrically necessary dislocation density in polycrystals" *Scripta mater.* **48**, 141.

Nye tensor to GND content

- Nye's original work also shows a precise connection between the dislocation tensor and the local dislocation network, formally expressed as:

$$\alpha_{ij} = \sum_{k=1}^{K} \rho^k \mathbf{b}_i^k \hat{\mathbf{z}}_j^k$$

- Here, ρ is the dislocation density of the $\mathrm{k^{th}}$ dislocation type, b is the associated Burgers vector and z is the corresponding line direction. There are 1 through K dislocations types.

- It is typical to make the line direction discrete, i.e. either edge (perpendicular to the Burgers vector) or screw type (parallel to b). In fcc metals with 6 distinct <110> Burgers vectors, this gives 18 dislocation types because each <110> edge can exist on two different slip planes.

- The analytical challenge is, therefore, the undetermined nature of the equation because there are more free variables on the RHS than (derived) observables on the LHS. Generally speaking, numerical methods such as simplex must be resorted to, combined with a constraint such as minimization of the total dislocation line length.

Disclination analysis

- Analyzing orientation gradients in terms of disclinations has been known for many years.

- Disclinations can be thought of as wedges on a continuum basis. Isolated disclinations have divergent strain fields but disclination dipoles are similar (but not the same as) arrays of edge dislocations.

- Disclination analysis has been developed by a number of people such as Romanov; most recently Fressengeas and Capolungo.

Disclinations, analysis

- To make a start, consider the gradient of the displacement field, formally the distortion tensor and equivalent to strain.

$$U = \mathrm{grad}(u)$$

- Consider the incompatible elastic distortion of the lattice that arises to maintain lattice continuity. The *curl* of this tensor provides the same Nye tensor as before.

$$\alpha = \mathrm{curl}(U_e^\perp) \approx \mathrm{curl}(g)$$

- There is a similar equation for the disclination density, θ, based on the curl of the elastic curvature, κ_e:

$$\theta = \mathrm{curl}(\kappa_e)$$

- The tricky part is how to obtain the elastic curvature from the observable, i.e. the orientation field, g. Here, ω_e is the rotation vector, obtained from the misorientation rotation matrix, Δg.

$$\kappa_e = grad(\vec{\omega}_e); \; \vec{\omega}_i^e = -e_{ijk}\Delta g_{jk}; \text{ thus } \kappa_{ij}^e \approx \Delta\omega_i / \Delta x_j; \theta_{ij} \approx e_{jkl}\Delta\omega_i / \Delta x_l / \Delta x_k$$

Disclinations, analysis, contd.

- It is useful to note that one can always compute the Nye tensor and fit a dislocation density to this value at each point. The curl of the curvature tensor, κ_e, which is the disclination vector, is assumed to be zero for this. If this field is non-zero, then a disclination field is present. This disclination field can be regarded as a quantification of the rotation defects present in the material.

- Recent papers on this topic include these:
  - M. Upadhyay, L. Capolungo, V. Taupin, C. Fressengeas, "Grain boundary and triple junction energies in crystalline media: A disclination based approach", *International Journal of Solids and Structures* **48** (2011) 3176–3193
  - C. Fressengeas, V. Taupin, M. Upadhyay, L. Capolungo, "Tangential continuity of elastic/plastic curvature and strain at interfaces", *International Journal of Solids and Structures* **49** (2012) 2660–2667