# Analysis of EBSD Data

27-750
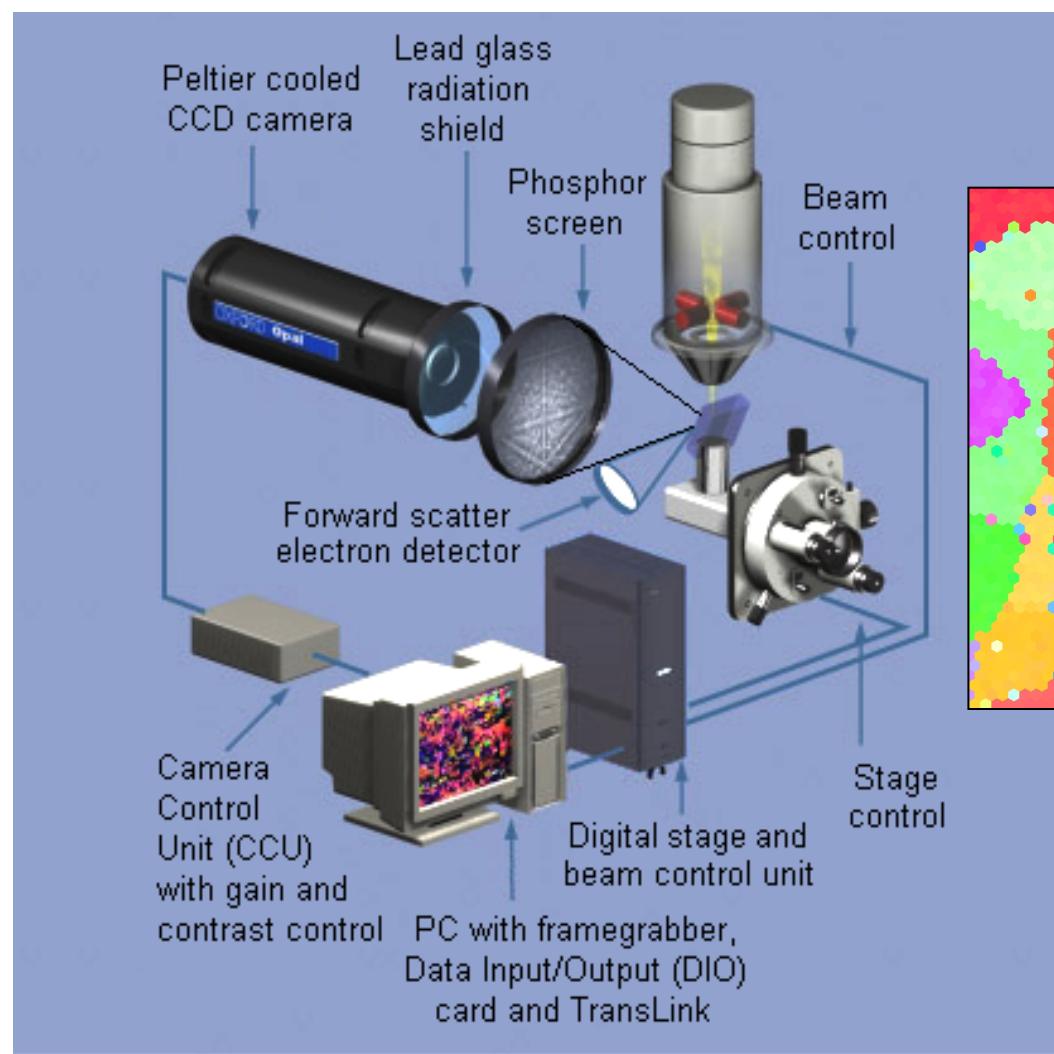
Texture, Microstructure & Anisotropy

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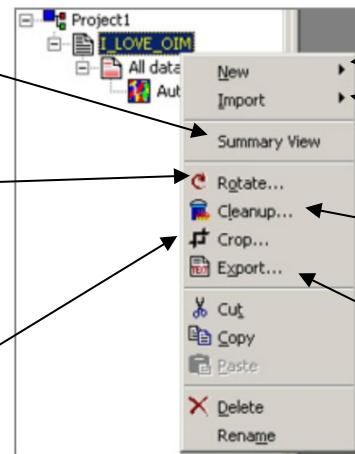
Rotate the *orientations* of each point about *sample frame*

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

Project1
  I_LOVE_OIM
    All data
      Aut
New
Import
Summary View
Rotate...
Cleanup...
Crop...
Export...
Cut
Copy
Paste
Delete
Rename

Project1
  I_LOVE_OIM
    All data
      Aut
New
Import
Summary View
Export Template...
Export Grain File...
Cut
Copy
Paste
Delete
Rename
Properties...
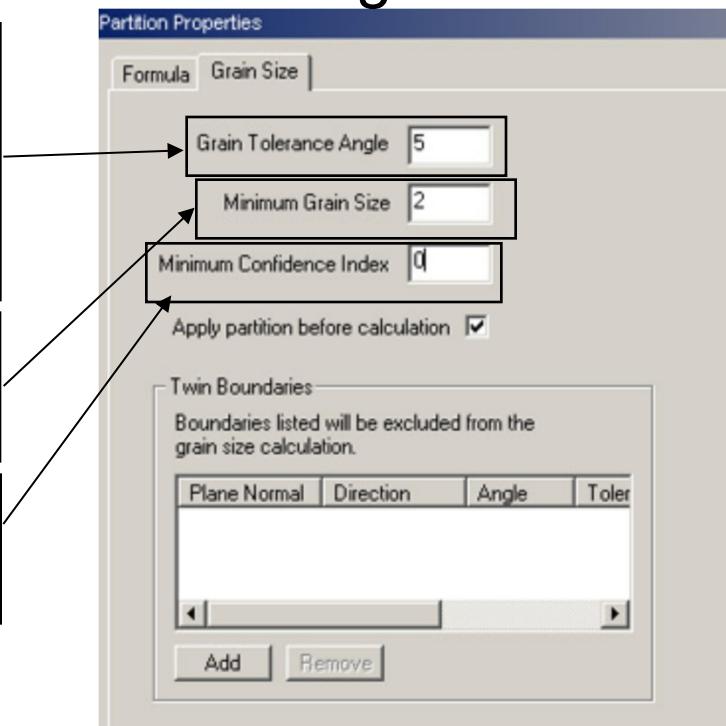
# Grain Definitions

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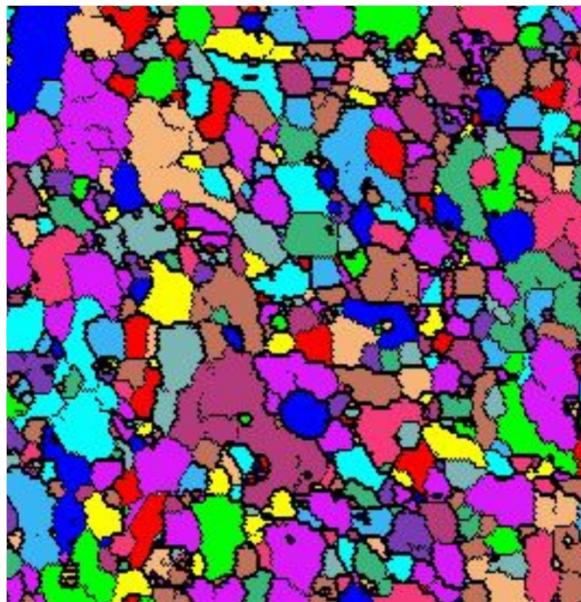
Points with a CI less than specified are excluded from *statistics*



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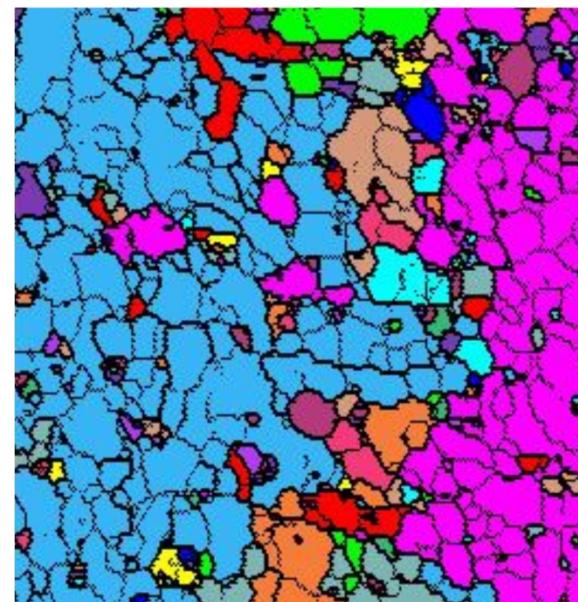
*Note:* Points that are excluded are given a grain ID of 0 (zero) in exported files

# Grain Definitions

Examples of definitions



3 degrees
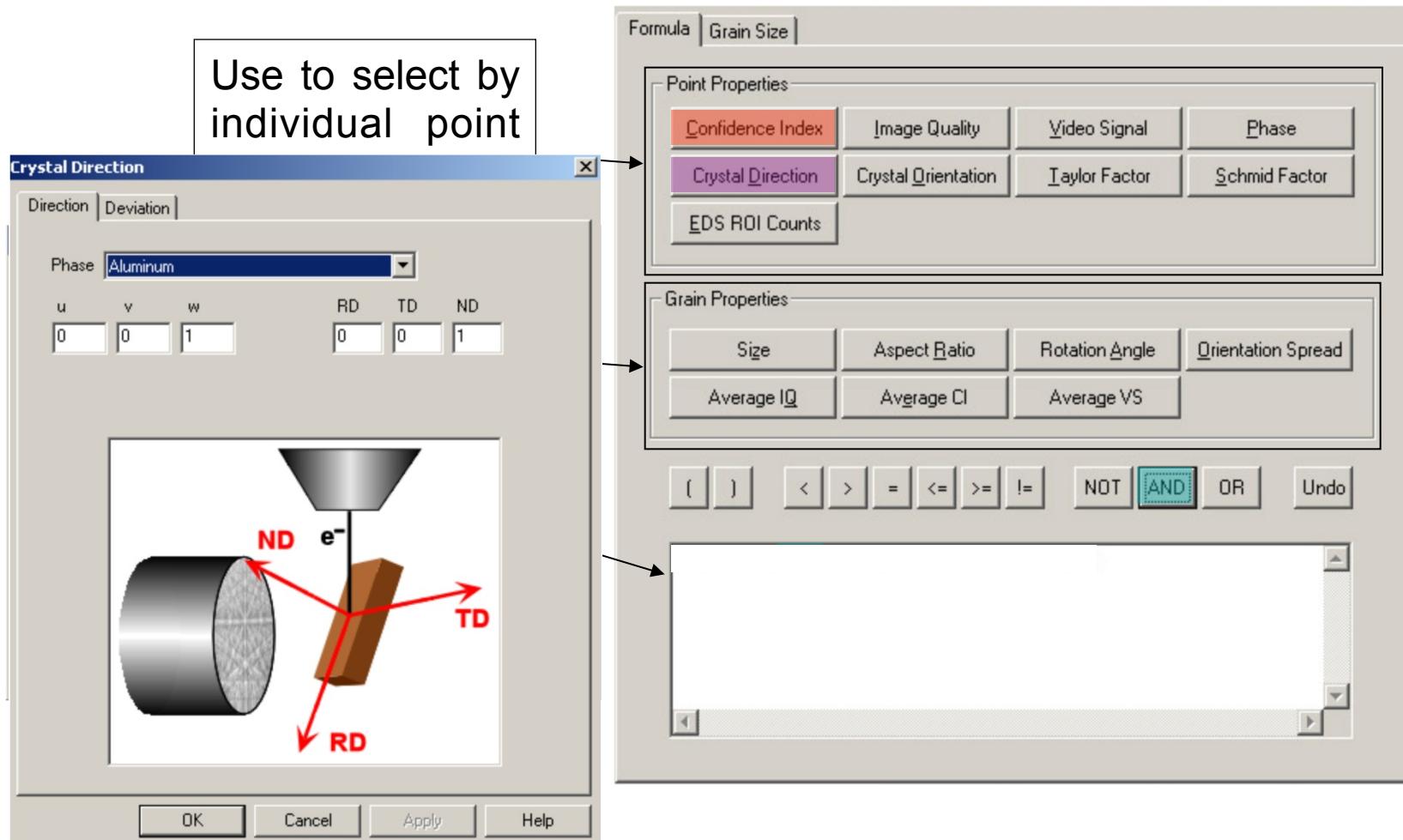
15 degrees

Note that each color represents 1 grain

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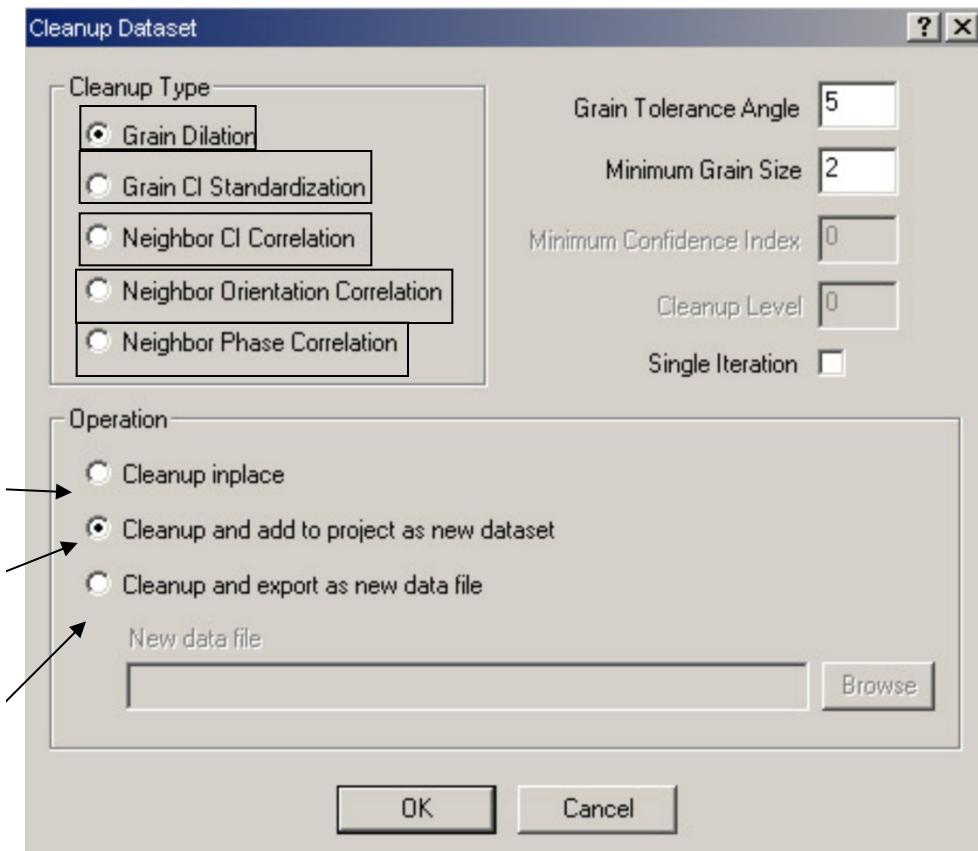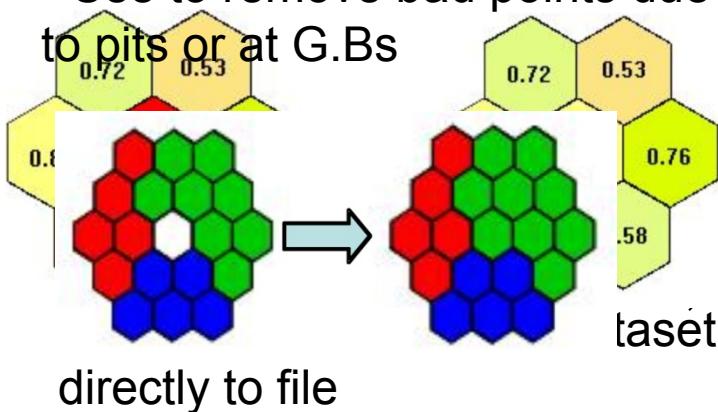
- Choose which points to include in analysis by setting up selection formula



Use to select by individual point

# 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
- Use to remove bad points due to pits or at G.Bs
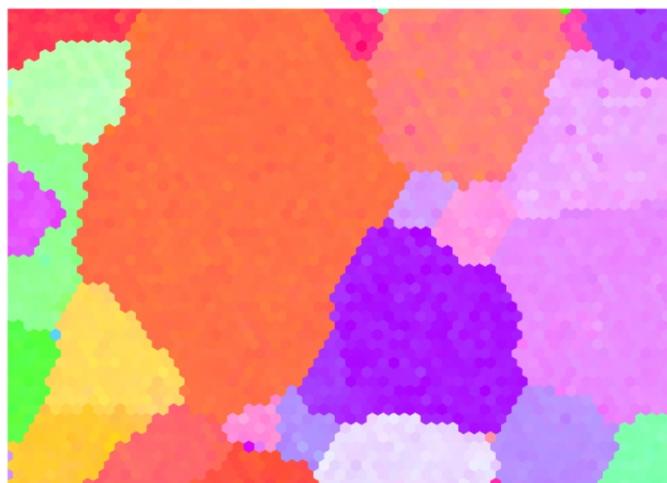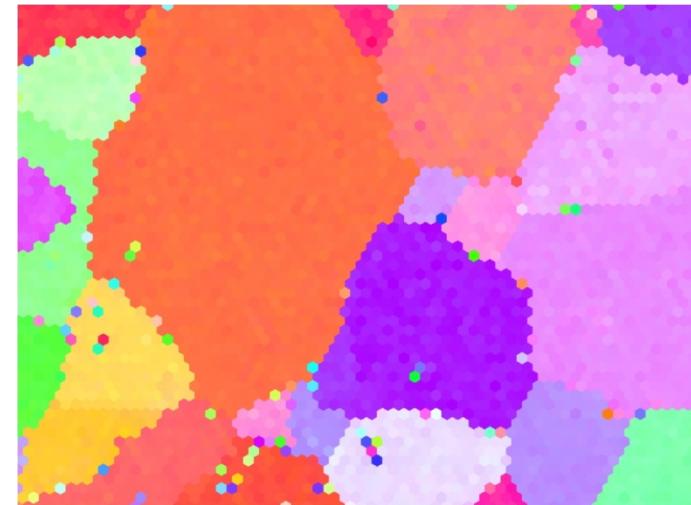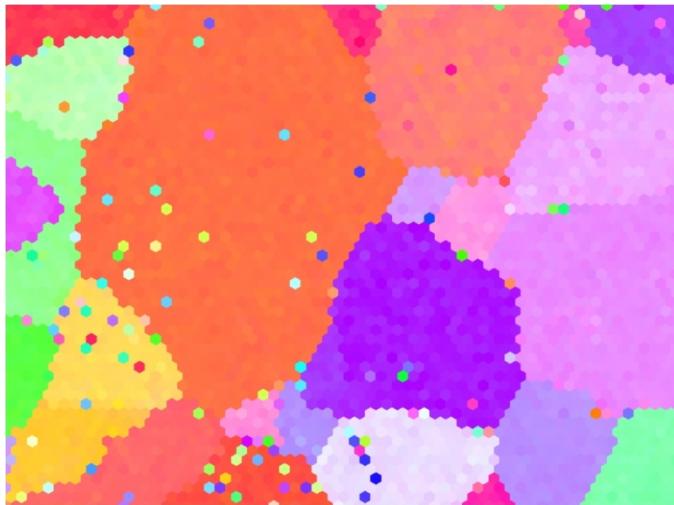
Neighbor CI Correlation
-- Performed only on points with CI less than a given minimum
-- The orientation and CI of the neighbor with highest CI is assigned to these points
-- Takes the orientation and CI of the neighboring point with highest CI

...taset
directly to file

**Cleanup Dataset** ? X

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

# Neighbor Correlation Example



No Cleanup
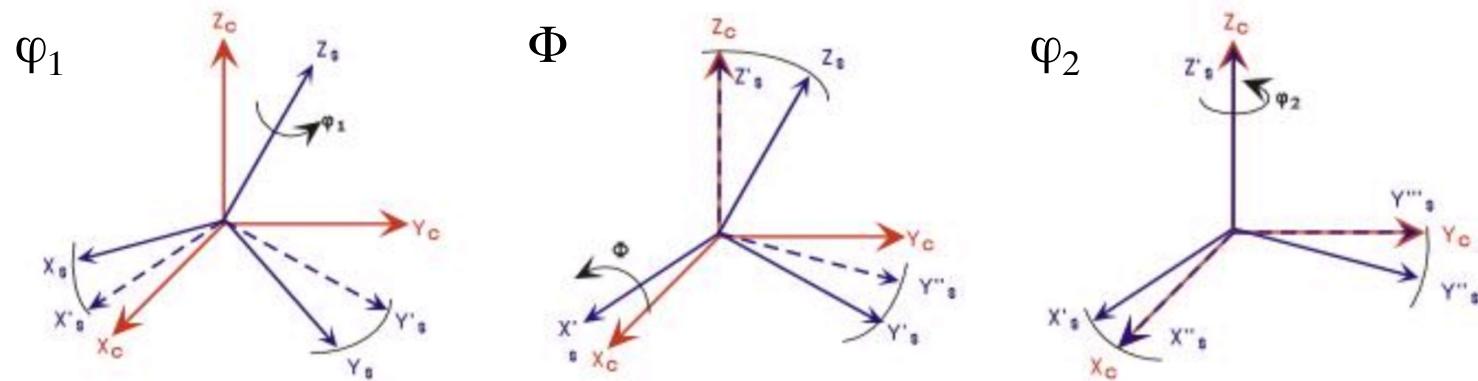


Level 0



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

$\varphi_1$



$\Phi$



$\varphi_2$



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

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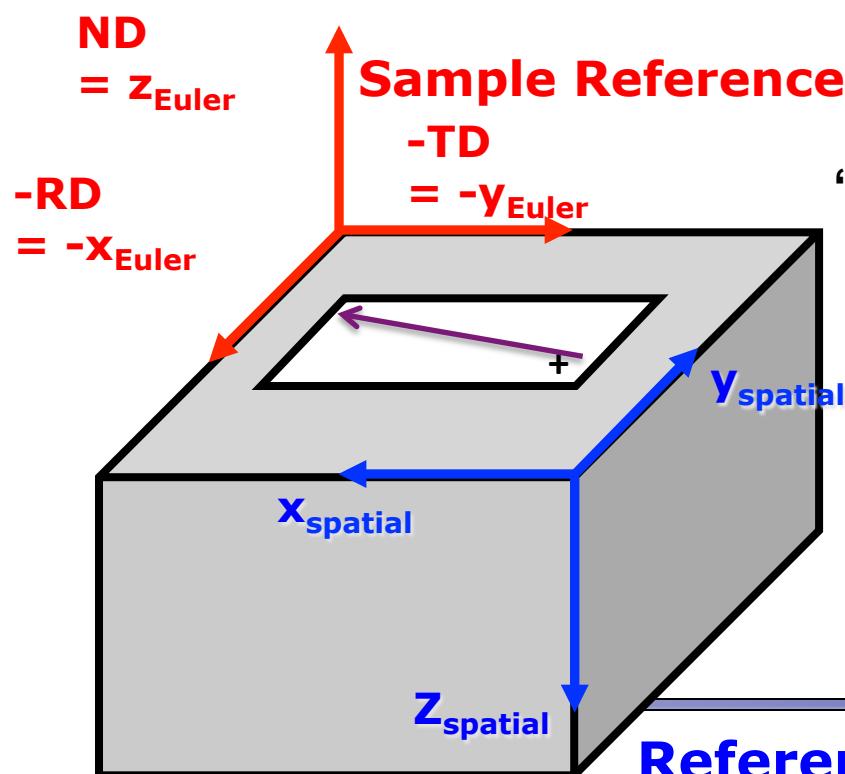
- This next set of slides is devoted to explaining, as best we can, how to relate features observed in EBSD images/maps to the Euler angles.

- 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.

$RD = x_{Euler}$
$= 100_{sample}$
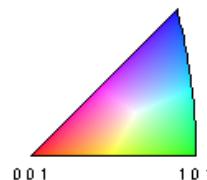
**Physical specimen:**
Mounted in the SEM, the tilt axis is parallel to "$x_{spatial}$"

+

111

$y_{spatial}$

001        101
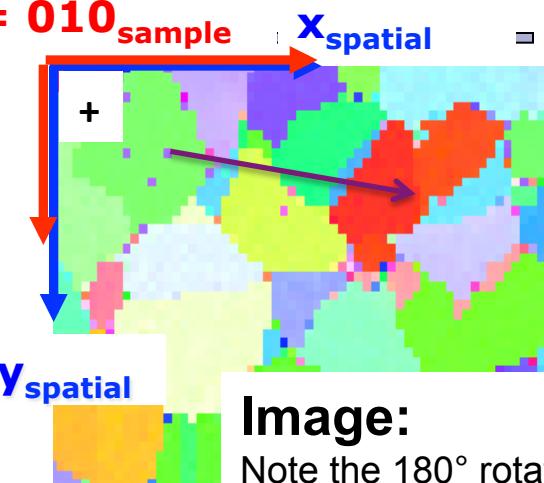
**Image:**
Note the 180° rotation.

ND
$= z_{Euler}$

**Sample Reference Frame for Orientations/Euler Angles**

-TD
$= -y_{Euler}$

"+" denotes the Origin

-RD
$= -x_{Euler}$

$y_{spatial}$

+

**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**
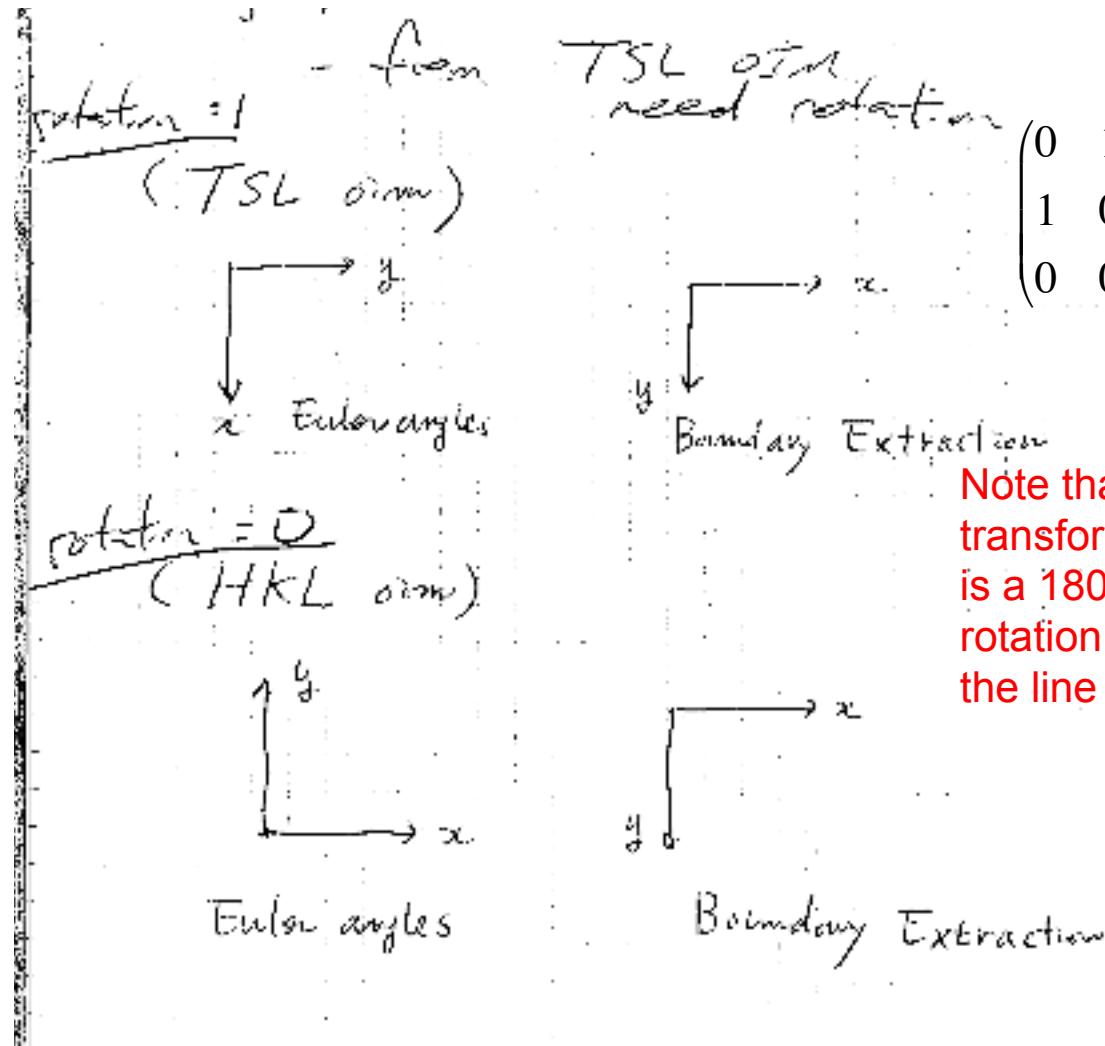
# TSL / OIM Reference Frames for Images

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.

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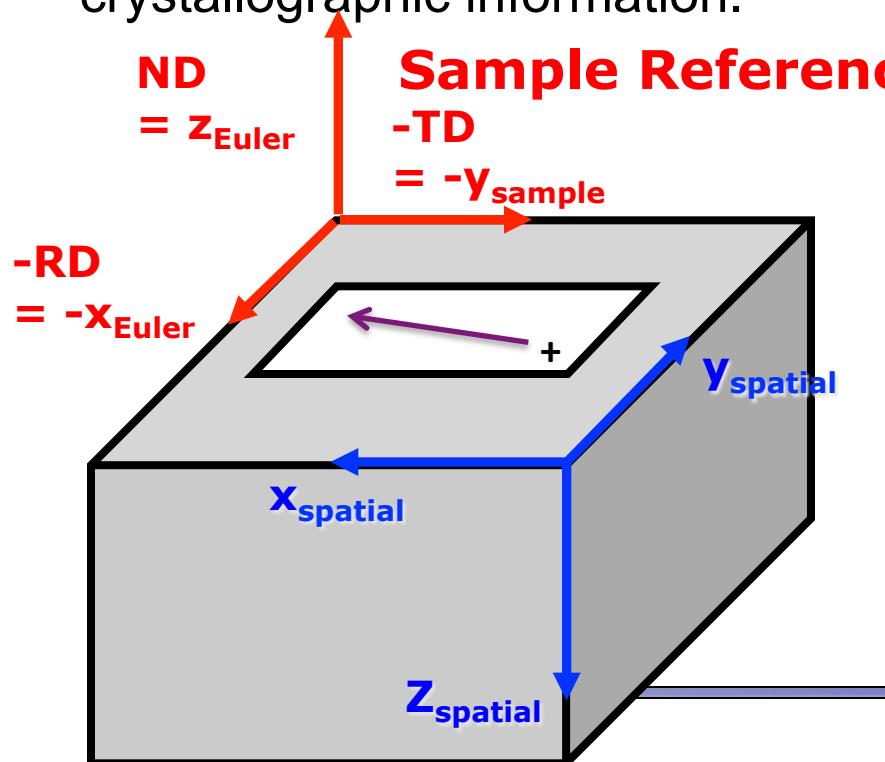


Note that the transformation is a 180° rotation about the line *x=y*

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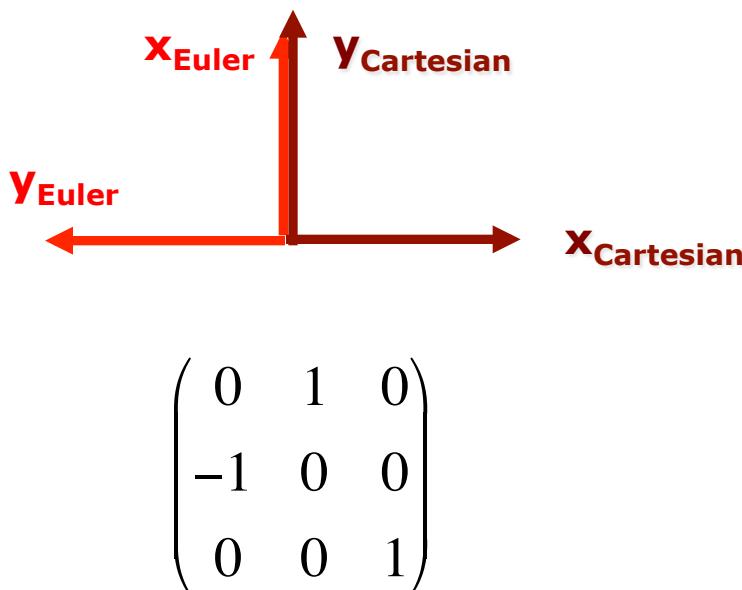
# TSL / OIM Reference Frames:
## Coordinates in Physical Frame, Conversion to Image

• 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.
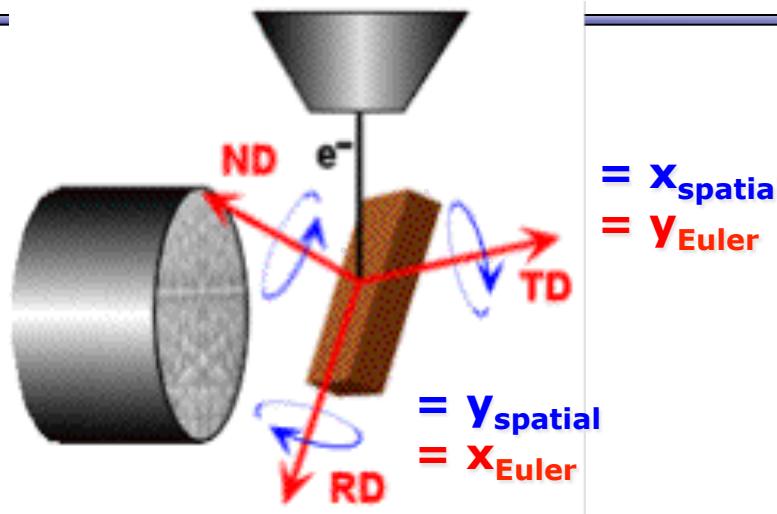
## Sample Reference Frame for Orientations

ND = $z_{Euler}$

-TD = $-y_{sample}$

-RD = $-x_{Euler}$

$y_{spatial}$

$x_{spatial}$

$z_{spatial}$

+

• 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

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

$\mathbf{y}_{Euler}$

$\mathbf{x}_{Cartesian}$

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

- 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



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

$= \mathbf{y_{spatial}}$
$= \mathbf{x_{Euler}}$
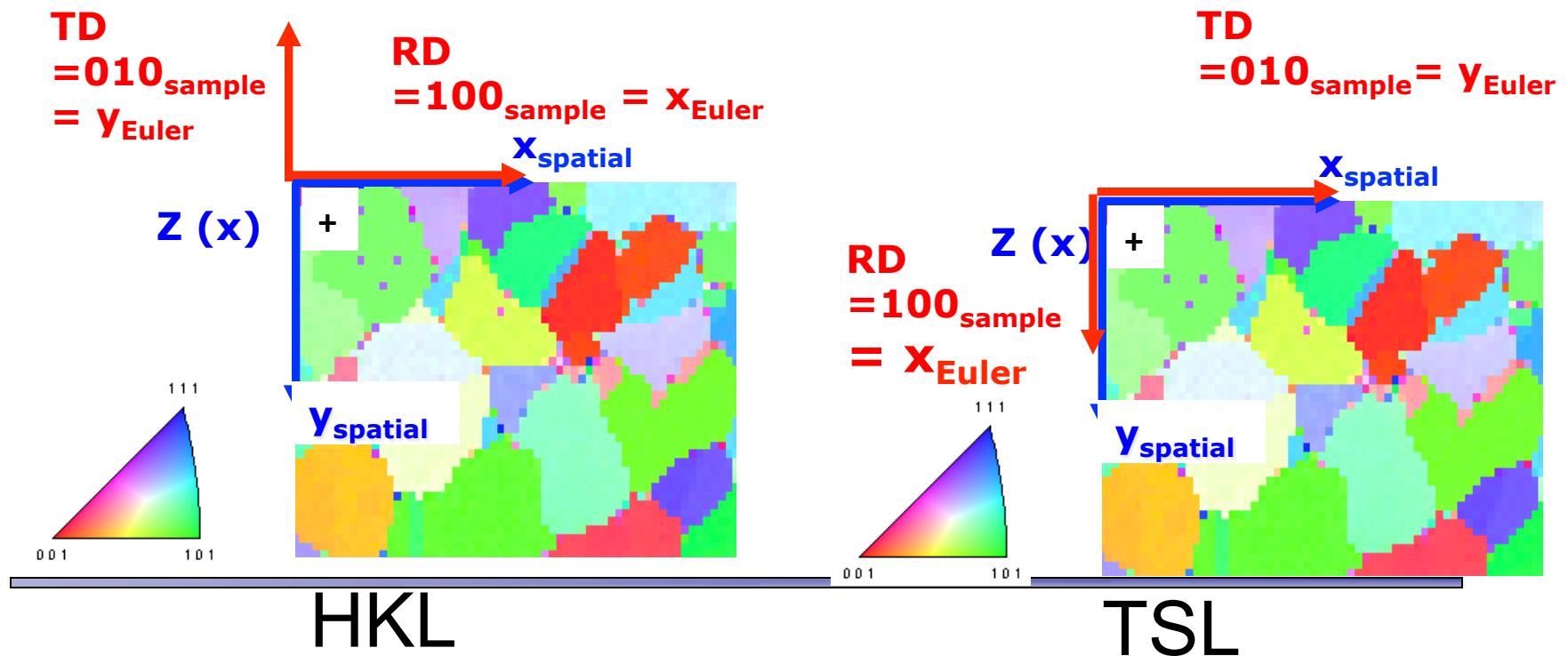
**The diagram is reproduced from the TSL Technical Manual (v5 and older); the designation of RD, TD and ND is only correct for Euler angles in reference to the plotted maps/ images, *not* the physical specimen**
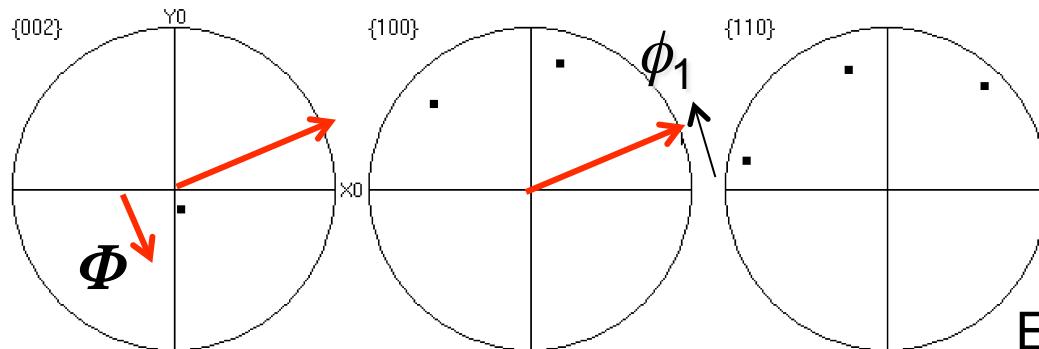
- What do the labels "RD", "TD" and "ND" mean in the TSL literature?
- The labels should be understood to mean that RD is the x-axis, TD is the y-axis and ND the z-axis, all for Euler angles (but *not* spatial coordinates).
- The labels on the Pole Figures are consistent with the maps/images (but NOT 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

TSL

# Test of Euler Angle Reference Frames



{002}  Y0  {100}  {110}  $\phi_1$

X0

$\Phi$

Pole Figures

[HEX_test_map_HKL_In
Zirc-alloy4 (6/mmm)
Complete data set
16 data points
Stereographic projection
Upper hemispheres
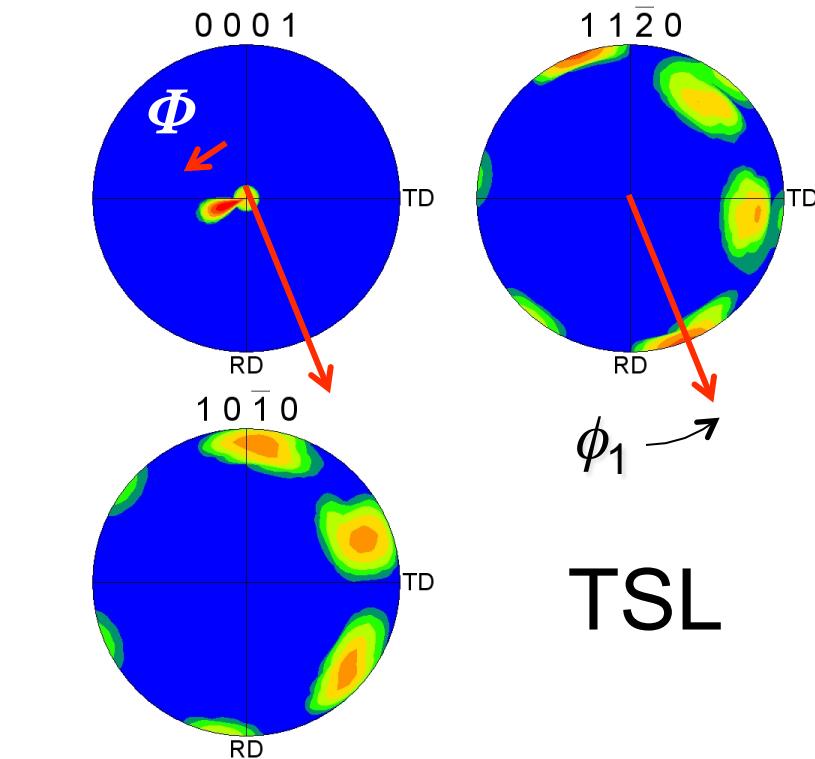
Hexagonal crystal symmetry (no sample symmetry)

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, $\Phi$.

Clearly, one has to add 90° to $\phi_1$ 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").

0 0 0 1          1 1 $\bar{2}$ 0

$\Phi$

TD          TD

RD          RD

1 0 $\bar{1}$ 0          $\phi_1$

TD          ## TSL

RD
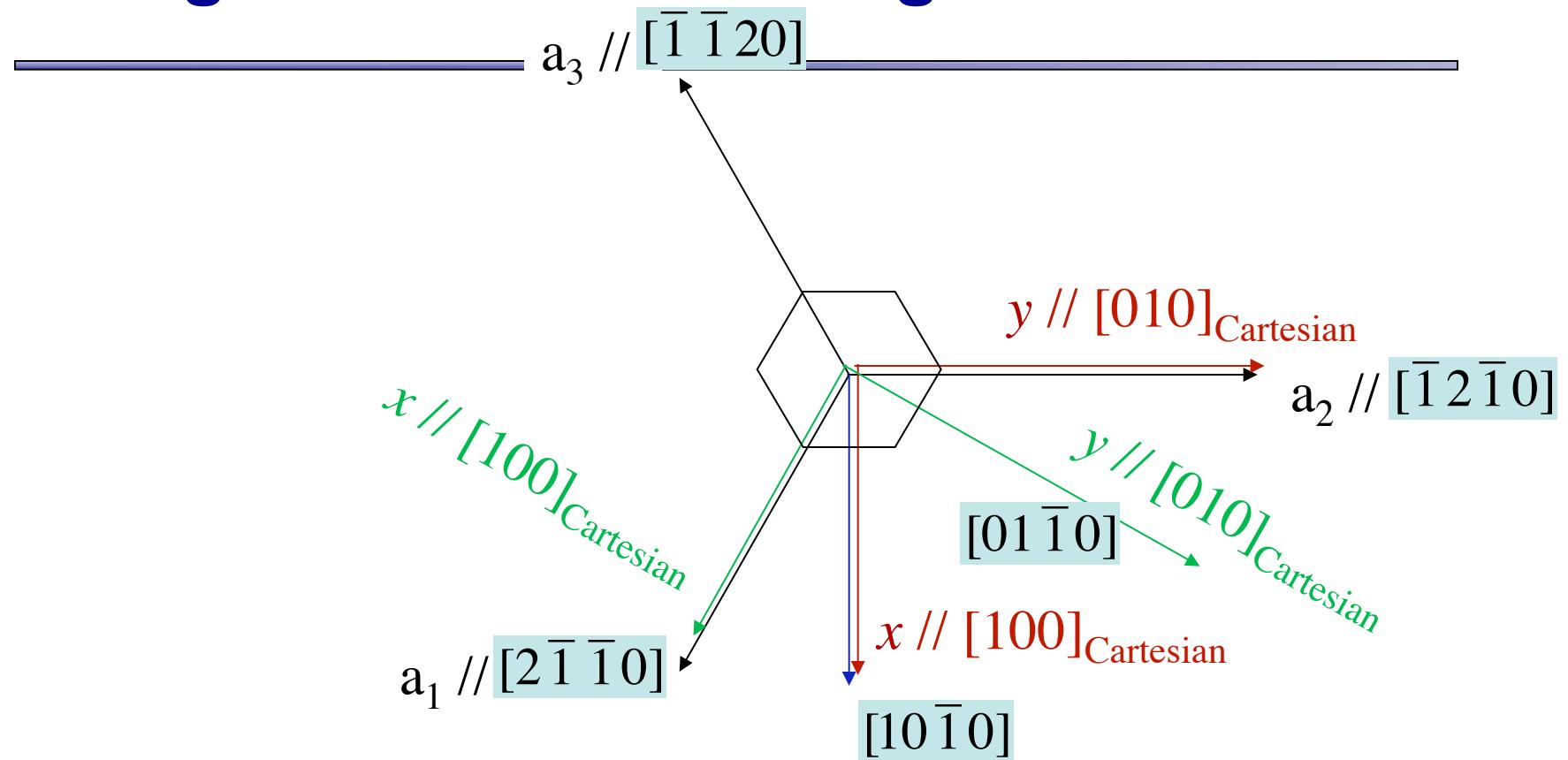
# The Axis Alignment Issue for Hexagonal

- 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.
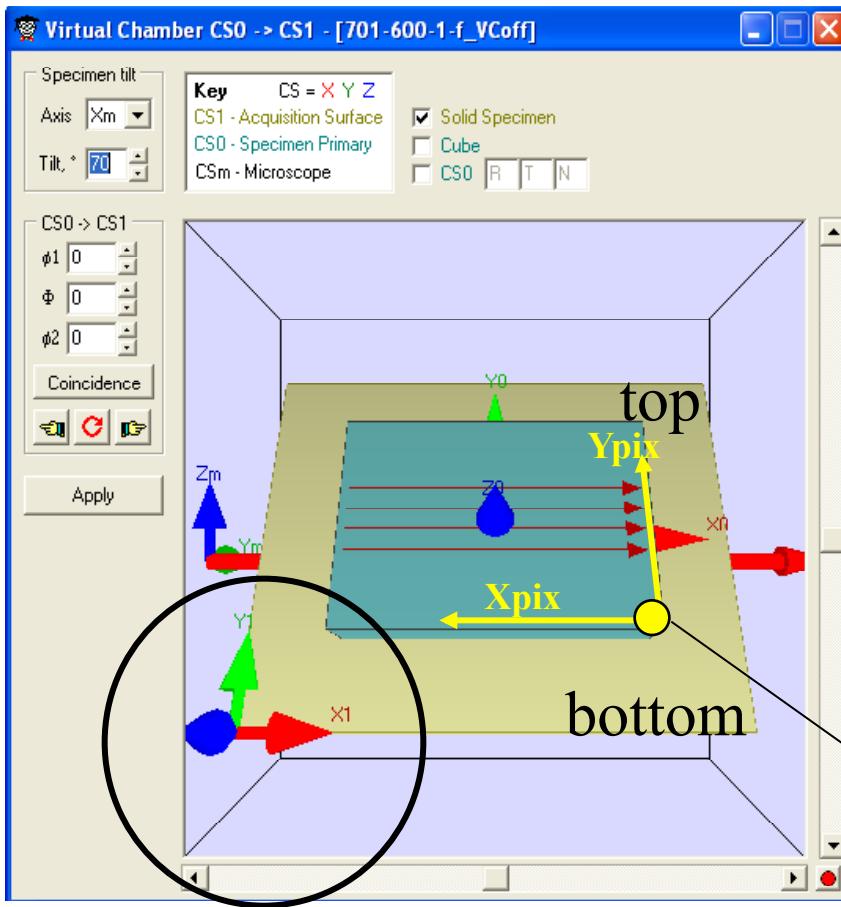
# Hexagonal Materials: Diagram of Axes

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

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

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

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

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

$[01\bar{1}0]$

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

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

$[10\bar{1}0]$

| [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 |
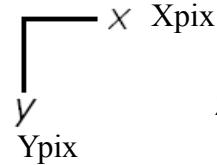
# Euler Angles

- 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



**Virtual Chamber CS0 -> CS1 - [701-600-1-f_VCoff]**

Key    CS = X Y Z
CS1 - Acquisition Surface    ☑ Solid Specimen
CS0 - Specimen Primary    ☐ Cube
CSm - Microscope    ☐ CS0 R T N

Specimen tilt
Axis  Xm
Tilt, °  70

CS0 -> CS1
φ1  0
Φ  0
φ2  0
Coincidence
Apply

section reference
X  Xpix
Y
Ypix

possible Euler angle reference frames

z pointing out

z pointing in

top
Ypix
Xpix
bottom

Euler angle reference frame

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

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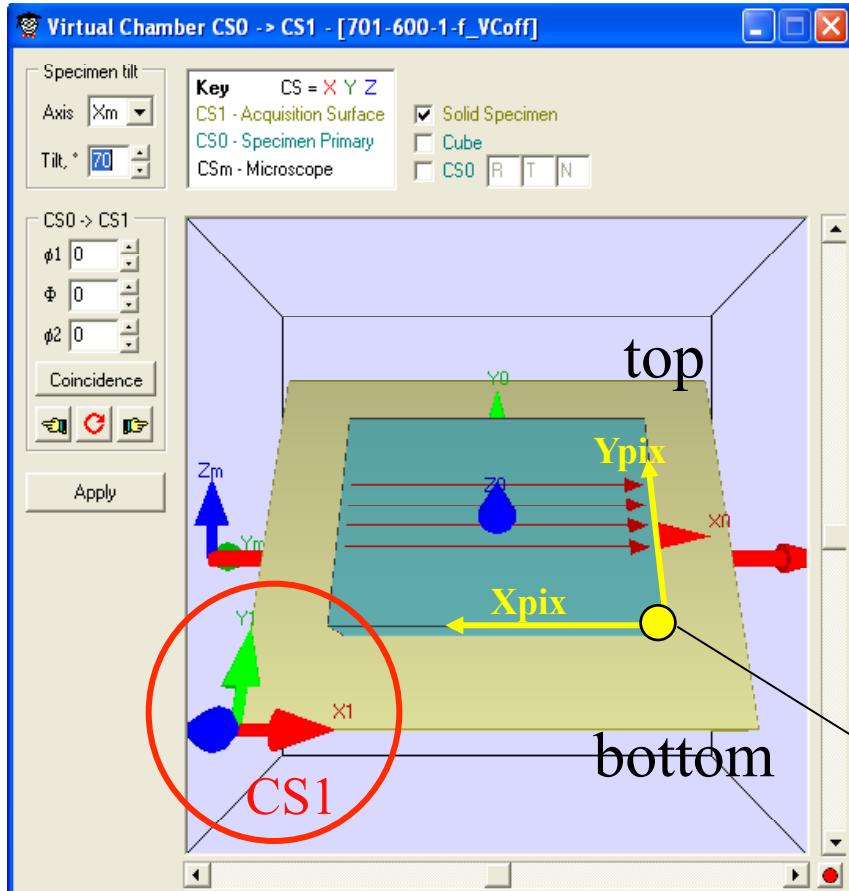
**- original Euler angles are given in frame_1** (also called CS1)

The ctf format is designed to export Euler angle into frame_0 (CS0), which is correct, provided that the specimen orientation is correctly defined.
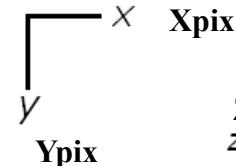
# HKL software
## keeping CS0 (sample frame) aligned with CS1(microscope frame)

- relying on what the virtual chamber is showing :
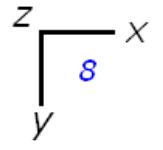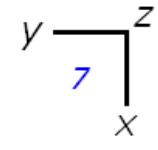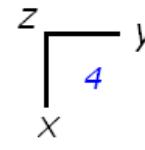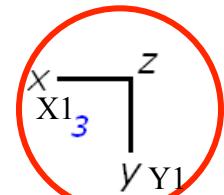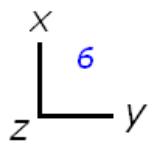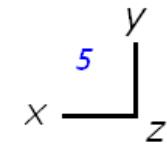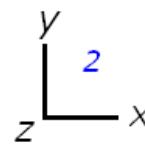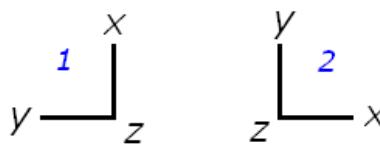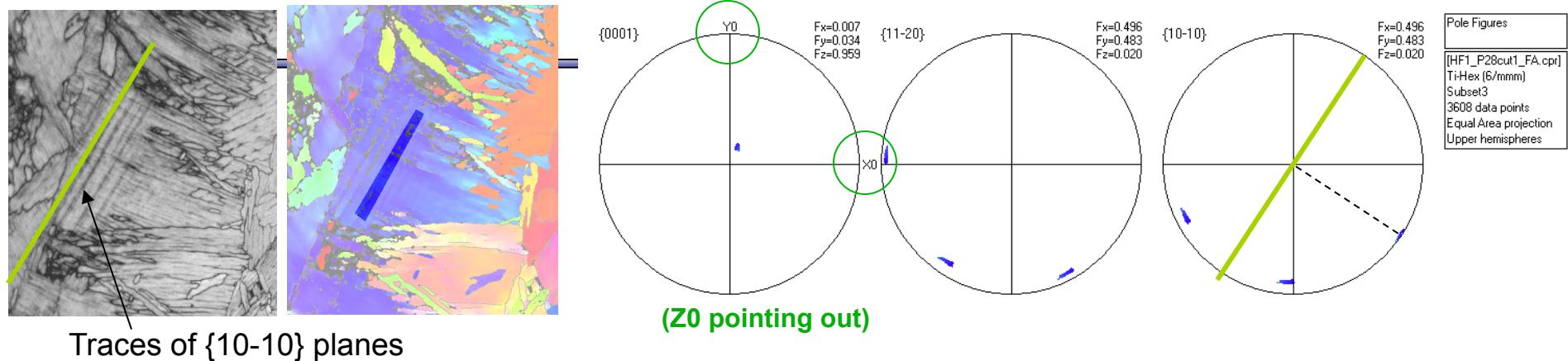


CS1 as shown in the virtual chamber
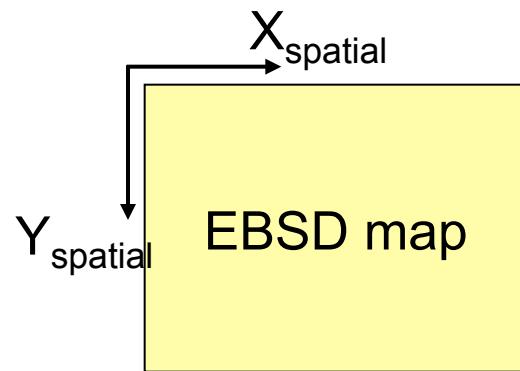
first acquired pixel ($X_{spatial}=1$, $Y_{spatial}=1$)
= top left pixel of the resulting map

- 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

{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

X0

**(Z0 pointing out)**

Pole Figures

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

$X_{spatial}$

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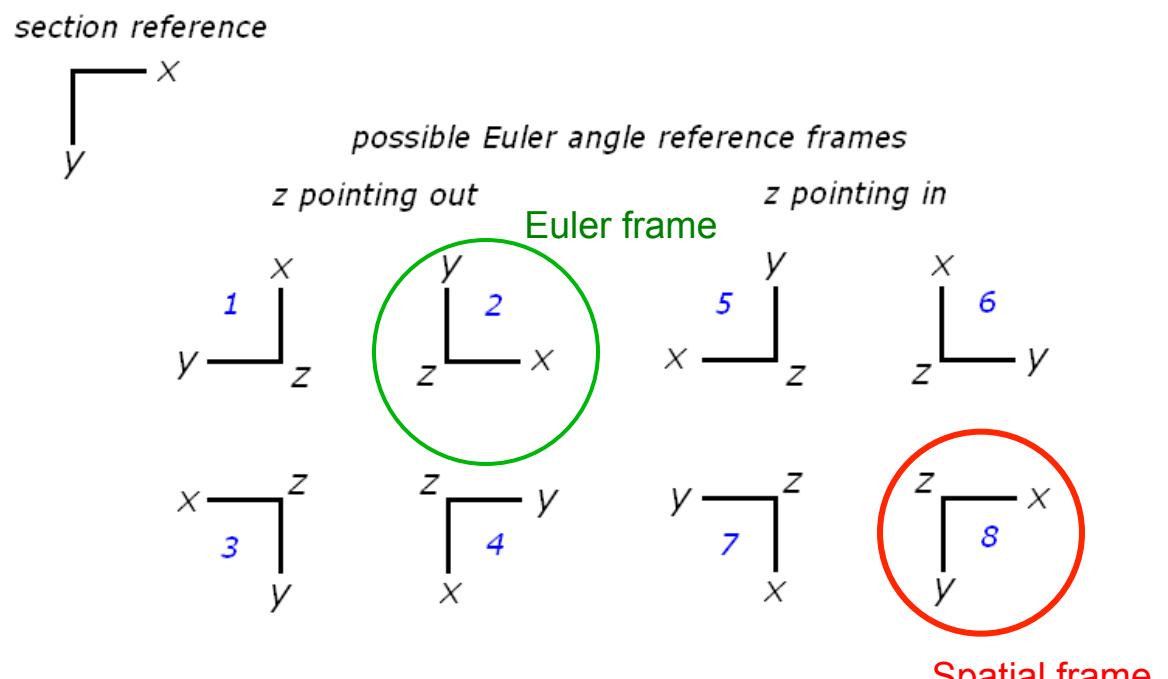
Xpix, Ypix = spatial frame
X0,Y0,Z0 = euler angle frame, supposed
to be aligned with X1,Y1,Z1 (µscope
frame)

section reference

X

y

possible Euler angle reference frames

z pointing out                z pointing in

Euler frame

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

x    z   z    y   y    z   z    x
3        4        7        8
y        x        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
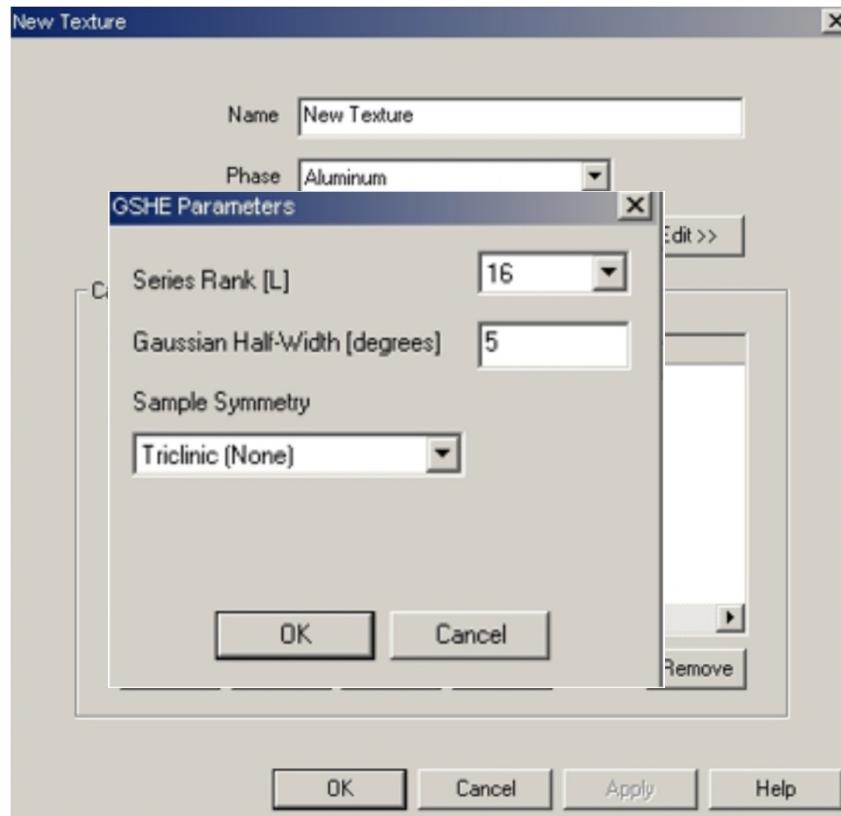
The difference is a rotation by 180° around the Z direction (frame numbered 2 versus frame 3)

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

# Orientation Distribution Functions

- The ODF displays how the measured orientations are distributed in orientation space
- Two types of distributions can be calculated:
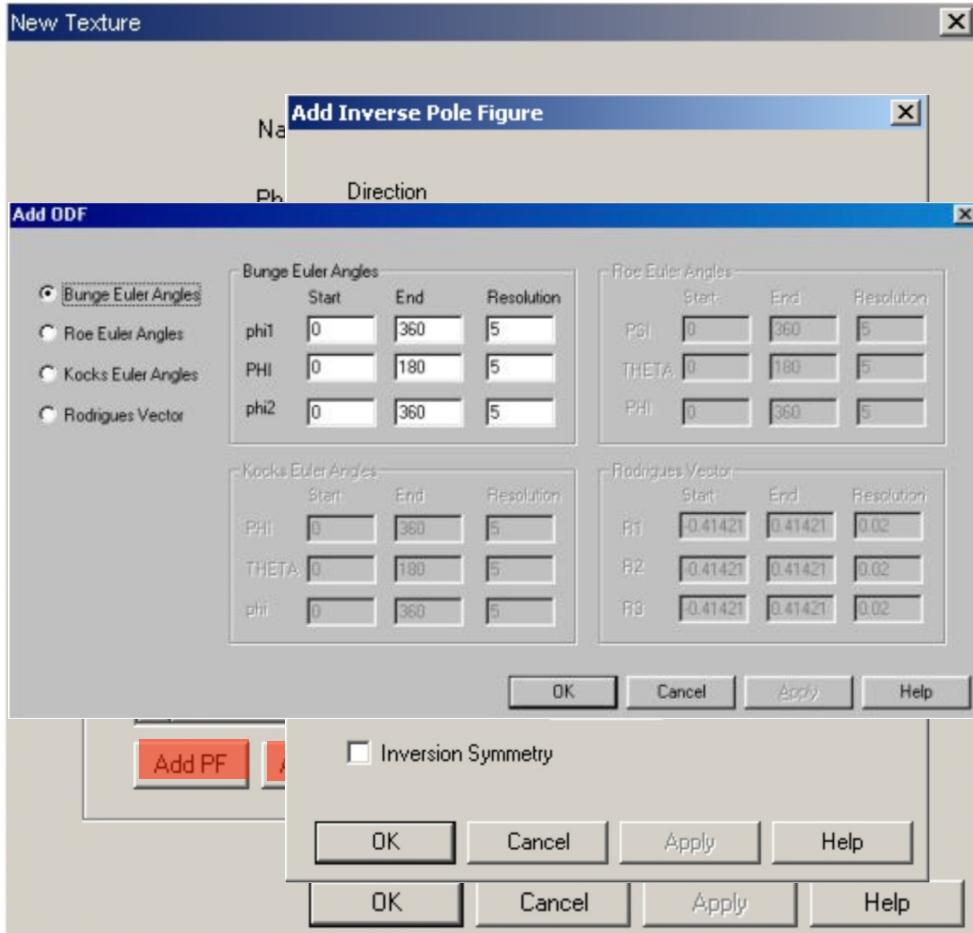


Continuous ODF:
• Generalized Spherical Harmonic Functions: Rank defines the "resolution" of the function
• Equivalent to a Fourier transform
• Calculation time rises steeply with rank number (32 is an effective maximum)
• Time intensive
• Mostly appropriate for weaker textures
• Some smoothing is inherent
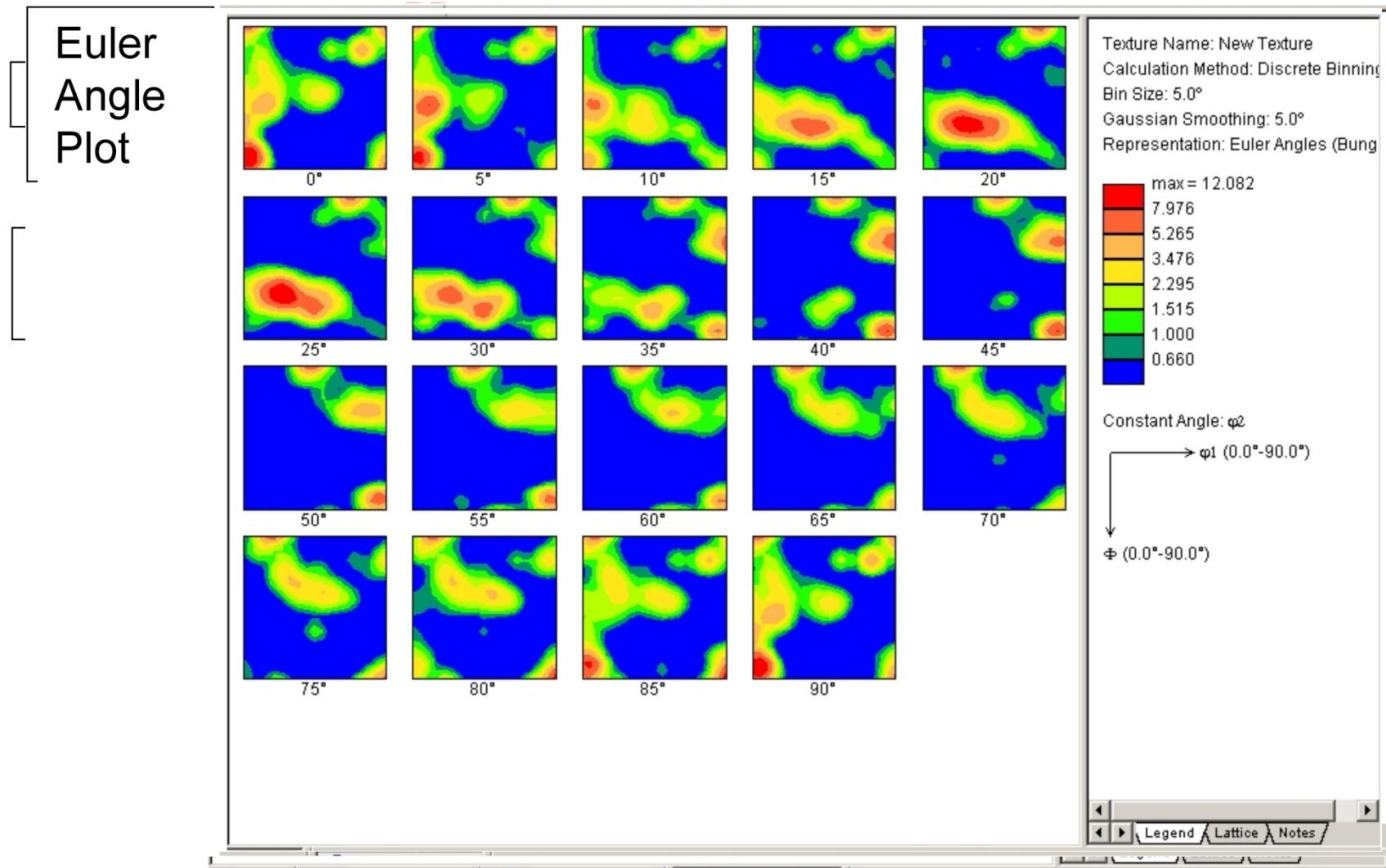
# Plotting Orientation Distributions

- 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:

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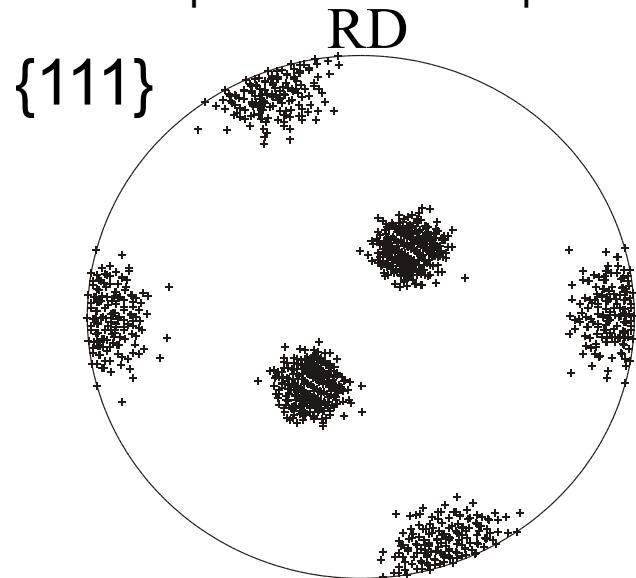
Very simple, n'est-ce pas?
However, there is a problem...
As a consequence of the crystal symmetry, there are several equivalent orientations.     *i=1,24*
This example illustrates the point:
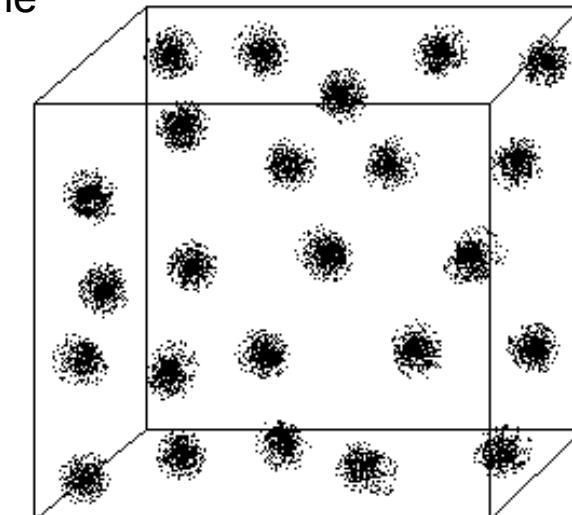
$$M(g)_{équivalent} = M(g)_{mesuré} \, [S_i]_{cristal}$$

RD

{111}
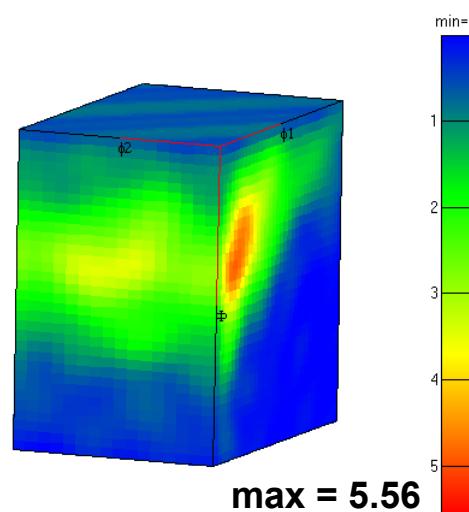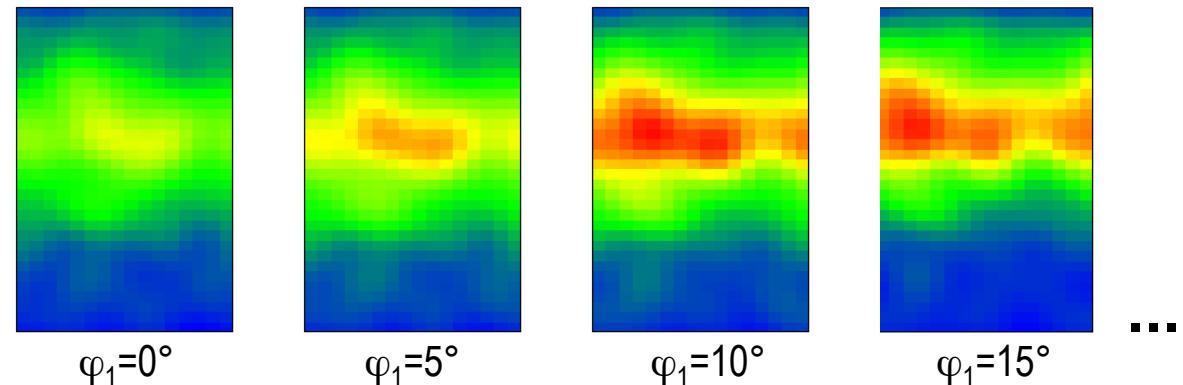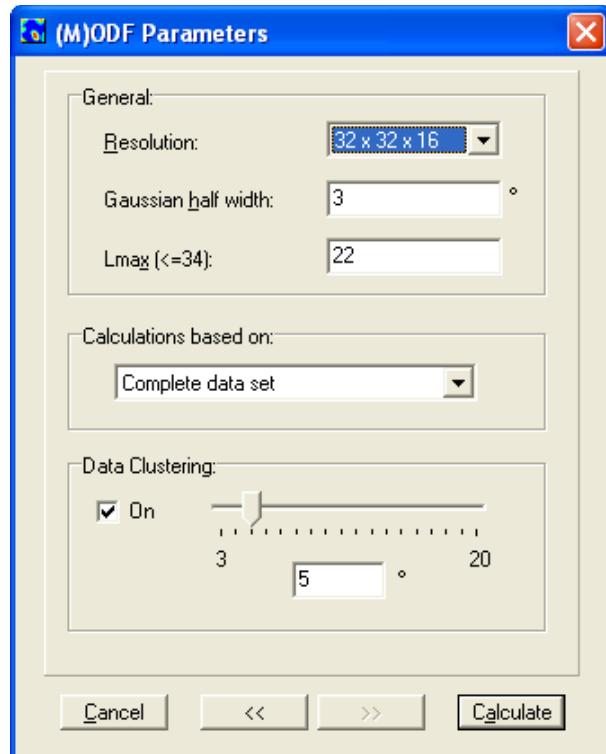


10 000 orientations near to the
Brass component:

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
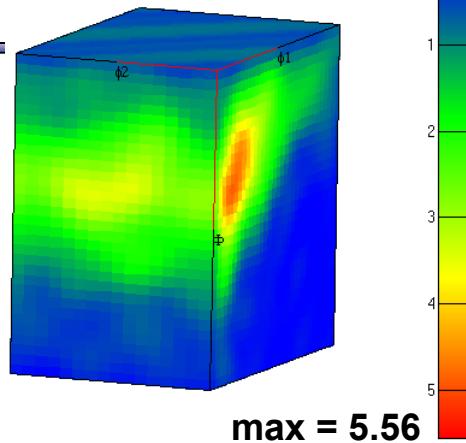


Courtesy of N. Bozzolo, CEMEF

# Parameters for texture analysis

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

max = 5.56
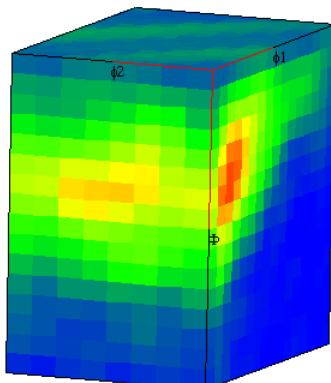
## Effect of the binning resolution

**16x16x8**
3°
22
5°

max = 5.37
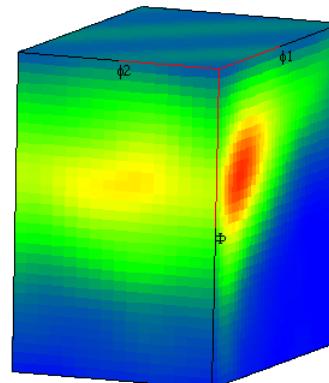
## Effect of the width of the Gaussian

32x32x16
**8°**
22
5°
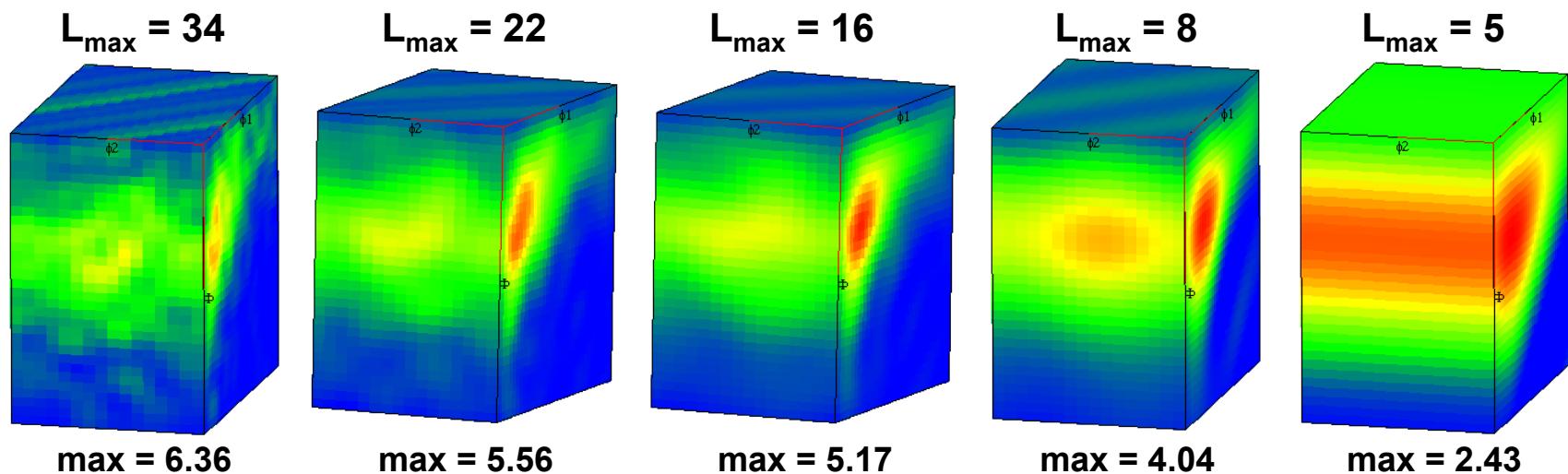
max = 4.44

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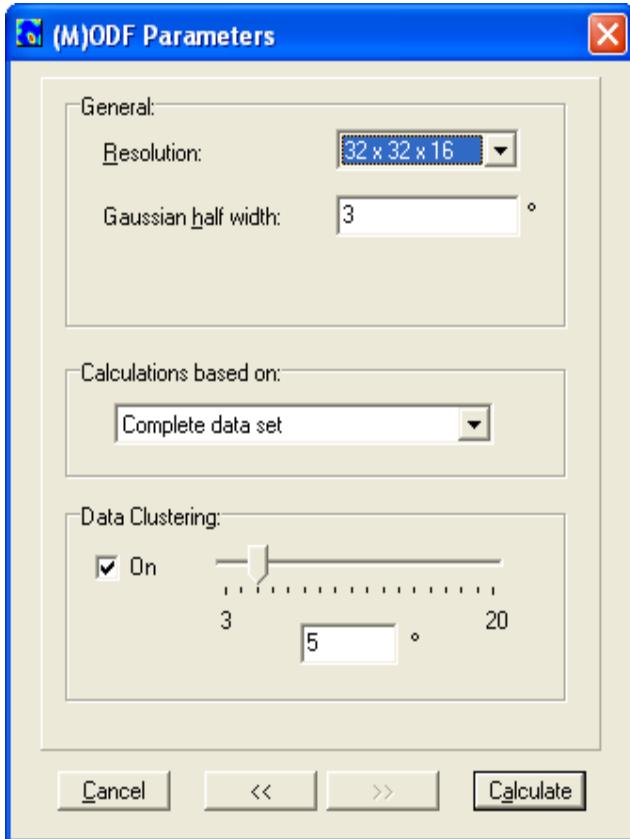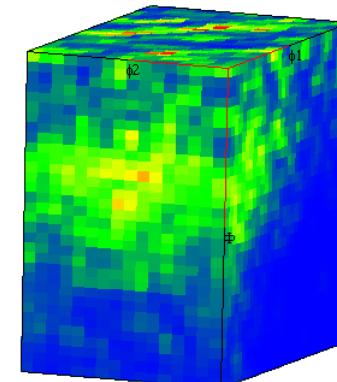
Clearly, taking the fitting to higher order (angular frequency) provides better resolution of the texture

# Direct Method
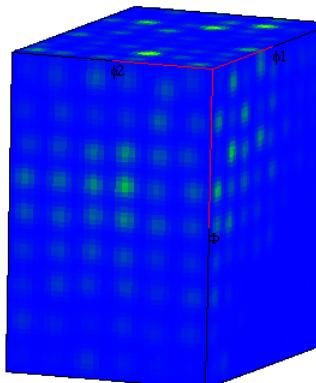
**max = 5.56**
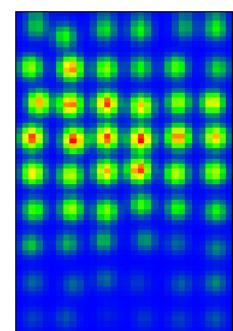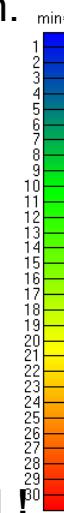
In effect the harmonic method gives some "smoothing" . Without this, a coarse binning of, say, 10°, produces a very "lumpy" result because the Gaussian applied around each point is not sufficiently wide to give a continuous distribution.

Same, with **10° binning** :

**max = 31 !**
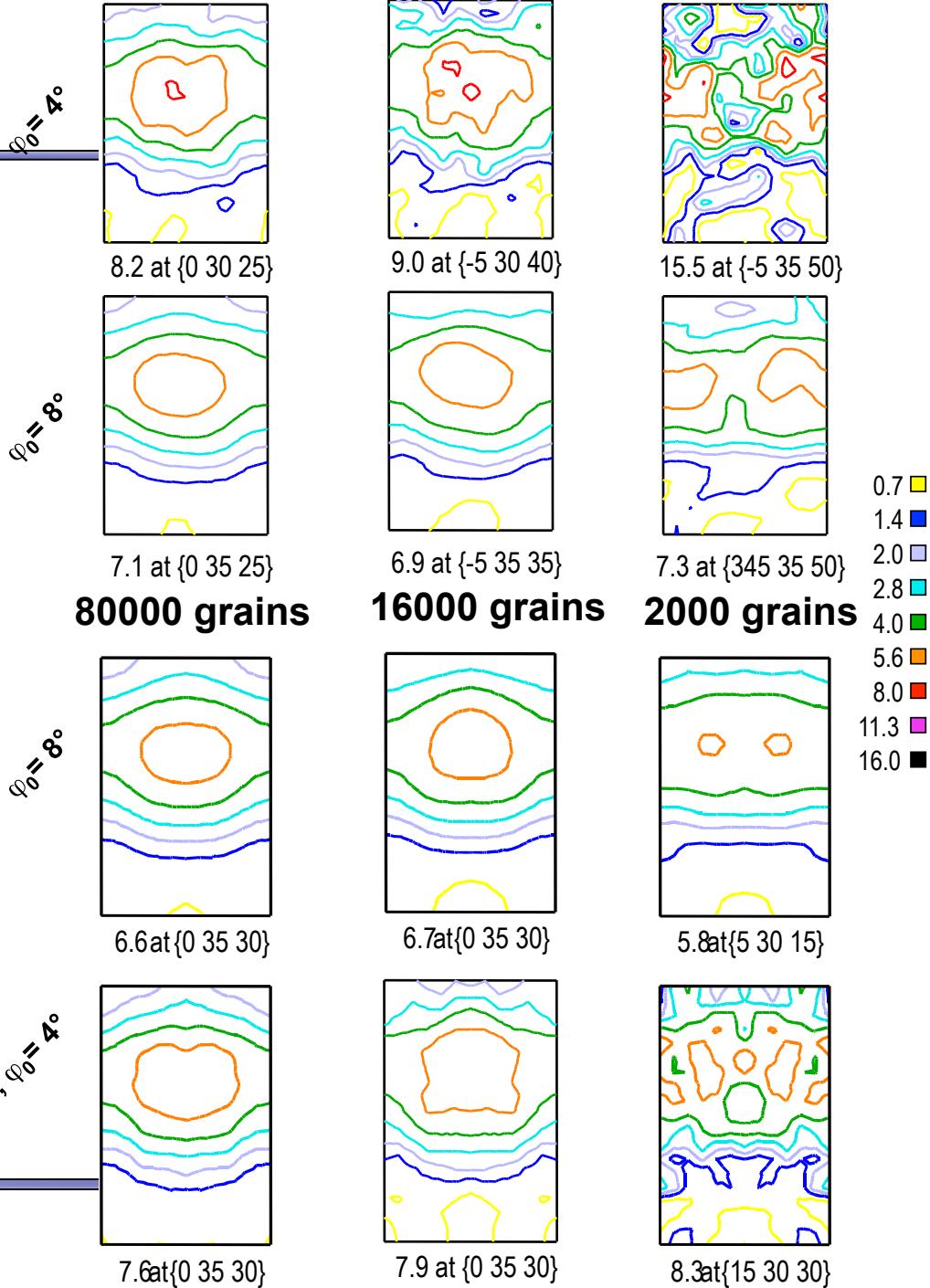
$\varphi_1 = 5°$

# 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 $\varphi_1$ ($L_{max}$ = 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}

*Gaussian, $\varphi_0 = 4°$*

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 | ⬛ |
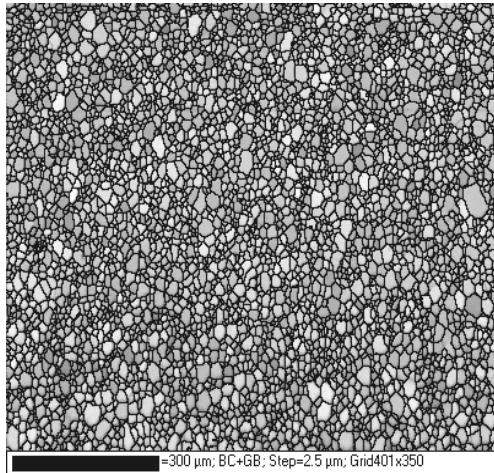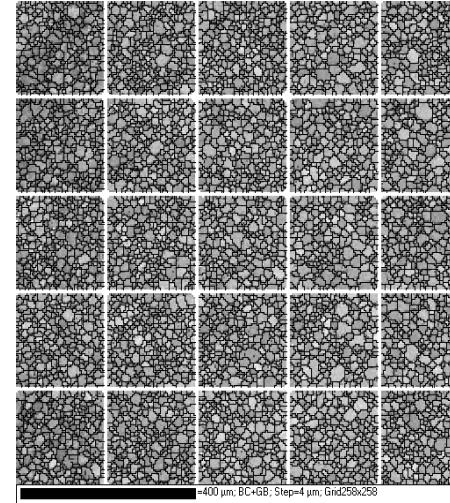
# Statistical Aspects Homogeneity/heterogeneity of the specimen...

Not just the number of grains must be considered but also their spatial distribution:
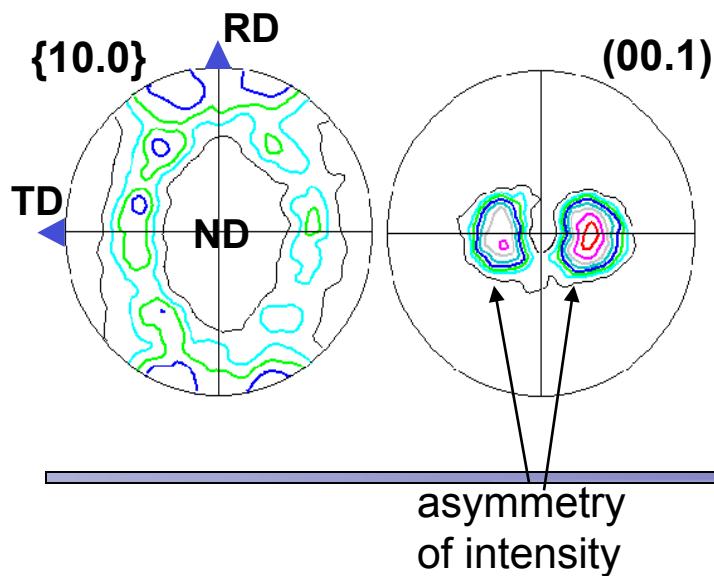
Single EBSD map (1 mm²)

Multiple maps, different locations ( total =1 mm²)



=300 µm; BC+GB; Step=2.5 µm; Grid401x350

=400 µm; BC+GB; Step=4 µm; Grid258x258

equiaxed Ti

**RD**

**{10.0}**

**(00.1)**

**TD**

**ND**

| | |
|---|---|
| 0.7 — | 4.0 |
| 1.4 | 5.6 |
| 2.0 | 8.0 |
| 2.8 | 11.3 |

asymmetry
of intensity
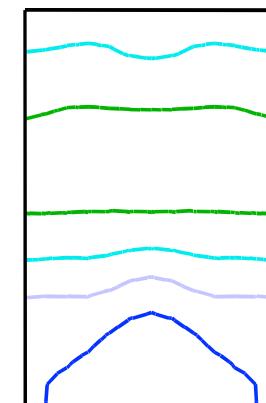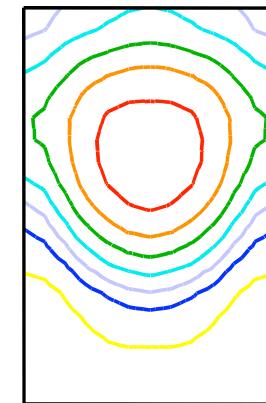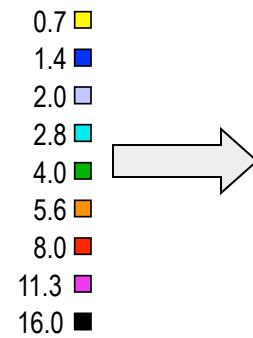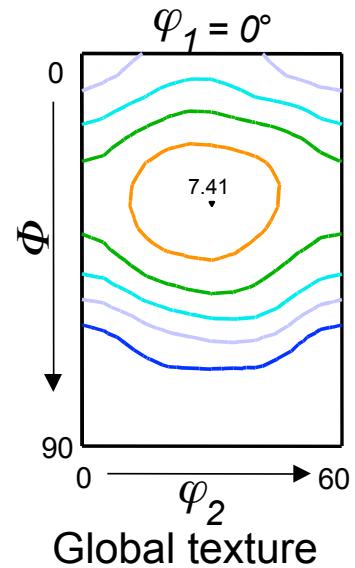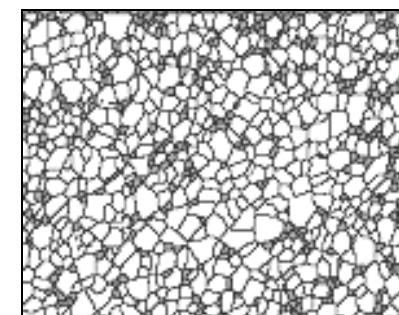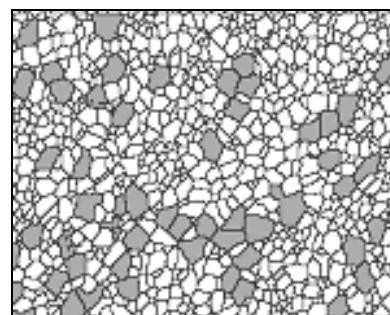
# Texture – Microstructure Coupling

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

$\varphi_1 = 0°$

$\Phi$

$\varphi_2$

0.7
1.4
2.0
2.8
4.0
5.6
8.0
11.3
16.0

7.41

Global texture

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

partial texture of the
**largest grains**

$D \leq \bar{D}/2$ (=2.75 µm)
14255 grains
1.7% surf.
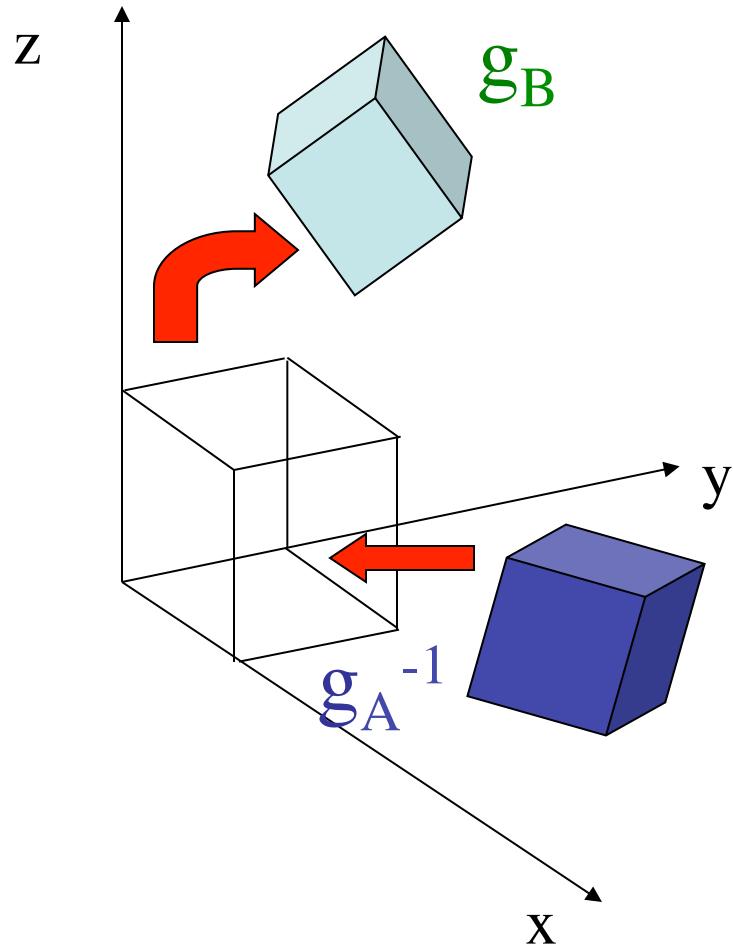
Partial texture of the
**smallest grains**

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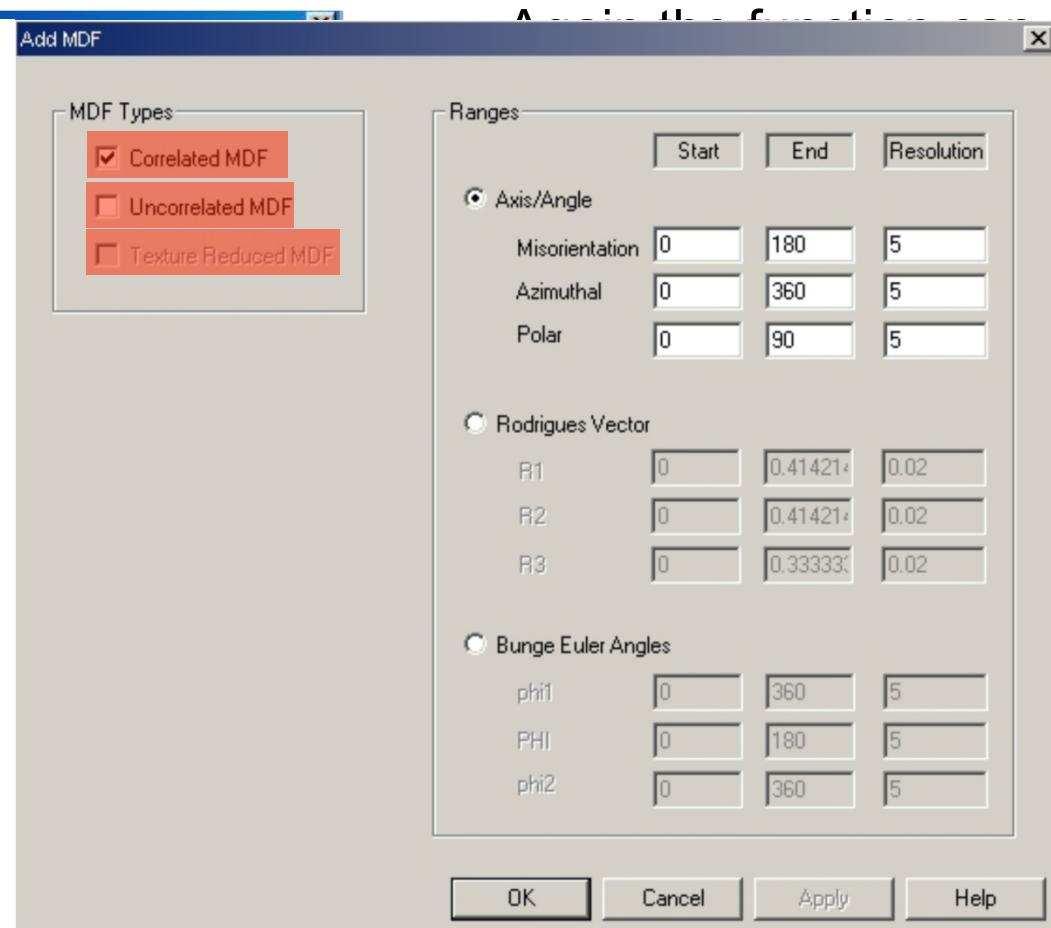
$$\text{Misorientation} = g_B g_A^{-1}$$

# Misorientation Distribution Functions

- Calculating MDFs is very similar to calculating ODFs

Again the function can

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.

**Add MDF**

**MDF Types**
- ☑ Correlated MDF
- ☐ Uncorrelated MDF
- ☐ Texture Reduced MDF

**Ranges**

| | Start | End | Resolution |
|---|---|---|---|
| ⦿ Axis/Angle | | | |
| Misorientation | 0 | 180 | 5 |
| Azimuthal | 0 | 360 | 5 |
| Polar | 0 | 90 | 5 |
| ○ Rodrigues Vector | | | |
| R1 | 0 | 0.414214 | 0.02 |
| R2 | 0 | 0.414214 | 0.02 |
| R3 | 0 | 0.333333 | 0.02 |
| ○ Bunge Euler Angles | | | |
| phi1 | 0 | 360 | 5 |
| PHI | 0 | 180 | 5 |
| phi2 | 0 | 360 | 5 |

OK    Cancel    Apply    Help
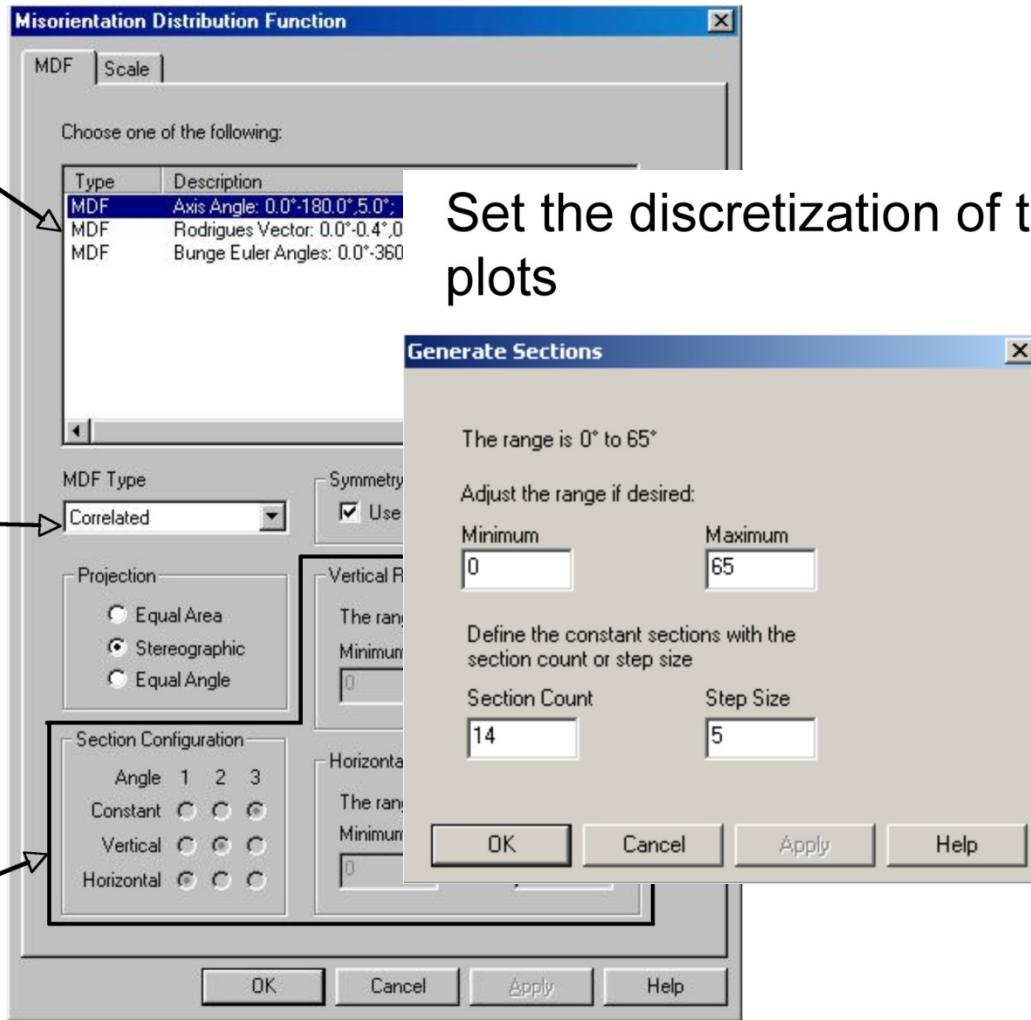
# Plotting MDFs



Select plot type (previously calculated)
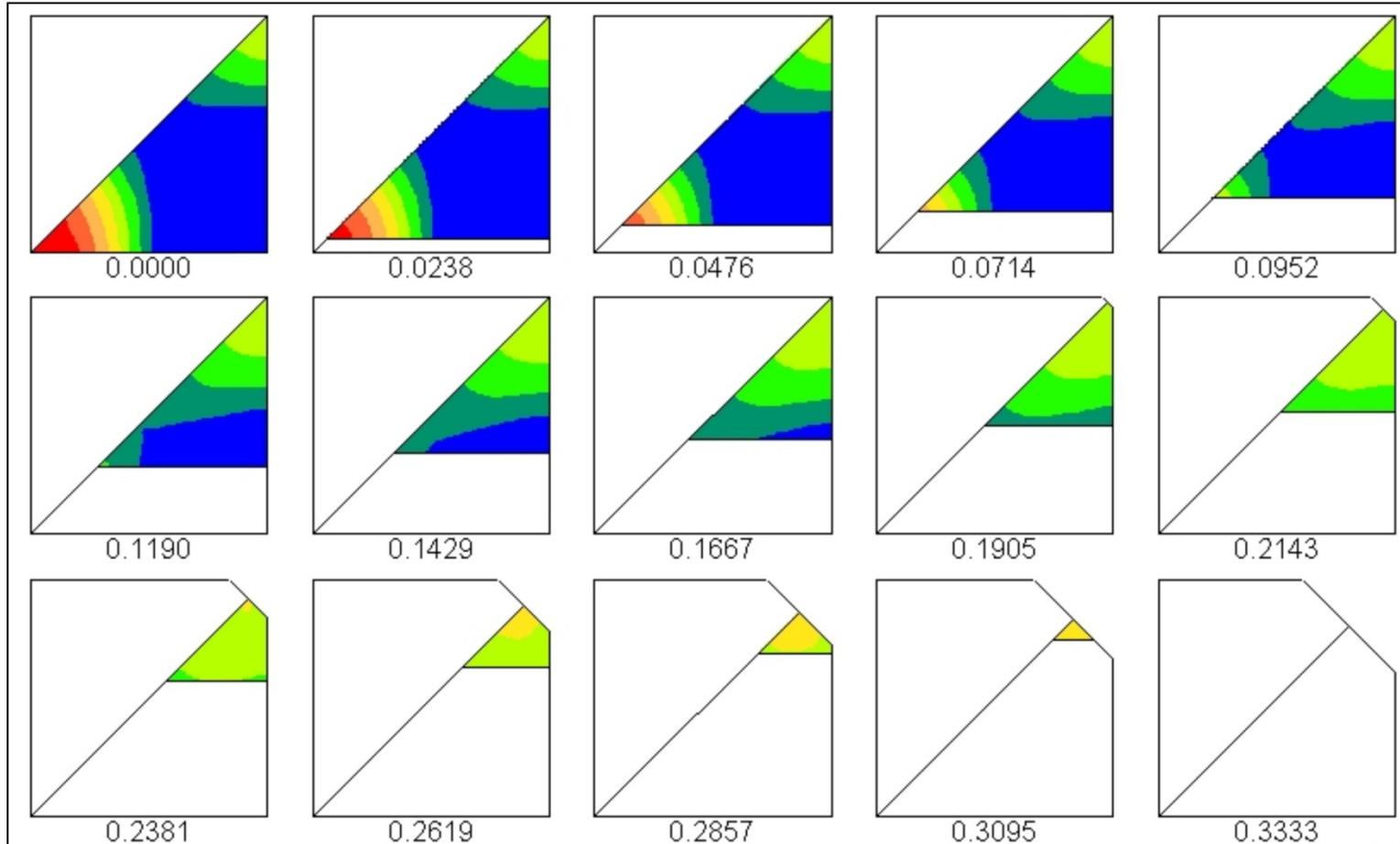
If different types calculated, choose

These only apply to Euler angle plots

Set the discretization of the plots
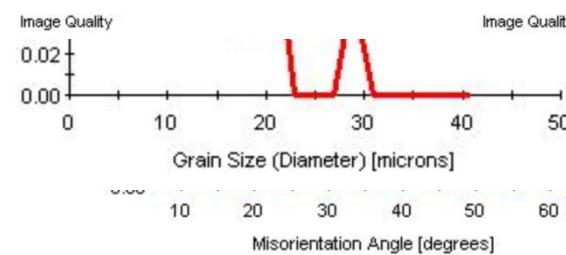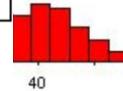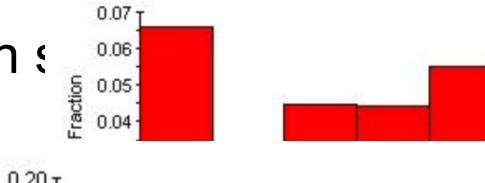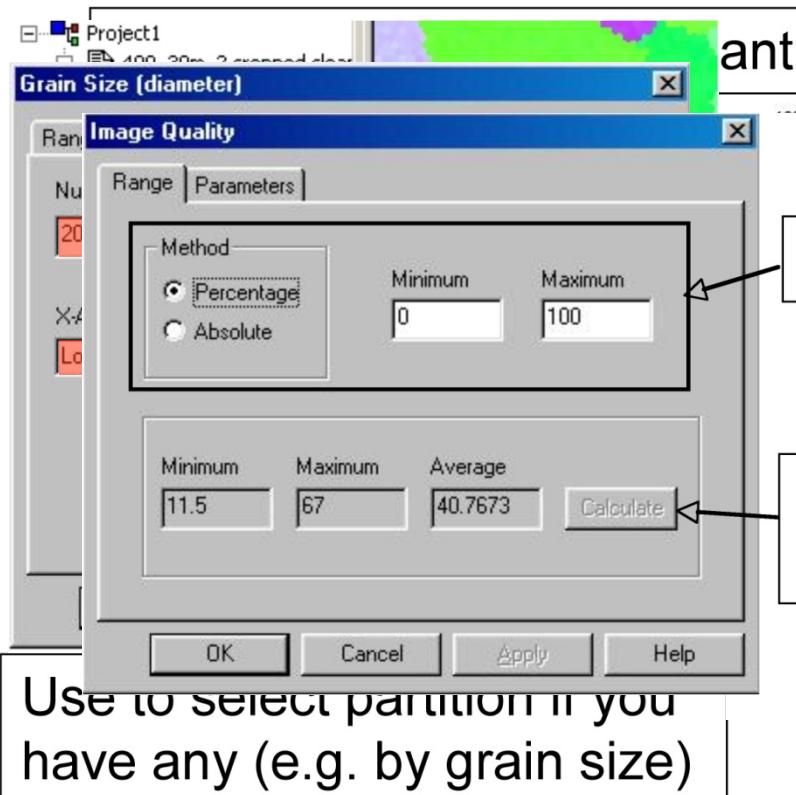
# Sections through Misorientation Space



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

# Charts
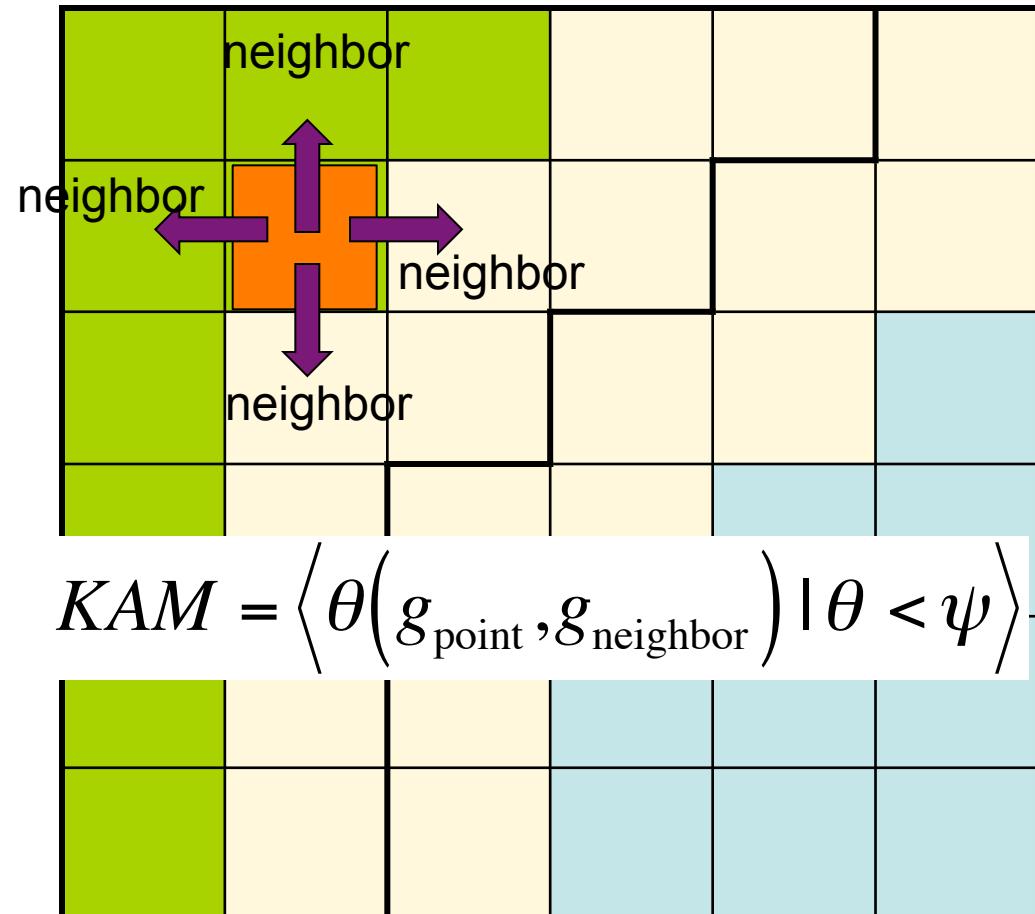
Charts are easy to use in order to obtain s

Project1

**Grain Size (diameter)** ✕

ant

**Image Quality** ✕

Range | Parameters

Method
- ⦿ Percentage
- ○ Absolute

Minimum
0

Maximum
100

Choose plot values and range

| Minimum | Maximum | Average |
|---------|---------|---------|
| 11.5 | 67 | 40.7673 |

Calculate

Displays data range. You can calculate the range

OK    Cancel    Apply    Help

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

Image Quality

Image Quality

Grain Size (Diameter) [microns]

Misorientation Angle [degrees]

# Kernel Average Misorientation (KAM)

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

- For each point (orange box), compute the misorientation ($\theta$, angle only, purple arrows) for each nearest neighbor (26 in 3D).
- For all values < chosen threshold ($\psi$, 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)

neighbor

neighbor

neighbor

neighbor

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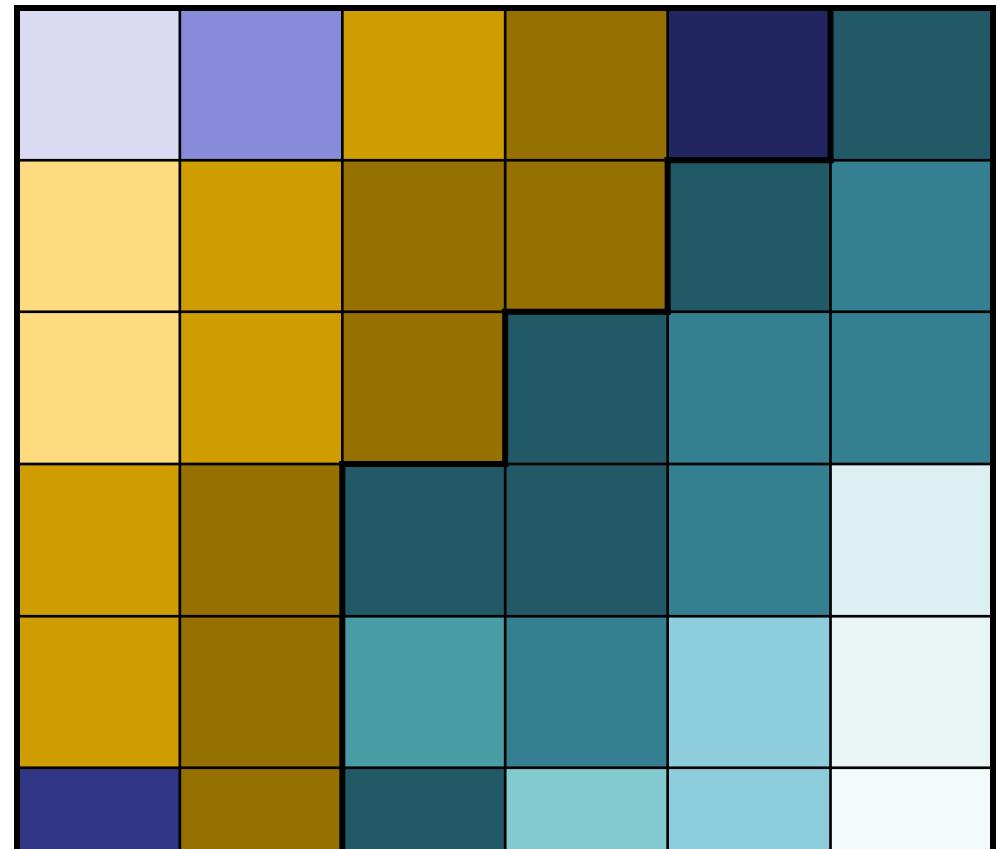
**Why is KAM important?  Nucleation of recrystallization, e.g.**

# 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 ($\theta$, 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).

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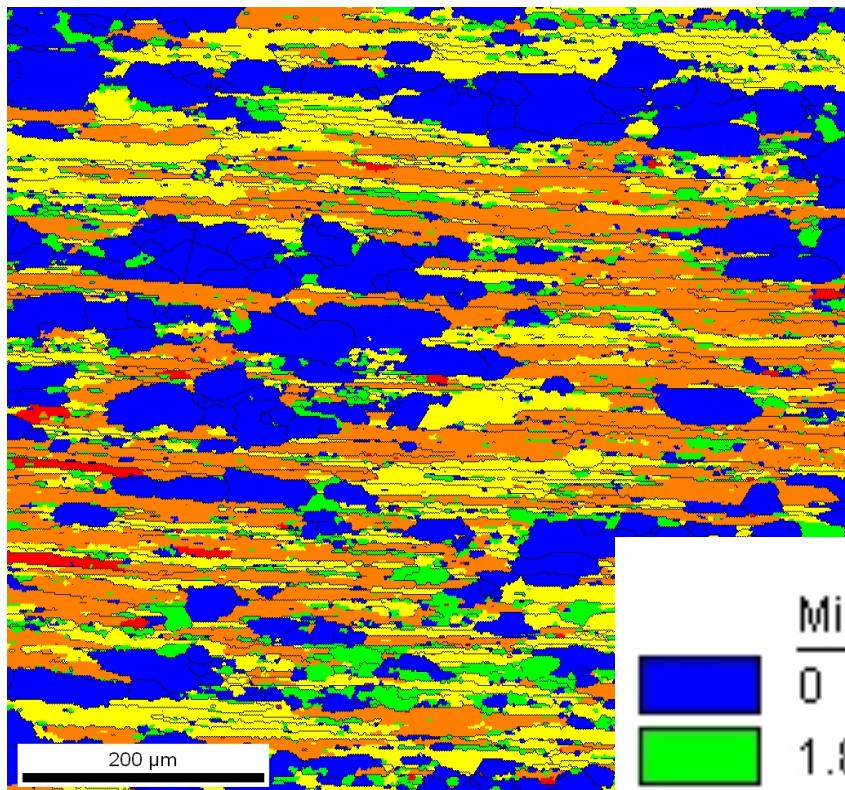
**Why is IGM important?  Long range orientation gradients, for example**

# GOS and GAM

$n$ = no. nearest neighbors
$N$ = number of pixels

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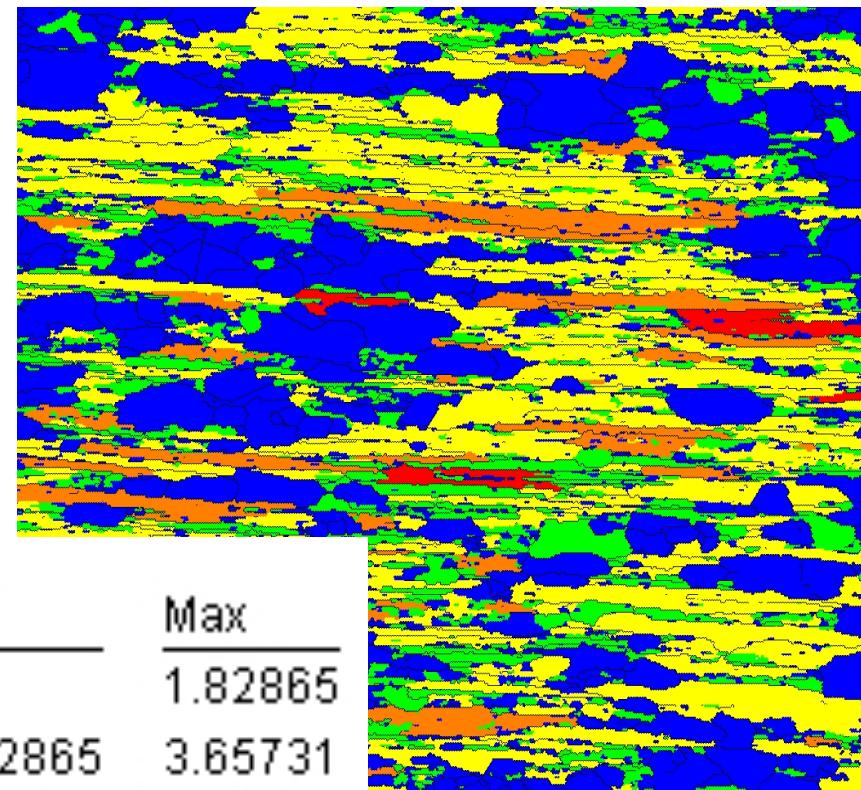
$$GOS = \frac{1}{N-1}\frac{1}{N}\sum_{j=1}^{N}\sum_{i=1}^{N}\Delta g_{ij}\left(g_i,g_j\right), \quad j \neq i$$



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 pairs
⇒ short range orientation
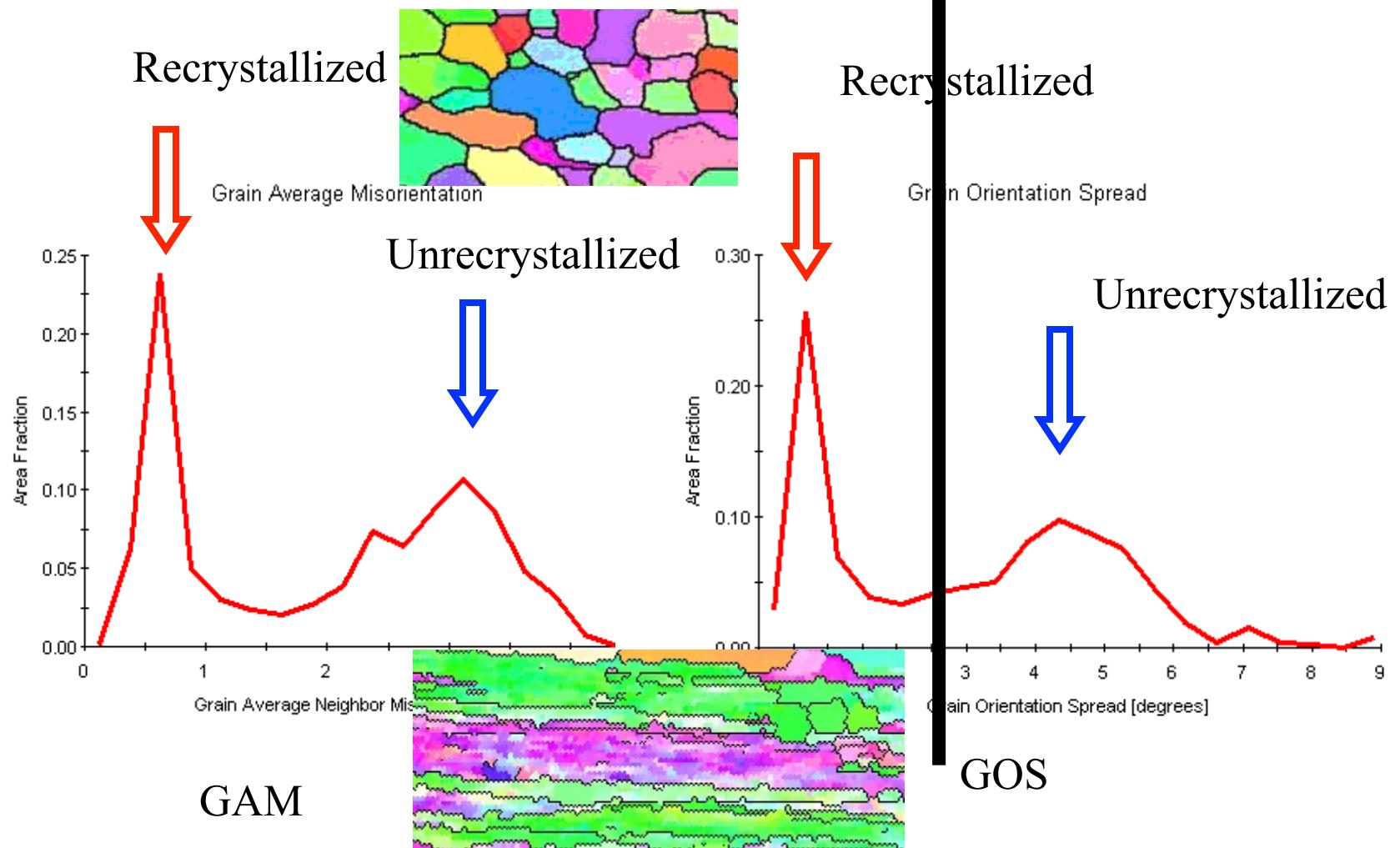
*M.H. Alvi*

irs
ge orientation gradients

# GOS and GAM



Recrystallized

Recrystallized

Unrecrystallized

Unrecrystallized

GAM

GOS
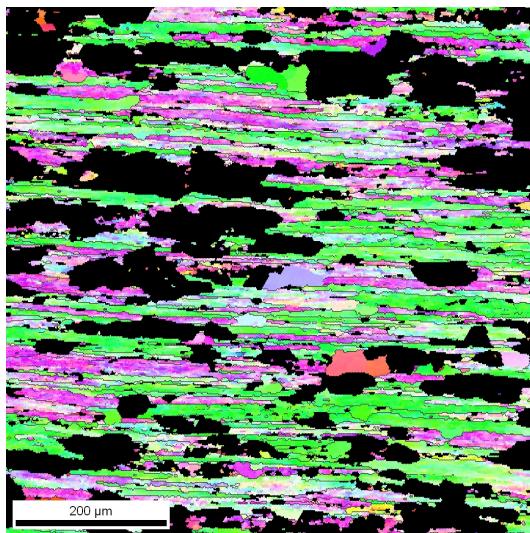
Overlapping peaks for deformed and recrystallized regions
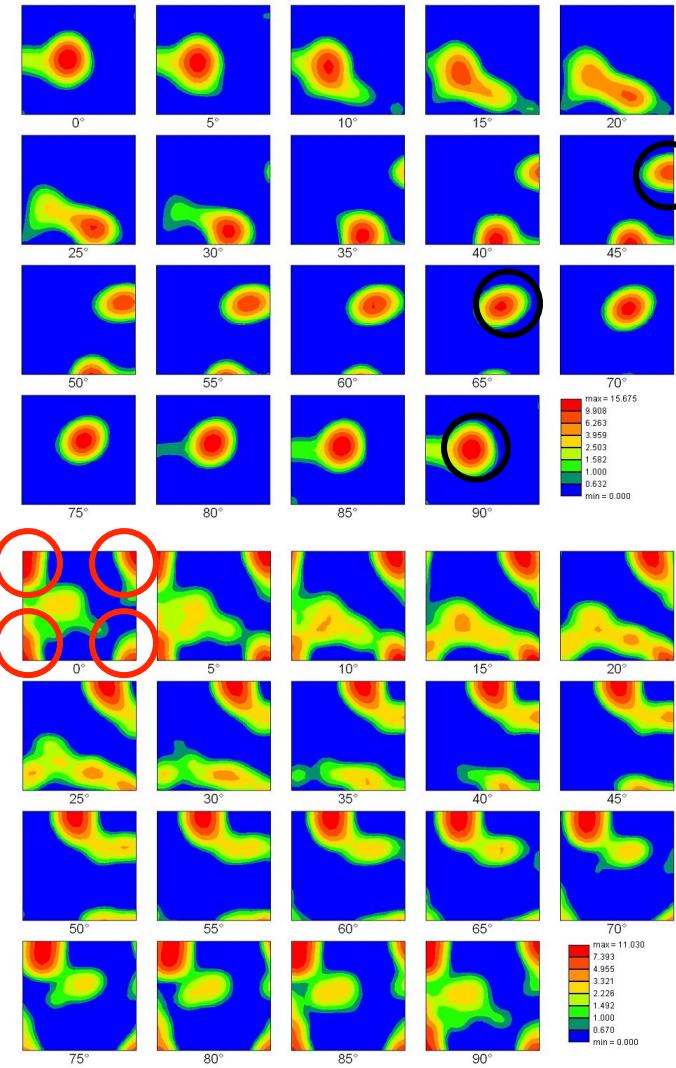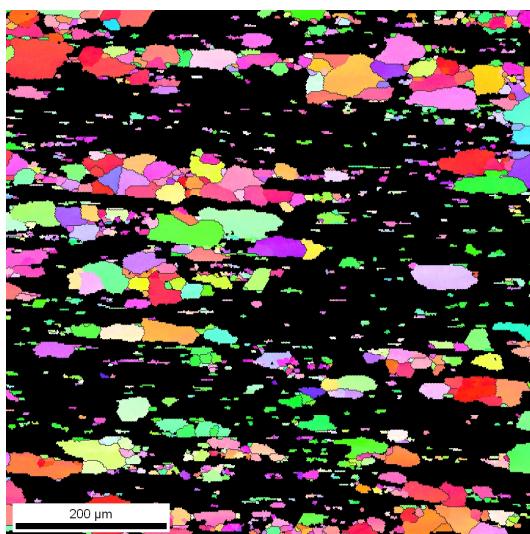
*M.H. Alvi*

# Partitioned scan: threshold GOS = 3°



Deformed Grains

Recrystallized Grains
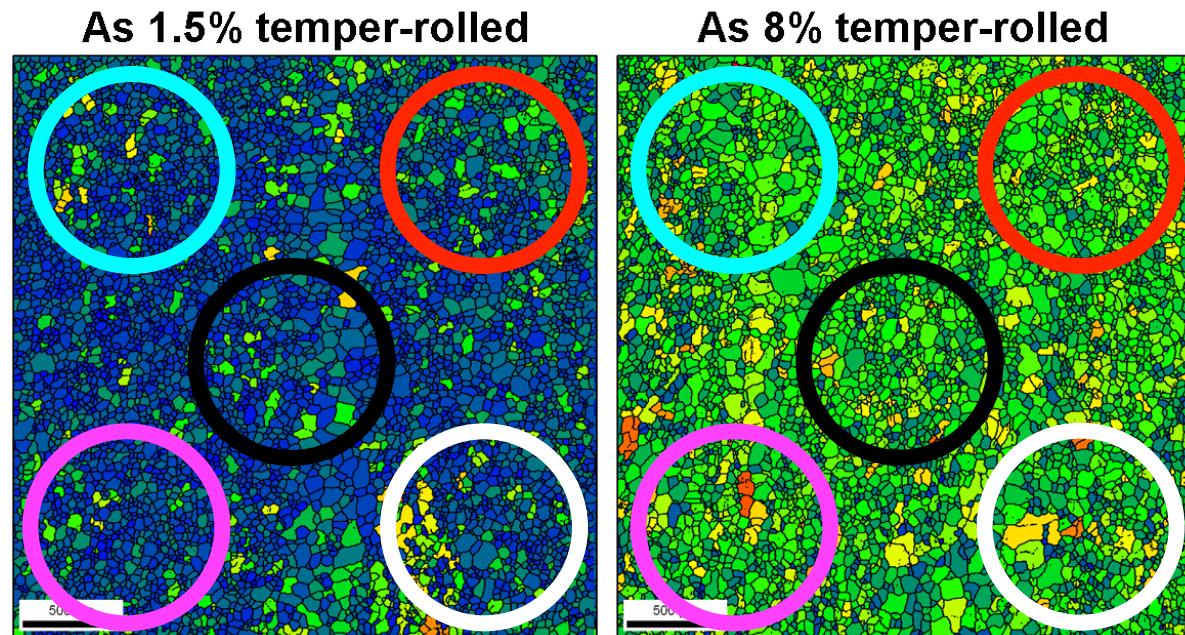
"Cube texture in hot rolled Aluminum Alloy 1050 (AA1050) - nucleation and growth behavior", M. H. Alvi, S. W. Cheong, J. P. Suni, H. Weiland, A. D. Rollett, *Acta materialia*, **56** 3098-3108 (2008).

# As-deformed Fe-1%Si



As 1.5% temper-rolled

As 8% temper-rolled

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

AGG is a local phenomenon.

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

**Maps shaded according to GOS.**

| | Min | Max |
|---|---|---|
| | 0.229345 | 7.85205 |
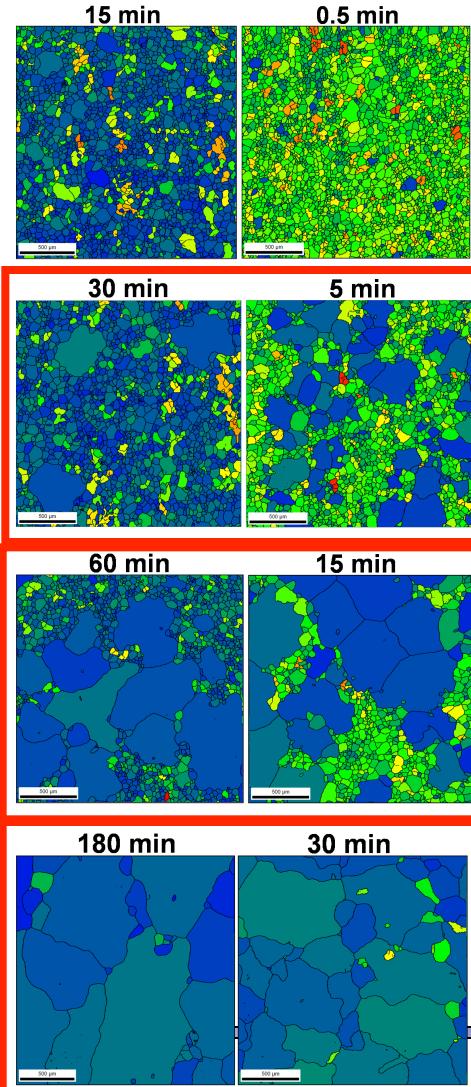
Density of abnormally large grains will be higher in the 8% material.

Presence of several same-stored-energy regions in 1.5% material leads to lower density of abnormally large grains.
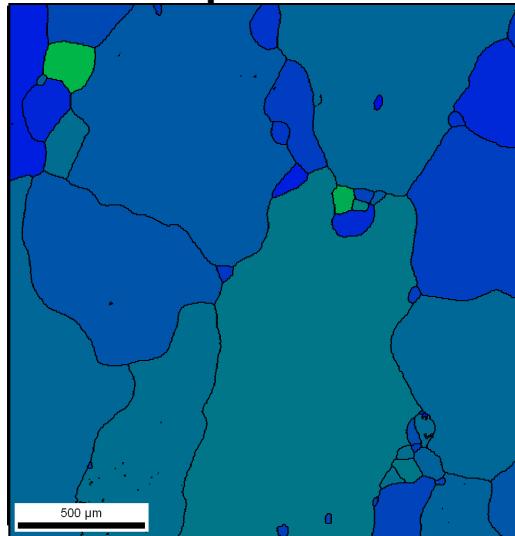
Grains that grow abnormally already exist in the as-deformed material.

"Strain-Induced Selective Growth in 1.5 % Temper-Rolled Fe similar to 1 % Si", Tricia A. Bennett, Peter N. Kalu; Anthony D. Rollett, *Microscopy and Microanalysis*, **17**(3) 362-367 (2011)

# Orientation Spread, Fe-1%Si
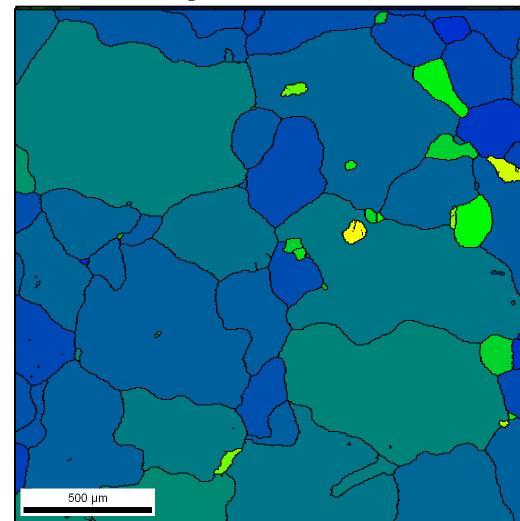


1.5% and 8% temper-rolled Fe-1%Si, annealed in air at 787°C for various times.

**1.5% temper-rolled**

**8% temper-rolled**

**180 min.**

**30 min.**

| Min | Max |
|---|---|
| 0.0337706 | 6.65443 |
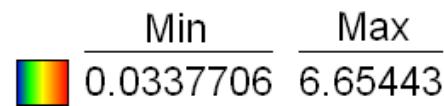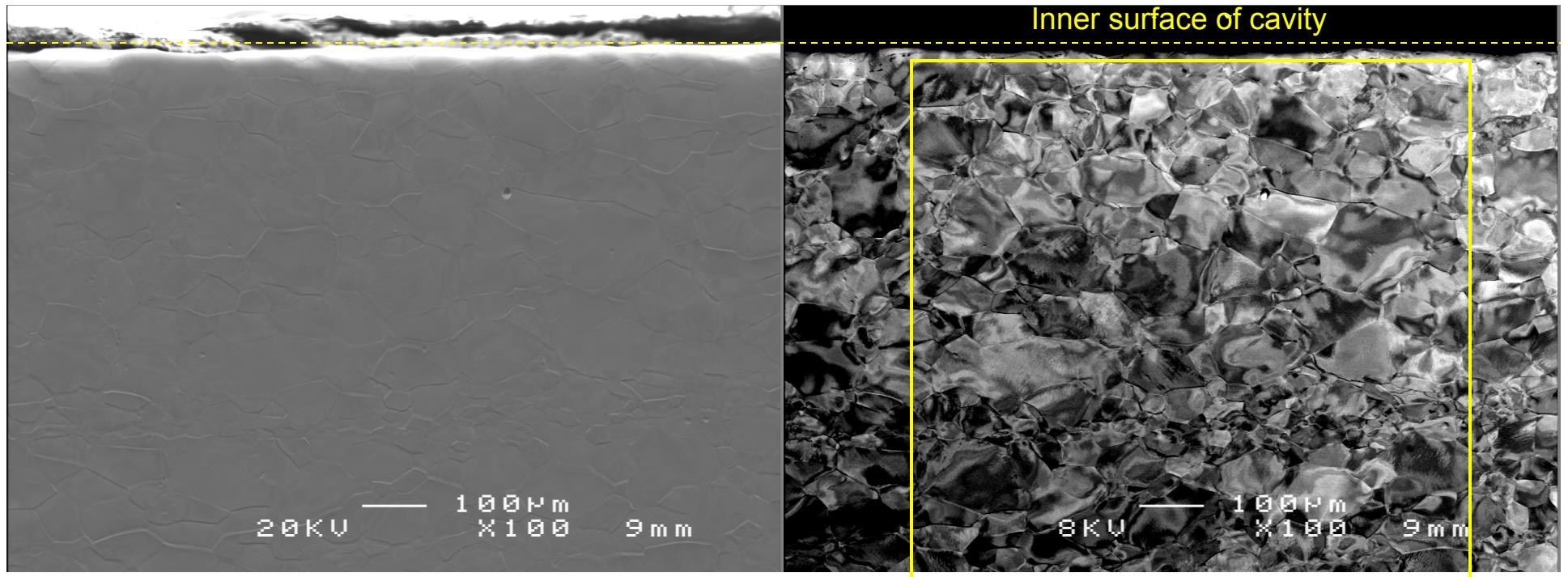
*T.A. Bennett*

**Overall, GOS decreases with annealing time.**
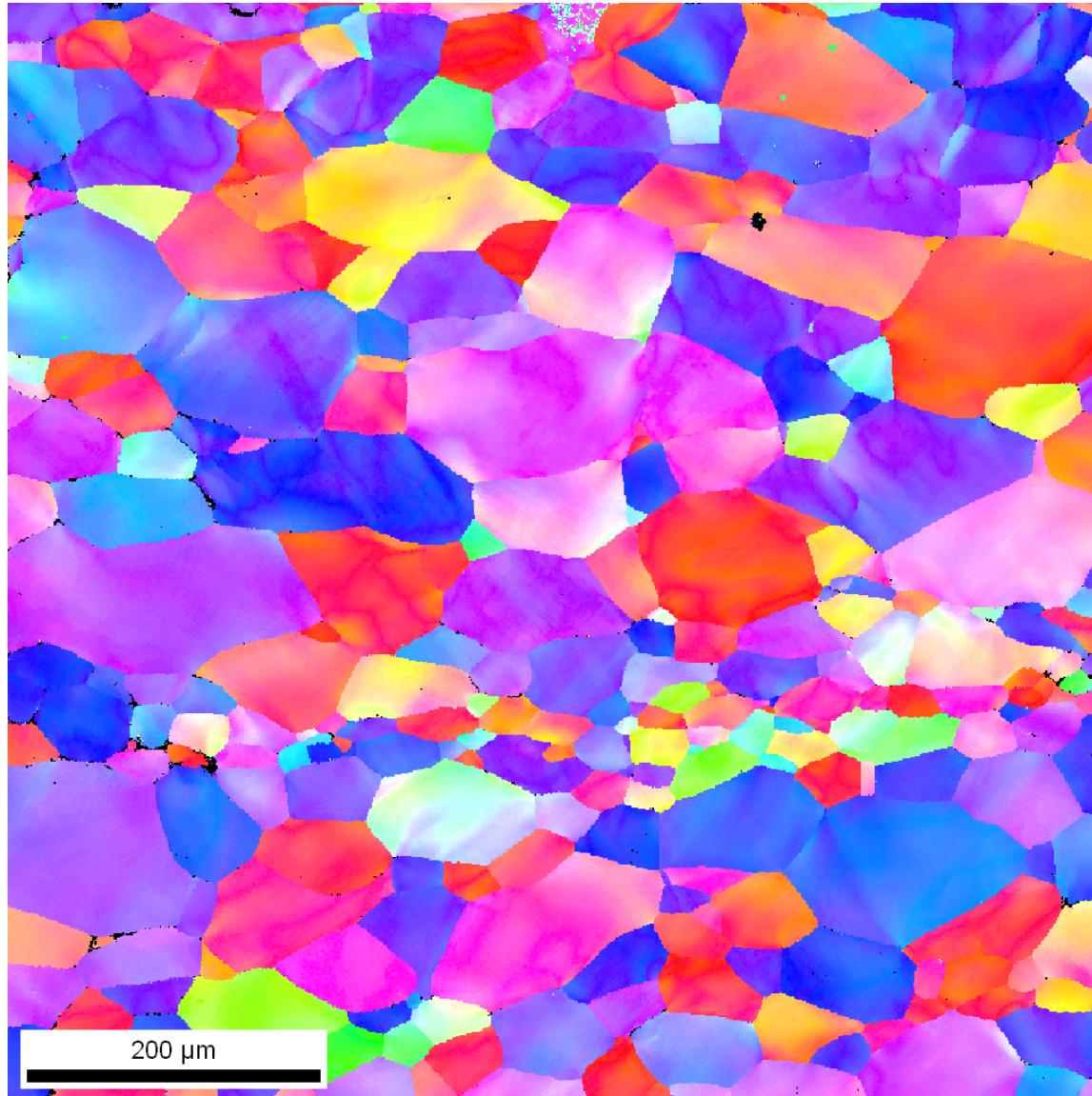
# Pure Nb: Longitudinal Section Etched

3mm from top of cavity



Secondary electron image      Backscattered electron image

EBSD Grid
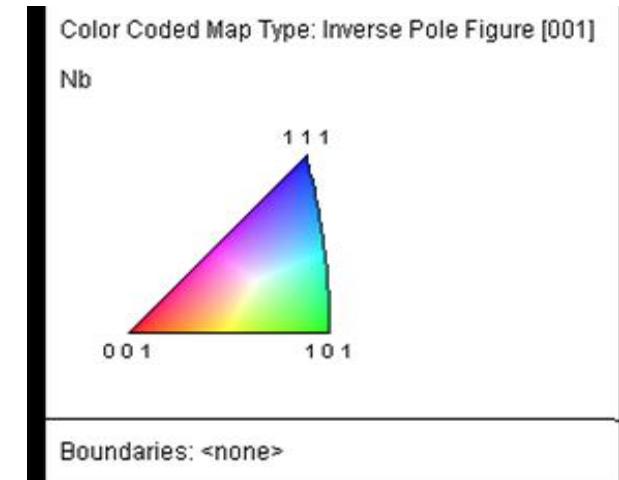
*R. Crooks*

# Nb: EBSD IPF Map

*R. Crooks*



Crystal directions normal to sheet surface

Color Coded Map Type: Inverse Pole Figure [001]

Nb

111

001      101

Boundaries: <none>
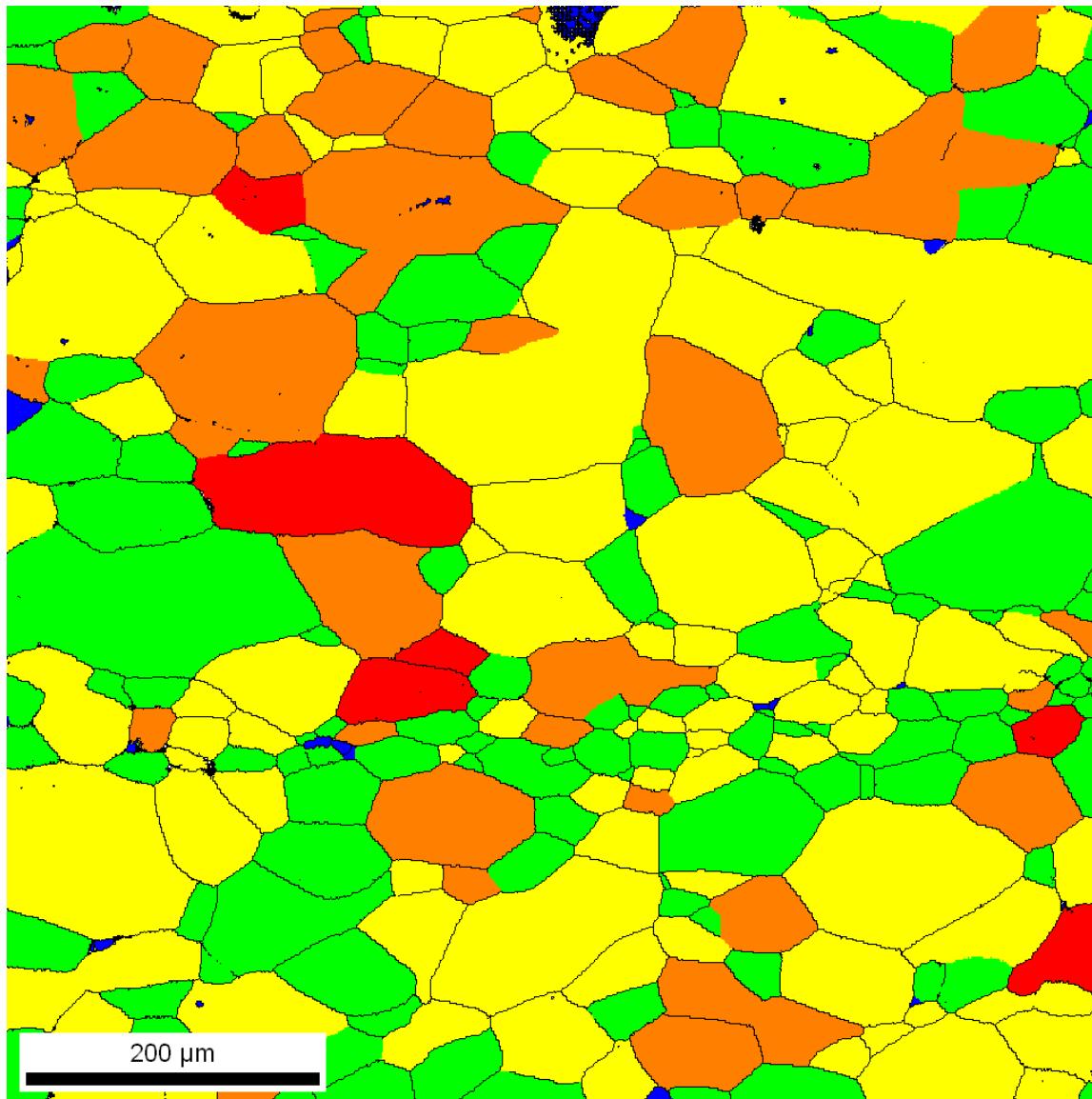
Color changes within grain show distortion of crystal

200 µm

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

# 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)

200 µm

**Stored Strain Energy very high at 500 µm from inner surface**

*R. Crooks*

1 µm spatial resolution

55

# Nb: EBSD IPF Map 500 μm deep



Color Coded Map Type: Inverse Pole Figure [001]
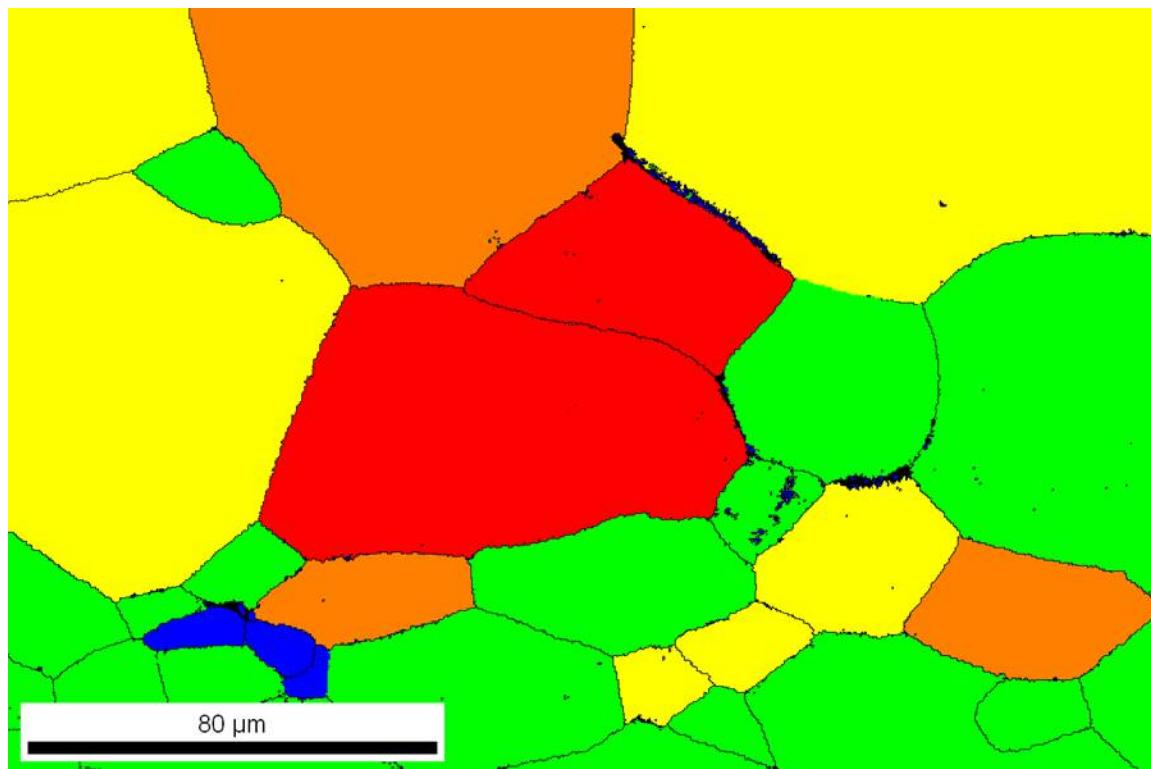
Nb

111

001    101

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

750 x 500, 0.3 μm spatial resolution

R. Crooks

# 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 |
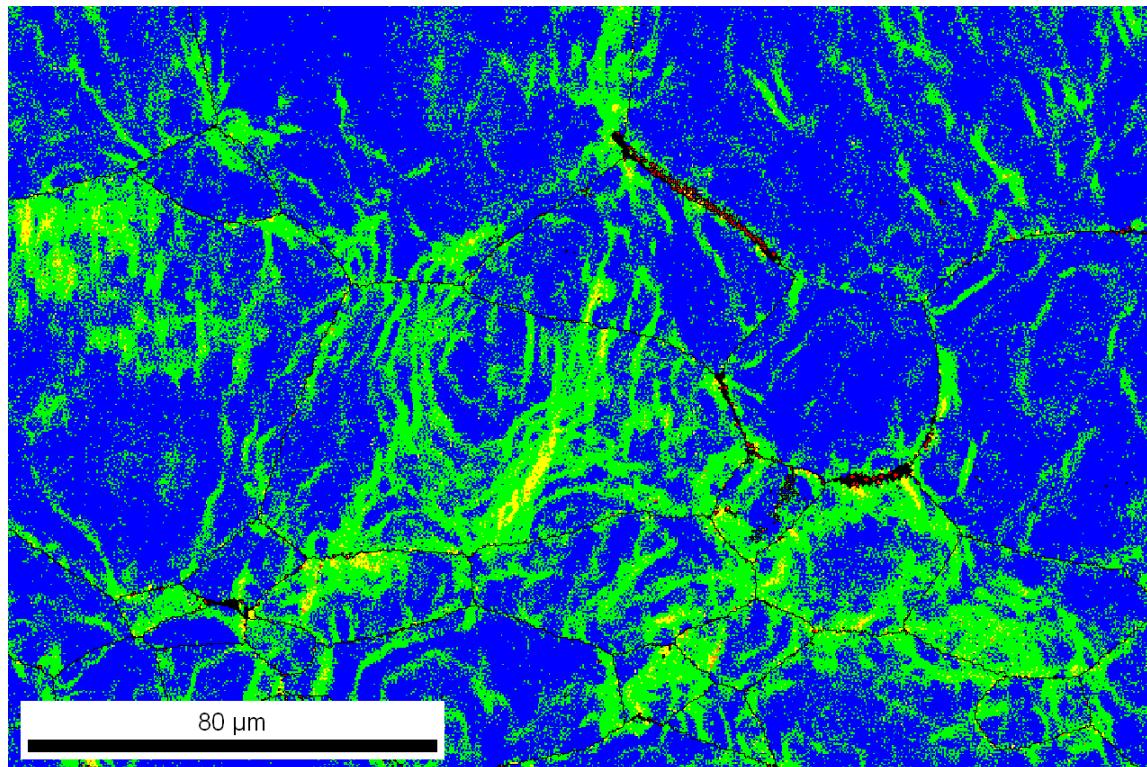
Boundaries: Rotation Angle

| | 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*

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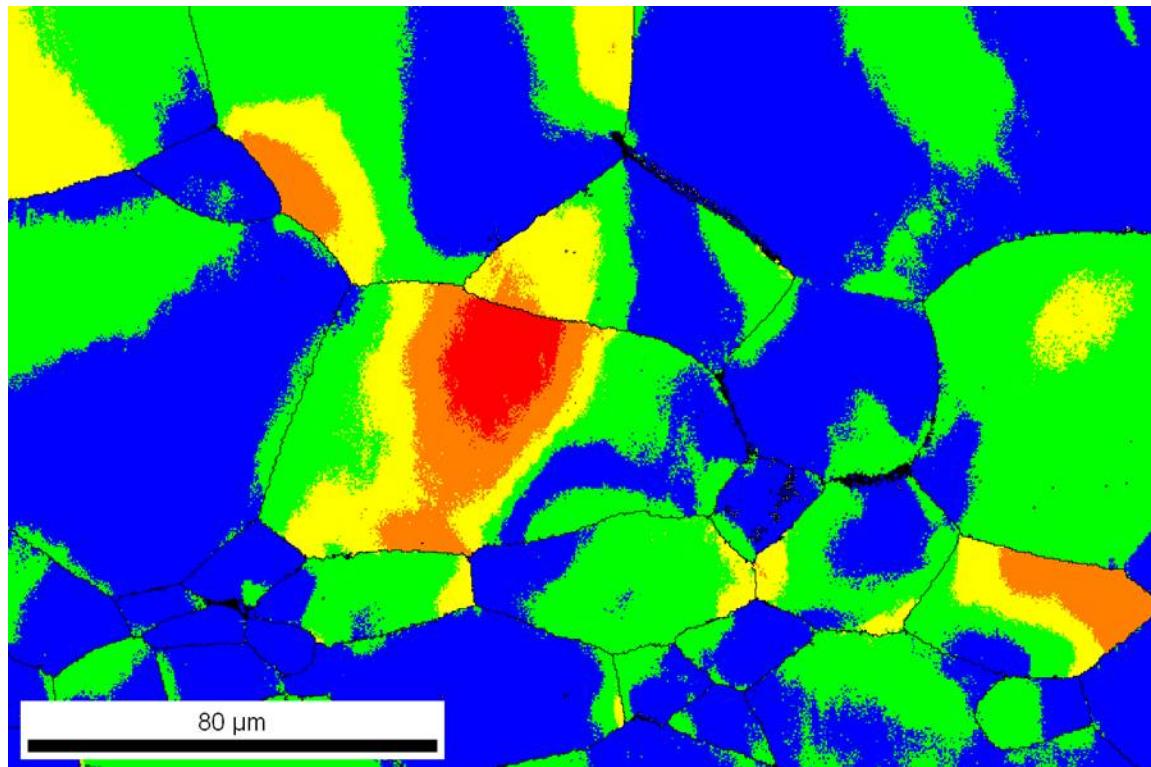
| | Min | Max | Fraction | Number | Length |
|---|---|---|---|---|---|
| — | 15° | 180° | 0.011 | 8093 | 2.43 mm |

*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 3$^{rd}$ neighbor x 0.3 μm spatial resolution

*R. Crooks*

# Nb: EBSD GROD Map 500 μm deep

*Severely deformed, >15° in 50 μm*
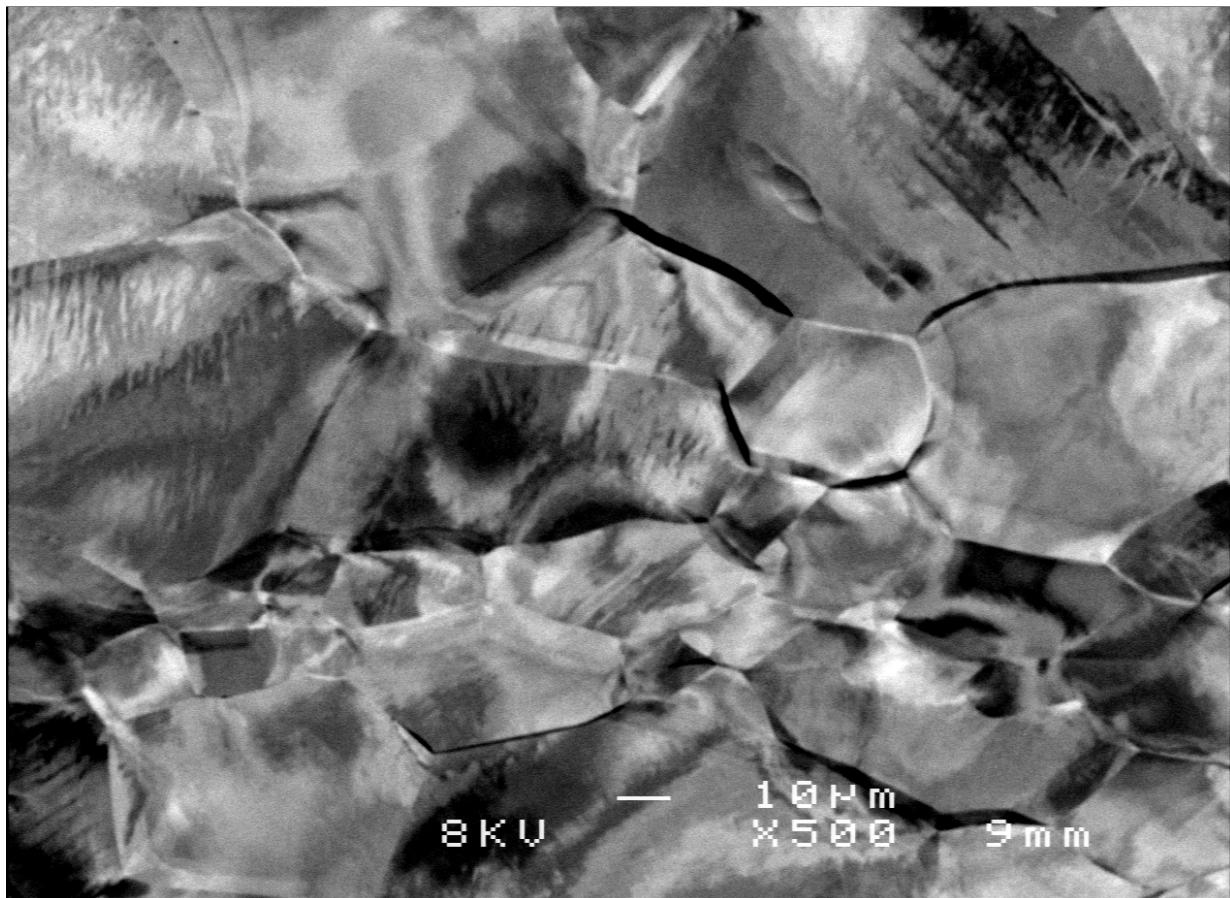


Color Coded Map Type: Grain Reference Orientation Deviation

| | 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
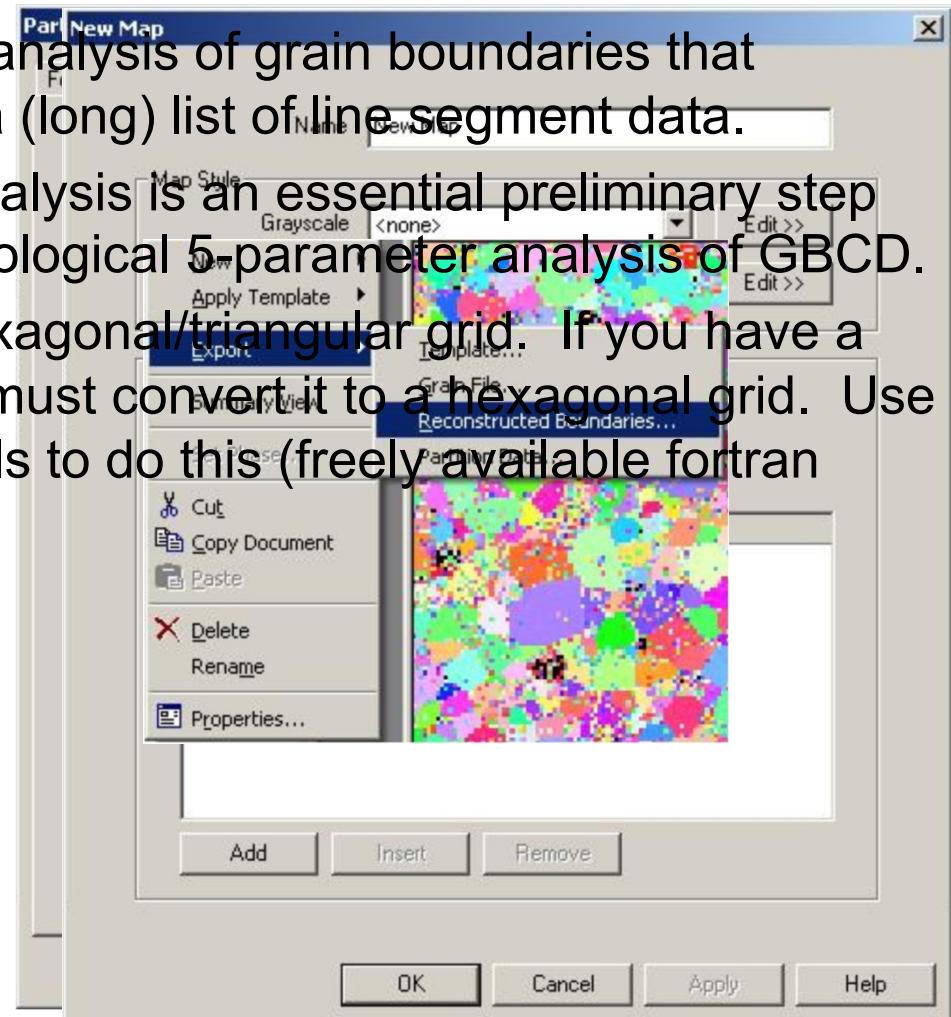


Channeling contrast of
Polished and etched
surface resembles
EBSD map

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

Greater strain at 300
and 500 $\mu$m
than at surface.

*R. Crooks*

# Reconstructed Boundaries

• The software includes an analysis of grain boundaries that outputs the information as a (long) list of line segment data.

• Data MUST be on hexagonal grid

• use of the GB segment analysis is an essential preliminary step before performing the stereological 5-parameter analysis of GBCD.

• Clean up the data to 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

# 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, $\alpha$.

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

- Here, $\varepsilon^e$ 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, $\rho$ is the dislocation density of the $k^{th}$ 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, $\theta$, based on the curl of the elastic curvature, $\kappa_e$:

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

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

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

# 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, $\kappa_e$, 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