

*Volume Fractions of  
Texture Components*

A. D. Rollett

27-731 (normally 27-750)

Texture, Microstructure & Anisotropy

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# *Lecture Objectives*

- Explain how to compute intensities in a discrete OD from counts of grains, points or volumes.
- Define *volume fraction* as the fraction of material whose orientation lies within a specified range of orientations.
- Explain how to calculate volume fractions given a discrete orientation distribution.
- Describe the calculation of *orientation distance* as a subset of the calculation of *misorientations*. Also discuss how to apply symmetry, and some of the pitfalls.
- Illustrate the binning scheme used for 5-parameter grain boundary description, as part of the discussion of how to obtain MRD values for specific examples.

# Notation

$g$  - orientation

$f(g)$  - orientation distribution

$O$  - symmetry operator

$O_{432}$  - 432 point group

$O_C$  - crystal symmetry operator

$O_S$  - sample symmetry operator

tr - trace of a matrix

$\Delta g$  - misorientation

$V_f$  - physical volume fraction of grain, material, orientation

$\phi_1, \Phi, \phi_2$  - Euler angles

$\Omega, \Delta\Omega$  - Volume of orientation space, increment of volume

popLA – preferred orientation package Los Alamos, a software package written in the early 1990s to analyze texture data, based on the DOS operating system.

# *In Class Questions*

- How do we compute intensities from volume fractions?
- What is the difference between cell-edge and cell-centered coordinates?
- What do we mean by the *volume fraction of a texture component*?
- How do we compute the volume fraction of a component?
- What is a *capture angle* or *tolerance angle* or *capture radius*?
- What is a *partition map*?
- Why is the density of randomly chosen orientations (in Euler space) not uniform?
- Describe two ways to compute *orientation distance*.
- Why is *misorientation* useful for computing orientation distance?
- How do we apply symmetry to compute misorientation?
- Why do different components (e.g. cube vs. S) have different volume fractions in a random texture?

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# *Intensity from Volume Fractions*

Objective: given information on volume fractions (e.g. numbers of grains of a given orientation), how do we calculate the intensity in the OD?

- General relationships:

Integrate odf to get  
volume fraction:

$$V_f(g) = \frac{1}{\Omega} \int_{\Delta\Omega} f(g) dg$$

Differentiate volume  
fraction to get odf :

$$f(g) dg = \frac{\Omega}{V} \frac{dV(g)}{dg} = \Omega \left. \frac{\Delta V_f}{\Delta\Omega} \right|_g$$

Reminder on units of the OD: the way that normalization is performed means that the units of the OD are Multiples of a Random Density (MRD). If there is no texture or preferred orientation then the value of “ $f$ ” is one everywhere. Note that the formulae given here differ from those in Bunge (who has very little to say about this topic). His correspond to a strict probability density formulation.

# *Discrete vs. Continuous Distributions*

- These notes emphasize the use of discrete distributions for obtaining volume fractions.
- If a continuous distribution is available, e.g., from fitting generalized spherical harmonics (from the “series expansion” method) then other ways of integrating over orientation space are used. Brief notes about how to use this approach are provided at the end.
- For data obtained as discrete points, e.g., from EBSD maps, performing calculations directly on the data makes the least assumptions about the material. On the other hand, prior knowledge may provide a justification for using a particular fitted function.

## *Intensity from $V_f$ , contd.*

- For each cell, we assign an intensity equal to the volume fraction in that cell,  $\Delta V$ , divided by the volume of orientation space associated with that cell,  $\Delta\Omega$  and multiplied by the total volume of orientation space .
- If we have points with equal area or volume (e.g. EBSD data) the volume fraction,  $\Delta V_i$ , is simply the number of points in the  $i^{\text{th}}$  cell,  $n_i$ , divided by the total number of points,  $N$ :  $\Delta V_i = n_i / N$ .
- For  $5 \times 5 \times 5^\circ$  discretization in a  $90 \times 90 \times 90^\circ$  space, we particularize to:

$$V_f(g) = \frac{1}{8100^{\circ 2}} \int f(g) \sin \Phi d\Phi d\varphi_1 d\varphi_2 \quad V_f(g) = \frac{1}{\Omega} \int_{\Delta\Omega} f(g) dg$$

$$f(g) = \frac{1}{V} \frac{dV(g)}{dg} = \Omega \left. \frac{\Delta V_f}{\Delta\Omega} \right|_g$$

$$= 8100^{\circ 2} \frac{\Delta V_f}{25^{\circ 2} (\cos[\Phi - 2.5^\circ] - \cos[\Phi + 2.5^\circ])}$$

## *Discrete OD*

- Normalization also required for discrete OD
- Normalization depends on the size of the sub-space of orientation, and on the measure used (radians versus degrees).
- Sum the intensities over all the cells.
- $0 \leq \phi_1 \leq 2\pi, 0 \leq \Phi \leq \pi, 0 \leq \phi_2 \leq 2\pi$

$$1 = \frac{1}{8\pi^2} \sum_{\phi_1} \sum_{\Phi} \sum_{\phi_2} f(\phi_1, \Phi_i, \phi_2) \Delta\phi_1 \Delta\phi_2 \left( \cos\left(\Phi_i - \frac{\Delta\Phi}{2}\right) - \cos\left(\Phi_i + \frac{\Delta\Phi}{2}\right) \right)$$

$$0 \leq \phi_1 \leq 90^\circ, 0 \leq \Phi \leq 90^\circ, 0 \leq \phi_2 \leq 90^\circ$$

$$1 = \frac{1}{8100} \sum_{\phi_1} \sum_{\Phi} \sum_{\phi_2} f(\phi_1, \Phi_i, \phi_2) \Delta\phi_1 \Delta\phi_2 \left( \cos\left(\Phi_i - \frac{\Delta\Phi}{2}\right) - \cos\left(\Phi_i + \frac{\Delta\Phi}{2}\right) \right)$$



## *Volume fraction calculations*

- Choice of cell size determines size of the volume increment, which depends on the value of the second angle ( $\Phi$  or  $\Theta$ ).
- Some grids start at the specified value.
- More typical for the specified value to be in the center of the cell.
- popLA: grids are cell-centered.

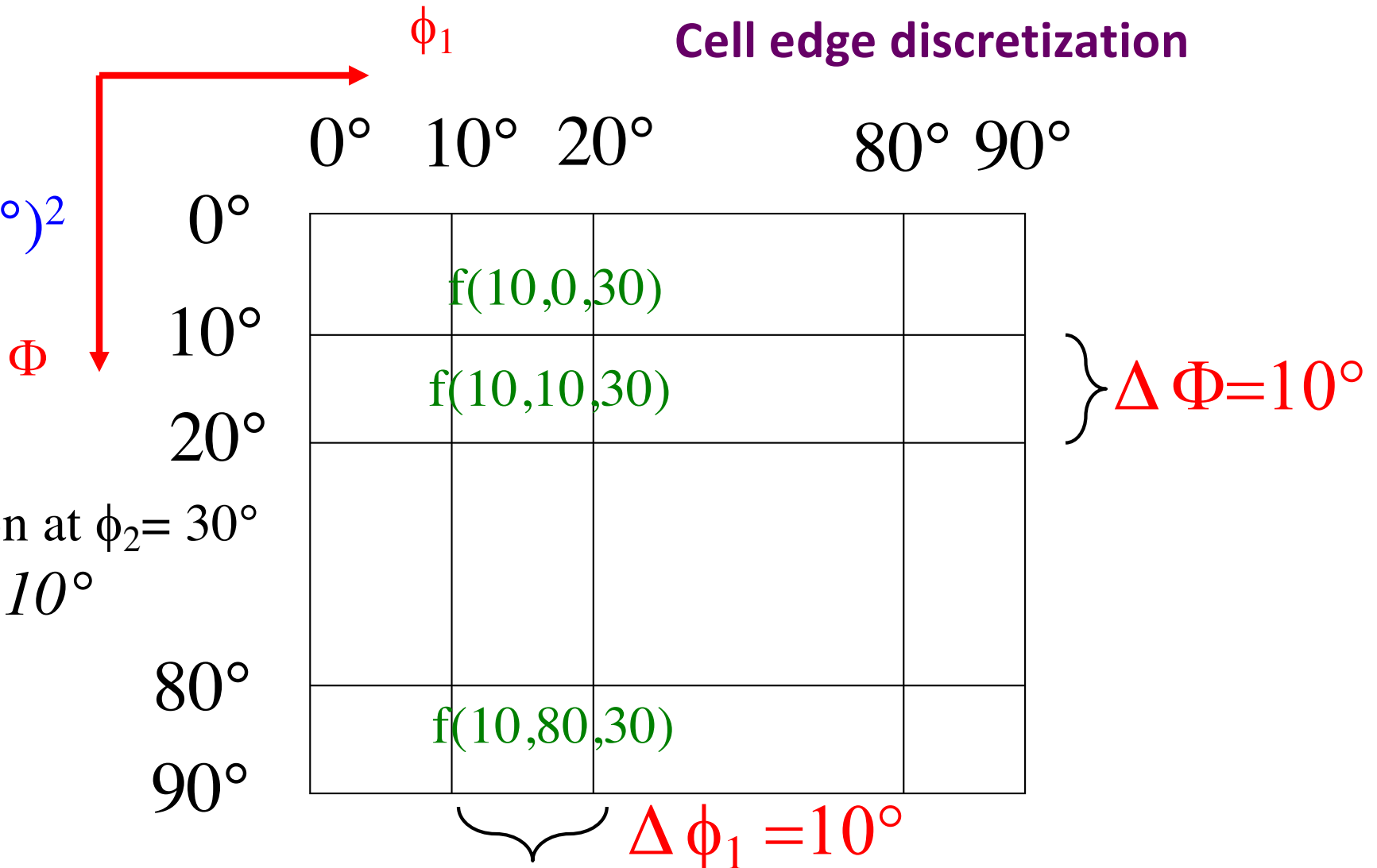
# Discrete ODs

$$dA = \sin \Phi d\Phi d\phi_1:$$

Each layer:  $\Delta\Omega = \sum \Delta A \Delta\phi_2 = 90(^{\circ})$   $\Delta A = \Delta(\cos \Phi) \Delta\phi_1$

Total:

$$\Omega = 8100(^{\circ})^2$$

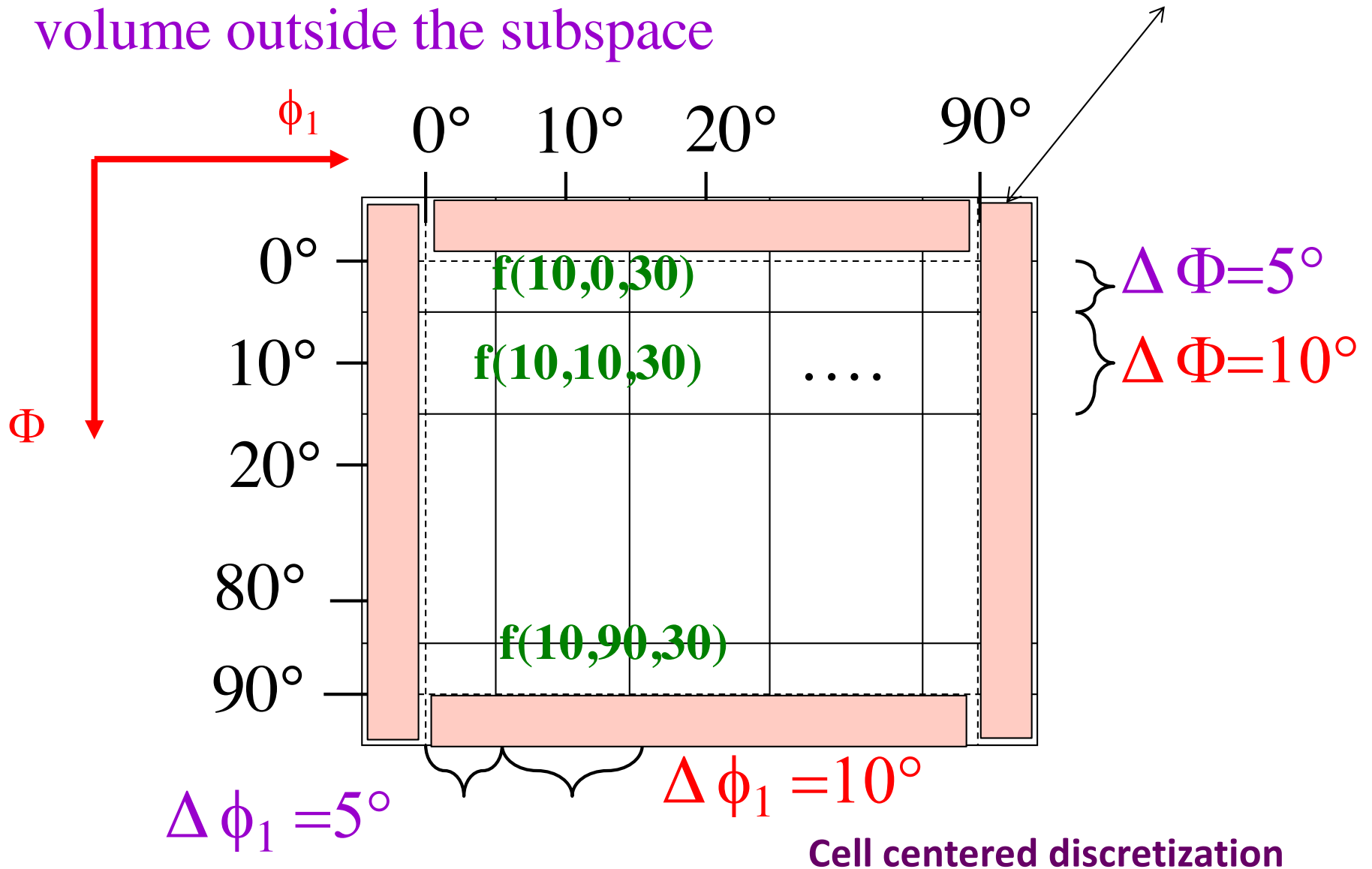


# Centered Cells

$$dA = \sin \Phi d\Phi d\phi_1:$$

$$\Delta A = \Delta(\cos \Phi) \Delta\phi_1$$

Different treatment of end and corner cells to exclude volume outside the subspace



# 12 *Discrete orientation information*

Typical text data. ANG file from TSL EBSD system

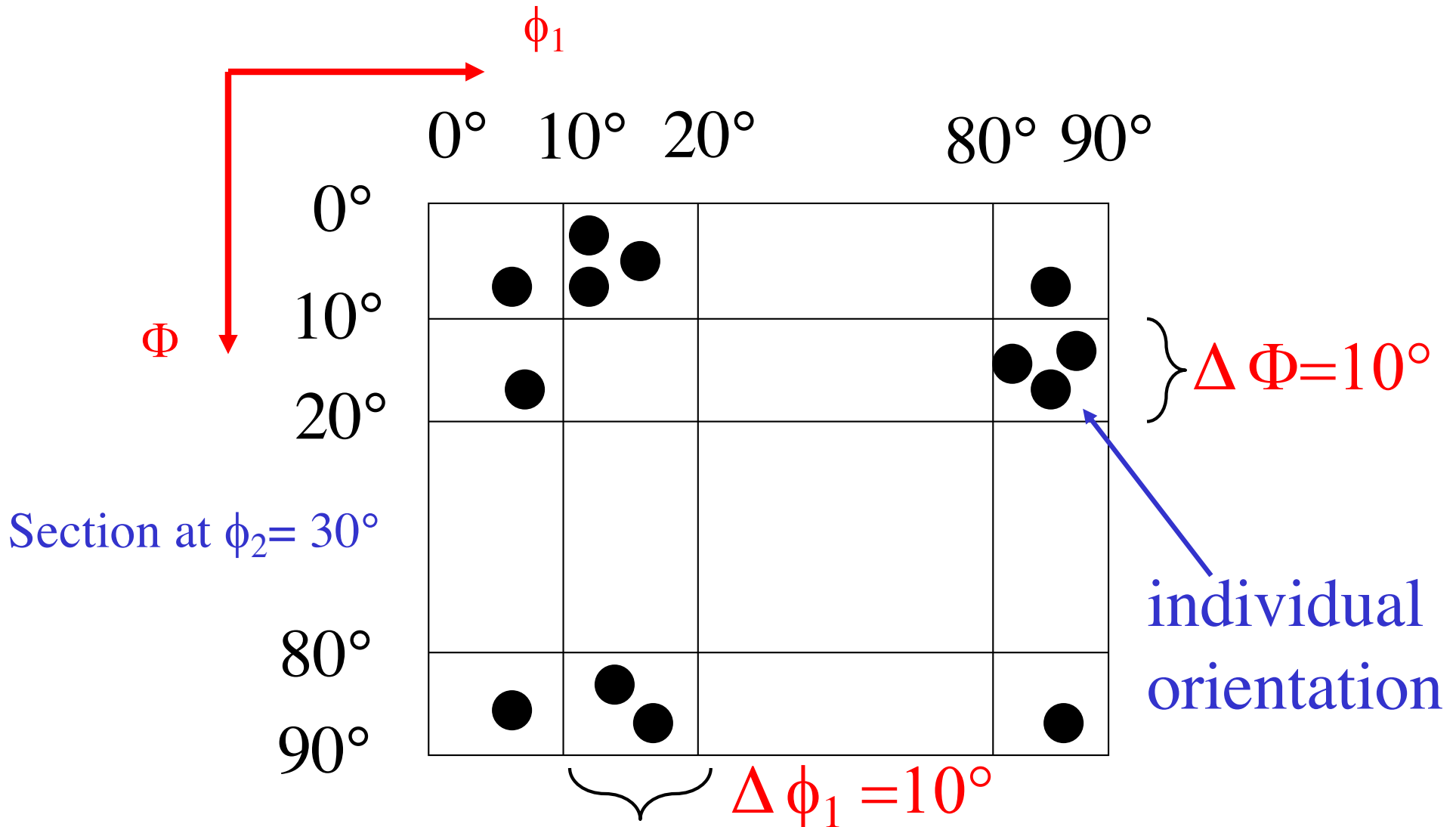
(e.g. SmallIN100/Slice\_1.ang available in SmallIN100.zip):

# WorkDirectory                    /usr/OIM/rollett     *Each dataset may*  
 # OIMDirectory                    /usr/OIM             *have millions of points*

#	$\phi_1$	$\Phi$	$\phi_2$	x	y				
4.724	0.234	4.904	0.500	0.866	1.0	1.000	0	0	
4.491	0.024	5.132	7.500	0.866	1.0	1.000	0	0	
4.932	0.040	4.698	19.500	0.866	1.0	1.000	0	0	
4.491	0.024	5.132	20.500	0.866	1.0	1.000	0	0	
4.491	0.024	5.132	21.500	0.866	1.0	1.000	0	0	
4.932	0.040	4.698	22.500	0.866	1.0	1.000	0	0	
4.932	0.040	4.698	23.500	0.866	1.0	1.000	0	0	
4.932	0.040	4.698	24.500	0.866	1.0	1.000	0	0	

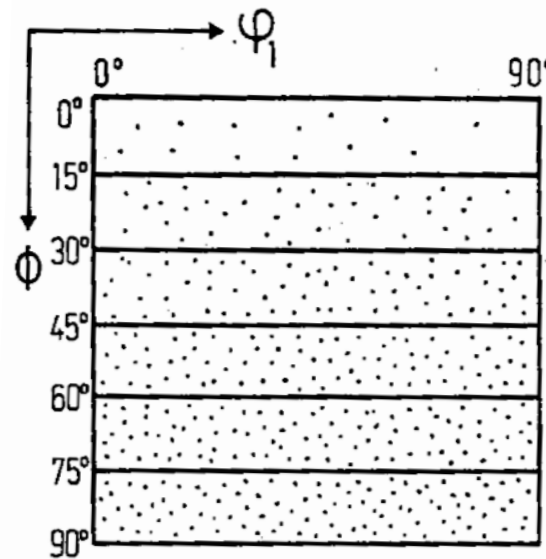
(Euler angles, radians)     (spatial coordinates, microns)

# *Binning individual orientations in a discrete OD*



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# Example of random orientation distribution in Euler space



[Bunge]

Figure 2.25 On the definition of the invariant measures by a random distribution in the EULER space  $\varphi_1\Phi\varphi_2$

Note the smaller densities of *points* (arbitrary scale) near  $\Phi = 0^\circ$ . When converted to *intensities*, however, then the result is a uniform, constant value of the OD (because of the effect of the volume element size,  $\sin\Phi d\Phi d\phi_1 d\phi_2$ ). If a material had randomly oriented grains all of the same size then this is how they would appear, as individual points in orientation space.

# *OD from discrete points: pseudo-code*

1. Compute the volume of the chosen orientation space, e.g. Euler space, e.g.  $90^\circ \times 90^\circ \times 90^\circ \Rightarrow \Omega = \int dg = 8100 \text{ }^\circ^2$ . Also compute the volume of each cell; in this case

$$d\Omega(\phi_1, \Phi, \phi_2) = \Delta(\cos \Phi) \Delta\phi_1 \Delta\phi_2$$

2. Bin each orientation into a cell in the OD
3. Sum number (or weight, if each orientation represents a different physical volume) in each cell
4. Divide the number (or physical volume) in each cell by the total number of grains (or total physical volume) to obtain  $V_f$
5. Convert from  $V_f$  to  $f(g)$ :

$$f(g) = V_f * \Omega / d\Omega = 8100 V_f / \{\Delta(\cos \Phi) \Delta\phi_1 \Delta\phi_2\}$$

$$\Omega = \int dg \quad \underbrace{\hspace{10em}}_{d\Omega = \text{cell volume}}$$

## *Discrete OD from points*

- The same  $V_f$  near  $\Phi=0^\circ$  will have much larger  $f(g)$  than cells near  $\Phi=90^\circ$ .
- Unless large number ( $>10^4$ , texture dependent) of grains are measured, the resulting OD will be noisy, i.e. large variations in intensity between cells.
- Typically, smoothing is used to facilitate presentation of results: always do this last and as a visual aid only!
- An alternative to smoothing an ODF plot is to replace individual points by Gaussians and then evaluate the texture. This is particularly helpful (and commonly applied) when performing a series expansion fit to a set of individual orientation measurements, such as OIM data.



## *Volume fraction calculation*

- In its simplest form: sum up the intensities multiplied by the value of the volume increment (invariant measure) for each cell.
- Check that when you compute this sum for the entire space the result is equal to one (else the normalization is not correct).

# Simple results

- What if all the orientations/grains/sets\_of\_Euler\_angles fall in one cell?
- Answer: the intensity (in units of Multiples of a Random Density, MRD) in that cell depends on its location in the space (assuming uniformly divided space by angle), and the intensity in all other cells is exactly zero.
- Example: cell-edge coordinates with  $10^\circ$  increments in a  $90 \times 90 \times 90$  space (total volume,  $\Omega = 8100$  ( $^\circ$ ));  
each cell has volume  $\Delta\Omega(g) = 100 \times \Delta\cos(\Phi)$ .  
Note that the sum of the second column is one, as it must be for the integral of  $\sin(\Phi)$  over the interval  $[0, \pi/2]$ .
- More exactly:  $f(g) = \Omega / \Delta\Omega(g)$
- The magnitude of the peak depends on the cell size in relation to the volume, not on the measure (*degrees versus radians*).

$\Phi$ ( $^\circ$ )	$\Delta\cos\Phi(g)$	Intensity (MRD)
0	0.0152	5331
10	0.0451	1795
20	0.0737	1100
30	0.1	810
40	0.1233	657
50	0.1428	567
60	0.1580	512
70	0.1684	481
80	0.1736	466

# Simple results: 2

- What if all, say, 9/10ths of the grains fall in one cell and the rest are randomly distributed?
- Answer: the intensity in that cell once again depends on its location in the space (assuming uniformly divided space by angle), and the intensity in all other cells is fixed at  $0.1/\{\text{remaining volume}\}$ , where the “remaining volume” is the total volume minus the volume of the individual cell that contains 9/10ths of the volume.
- Example: cell-edge coordinates with  $10^\circ$  increments in a  $90 \times 90 \times 90$  space (total volume = 8100; each cell has volume  $100 \times \Delta \cos(\Phi)$ ). Note that the sum of the second column is one.
- More exactly (in the single cell):  
 $f(g) = 0.9 \Omega / \Delta \Omega(g)$ , - “peak”  
 or elsewhere, since  $\int f(g) = \Omega$   
 $f(g) = 0.1 \Omega / (\Omega - \Delta \Omega(g))$  - “random”

$\Phi$ ( $^\circ$ )	$\Delta \cos \Phi(g)$	Intensity in Cell (MRD)	$f(g)$ elsewhere ( $10^{-5}$ MRD)
0	0.0152	4779	0.10002
10	0.0451	1615	0.10006
20	0.0737	990	0.10009
30	0.1	729	0.10012
40	0.1233	591	0.10015
50	0.1428	510	0.10017
60	0.1580	461	0.10019
70	0.1684	433	0.10020
80	0.1736	420	0.10021

# *Grain Boundary Space*

- As a preview to dealing with grain boundaries, we explain the binning scheme and show how to compute intensities and expected area fractions.
- A grain boundary requires five (5) macroscopic parameters to describe its crystallographic character (which ignores translational parameters at the atomic scale).
- Generally, it is convenient to separate these parameters into the disorientation and the normal of the boundary plane.
- For the purposes of this lecture, assume that the disorientation is the difference in orientation across the boundary, reduced to a fundamental zone (FZ). Assume that the normal is a unit vector described by two spherical angles, which can be referred to either one of the two crystal lattices (orientations).
- Assume a binning scheme in which the disorientation is expressed as Euler angles thus  $(\phi_1, \cos(\Phi), \phi_2)$ ; each dimension is divided into equal size cells. The use of the cosine provides cells of equal volume. We bin the normal according to  $(\beta, \cos(\alpha))$ , where alpha is the co-latitude and beta the longitude.
- For cubic materials, we can use a  $90^\circ \times 90^\circ \times 90^\circ$  space for disorientation (which contains multiple copies of the FZ) and a  $90^\circ \times 360^\circ$  space for the normal (which has only one copy of the FZ).

# *Area Fractions of Grain Boundaries*

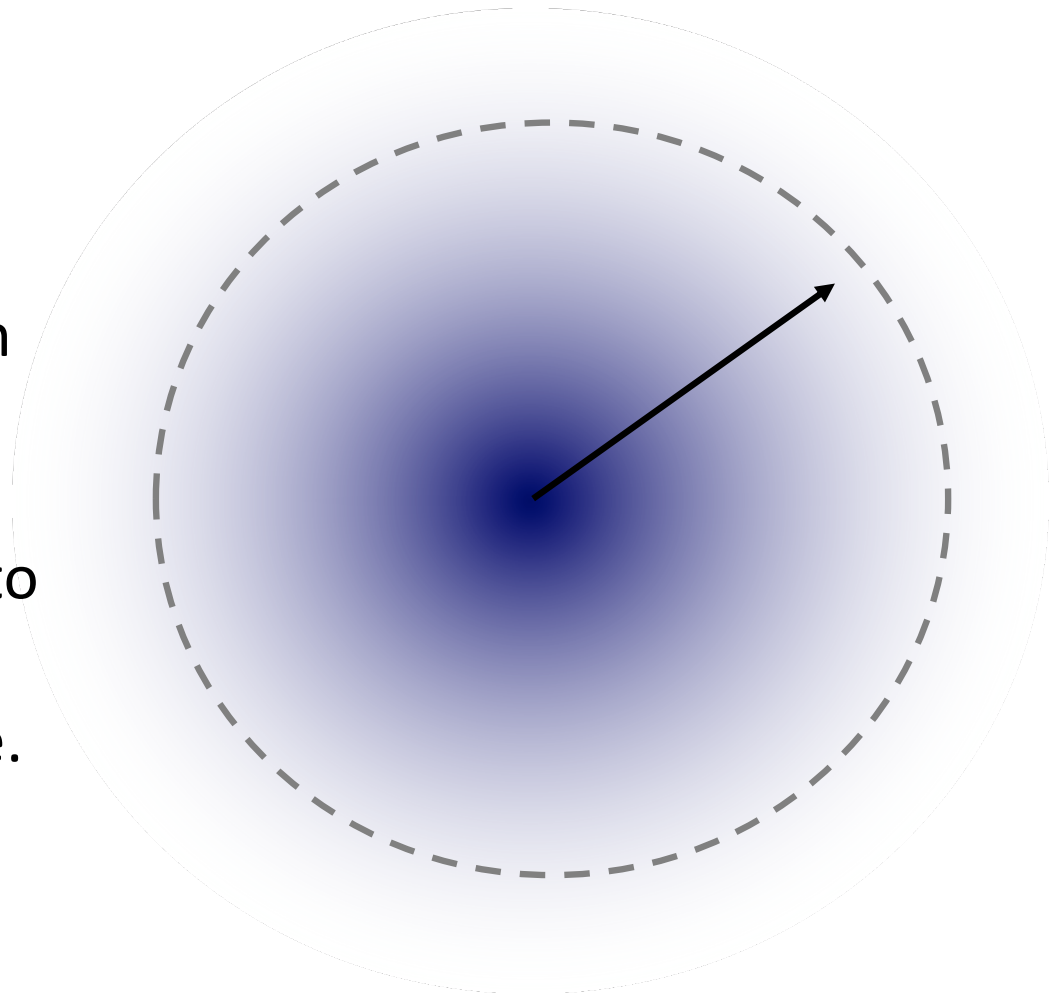
- A reasonable discretization uses 9 intervals (cells) in all dimensions except we use 36 for the longitude of the normal. This provides an approximate  $10^\circ$  resolution.
- Multiplying out the dimensions,  $9*9*9*9*36 = 288,684$ . Crystal symmetry provides a reduction of a factor of 36 (1152/96, the number of copies of the FZ in the disorientation space), down to 8,019 independent cells. This means that, if we want an average of ten data points per bin (on average) then we need of order 80,000 points.
- Consider the intensity associated with coherent twin boundaries in an fcc metal, such as copper or silver. This GB type corresponds to a single disorientation (S3, explained elsewhere) and a single normal, (111). If 1/3 of the boundaries are of this type (i.e. the area fraction is 1/3) then all the corresponding data points fall into a single bin/cell. Therefore the intensity associated with that cell is the area fraction divided by the fraction of bins for that type, but there is only 1 cell. Therefore the intensity in units of MRD is  $8019/3 = 2,673$  (“times random”).

# *Texture Component Fractions: Partitioning by Misorientation*

- Now we discuss how to compute the **volume fraction of material associated with a particular texture component**.
- The physical analogy is, how many (equal sized) grains will we find in a material that correspond to a particular texture component?
- The simplest way to think about volume fractions is to consider that all cells within a certain angle of the location of the position of the texture component of interest belong to that component.
- Although we will need to use the concept of orientation distance (equivalent to misorientation), for now we can use a fixed angular distance or *acceptance angle* to decide which component a particular cell belongs to.
- This latter approach introduces the concept of *orientation distance*, or the difference between two rotations/orientations, which is itself a rotation or *misorientation*. Note that rotations are not Cartesian vectors and so we cannot use Euclidean distance; however, the angle associated with the difference in orientation (misorientation angle) provides a suitable measure of orientation distance. *Symmetry* has to be included in order to find the smallest possible misorientation angle.

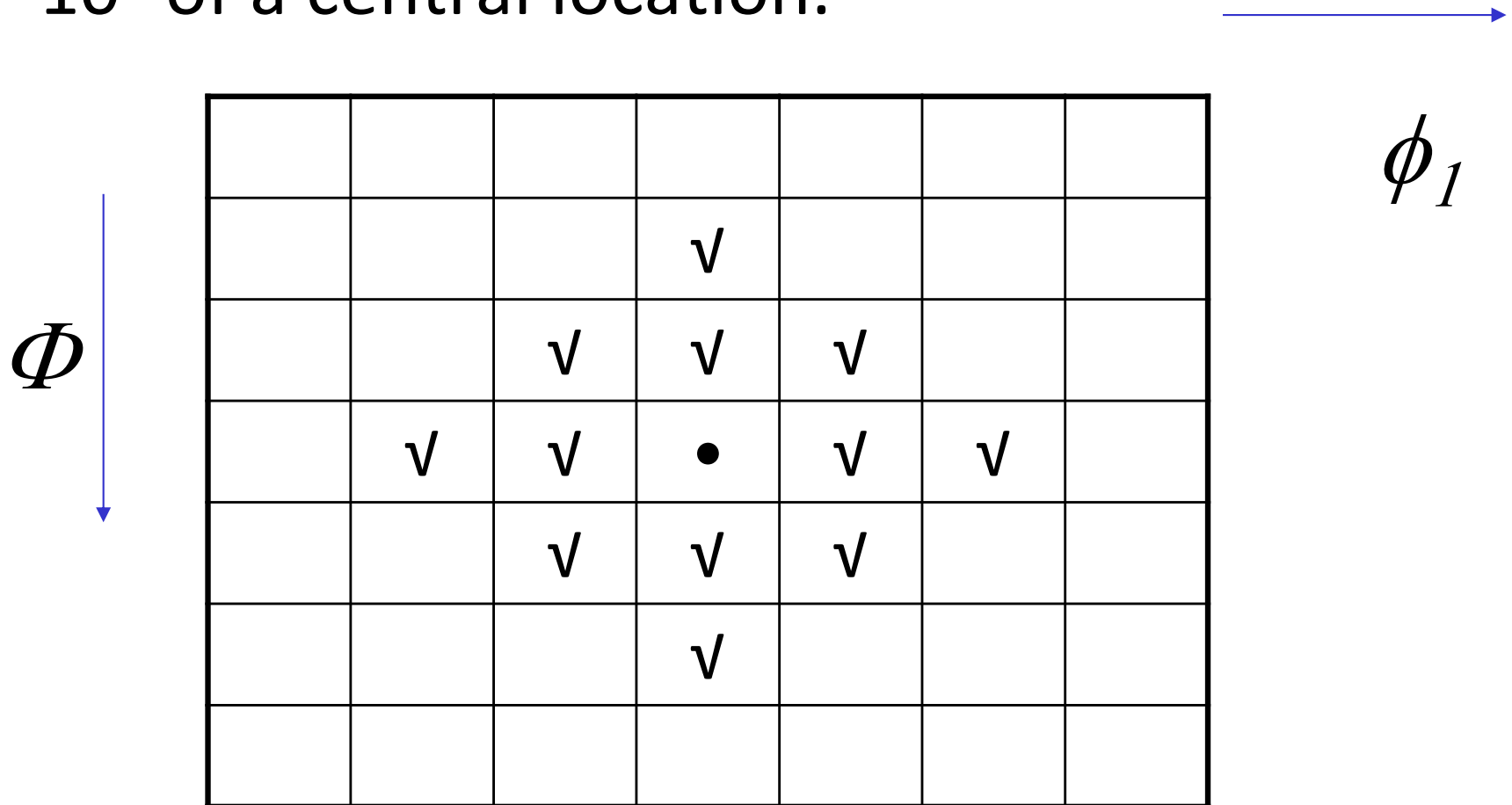
# *Acceptance Angle Schematic*

- In principle, one might want to weight the intensity in each cell as a function of distance from the component location.
- For now, however, we will assign equal weight to all cells included in the volume fraction estimate.



# *Illustration of Acceptance Angle*

- As a basic approach, include all cells within  $10^\circ$  of a central location.





# Copper component example

15° acceptance angle; location of maximum intensity 5° off ideal position

CUR80-2 6/13/88 35 Bwimv iter: 2.0%FON= 0 13-APR-\*\* strength= 2.43  
 CODK 5.0 90.0 5.0 90.0 1 1 1 2 3 100 phi= 45.0

15	12	8	3	3	6	14	42	89	89	89	42	14	6	3	3	8	12	15
5	5	5	6	8	20	43	53	57	65	65	45	21	14	12	10	8	9	7
12	11	10	14	20	30	60	118	136	84	49	16	2	1	1	1	2	4	5
22	21	32	49	68	81	100	123	132	108	37	12	6	3	3	3	3	2	1
321	284	228	185	172	190	207	178	109	48	19	7	5	5	4	3	3	1	1
955	899	770	575	389	293	223	131	55	12	3	2	2	1	1	1	0	0	0
1730	1547	1100	652	382	233	132	62	23	7	2	1	1	1	1	0	1	0	0
1513	1342	881	436	191	90	53	29	17	6	2	1	0	0	1	0	0	0	0
137	135	109	77	59	41	24	10	4	2	1	0	0	0	0	0	0	0	0
1	0	1	3	5	10	13	14	10	3	1	1	0	0	0	0	0	0	0
0	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0
0	0	0	1	1	1	1	1	1	1	0	0	0	0	0	1	1	1	1
0	0	0	0	1	0	1	2	2	1	1	1	2	2	3	4	5	6	7
0	0	0	0	1	1	2	4	5	5	5	4	3	6	8	6	6	7	5
2	2	2	2	2	2	2	2	4	3	3	3	4	7	9	6	12	17	16
3	4	4	4	4	7	33	80	86	66	42	29	29	31	33	40	51	46	40
7	7	9	14	31	71	144	179	145	81	31	11	7	7	10	17	25	23	23
203	190	188	193	224	304	417	486	410	249	109	51	36	26	16	12	12	12	8
301	315	404	559	752	1005	1180	1140	861	494	237	132	65	42	29	26	31	30	30

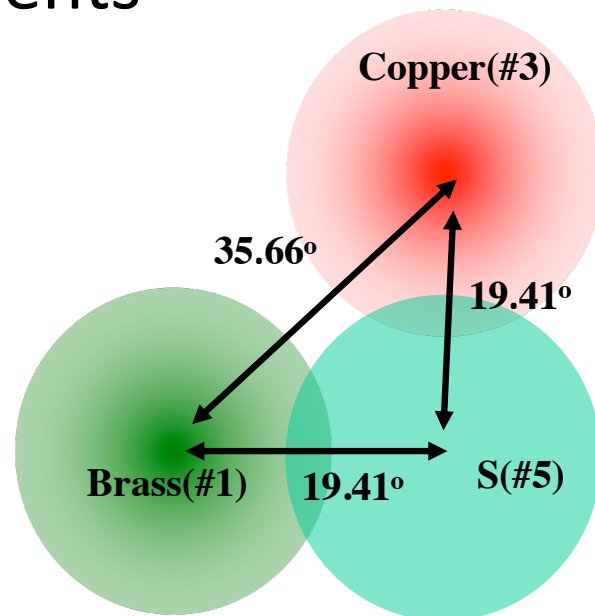
$\Phi$  (vertical arrow pointing down)

$\phi_1$  (red symbol next to the 1st column)

Red arrow pointing right from the 17th column.

# Partitioning Orientation Space

- Problem!
- If one chooses too large an acceptance angle, overlap occurs between different components
- Solution:
- It is necessary to go through the entire space and *partition* the space into separate regions with one subregion for each component. Each cell is assigned to the “nearest” component.



# *Distance in Orientation Space*

- What does “distance” mean in orientation space?
- Note: distance is *not* the Cartesian distance (Pythagorean,  $\sqrt{\Delta x^2 + \Delta y^2 + \Delta z^2}$ )
- This is an issue because the volume increment varies with [the *sine* of the] the 2nd Euler angle.

- Answer:
- Distance in orientation space is measured by *misorientation*.
- This provides a better method for partitioning the space.
- Misorientation distance is the *minimum available rotation angle* between a pair of orientations.
- Symmetry must be included.

# Misorientation Calculation

- Compute misorientation by “reversing” one orientation and then applying the other orientation. More precisely stated, compose the inverse of one orientation,  $g_A$ , with the other orientation,  $g_B$ .
- $|\Delta g| = \min_{ij} \{ \cos^{-1} ( \{ \text{tr}([O_i^{xtal} g_A O_j^{sample}] g_B^T) - 1 \} / 2 ) \}$
- The symbol “ $\text{tr}()$ ” means the trace of (sum of leading diagonal entries) of the **matrix** within the parentheses. The *minimum* function indicates that one chooses the particular combination of crystal symmetry operator,  $O_i \in O_{432}$ , and sample symmetry operator,  $O_j \in O_{222}$ , that results in the smallest angle (for cubic crystals, computed for all 24 proper rotations in the crystal symmetry point group). Thus  $i=1..24$  and  $j=1..4$ .
- Superscript  $T$  indicates (*matrix*) *transpose* which gives the inverse rotation. Subscripts  $A$  and  $B$  denote first and second component. For this purpose, the order of the rotations does not matter (but it will matter when the rotation axis is important!).
- Note that including the symmetry operators allows points near the edges of orientation space to be close to each other, even though they may be at opposite edges of the space.
- Including sample symmetry ensures that a given cell in orientation space is associated with the nearest of any variant of a given component.
- More details provided in later slides.

# *Partitioning by Misorientation*

- For each point (cell) in the orientation space, compute the misorientation of that point with every component of interest (including all 3 variants of that component within the space); this gives a list of, say, six misorientation values between the cell and each of the six components of interest.
- Assign the point (cell) to the component with which it has the smallest misorientation, provided that it is less than the acceptance angle.
- If a point (cell) does not belong to a particular component (because it is not close enough), label it as “other” or “random”.

# Partition Map, COD, $\phi_2 = 0^\circ$

Acceptance angle (degrees) = 15.

AL 3/08/02 99 WIMV iter: 1.2%, Fon= 0 20-MAY-\*\* strength= 3.88

CODB 5.0 90.0 5.0 90.0 1 1 1 2 3 0 6859Phi2= 0.0

1	1	1	4	4	4	4	0	0	0	0	4	4	4	4	1	1	1
1	1	1	4	4	4	4	0	0	0	0	4	4	4	4	1	1	1
2	2	2	4	4	4	4	0	0	0	0	4	4	4	4	5	5	5
2	2	2	2	4	0	0	0	0	0	0	0	0	0	0	5	5	5
2	2	2	0	0	0	0	0	0	0	0	0	0	0	0	5	5	5
2	2	2	0	0	0	9	9	9	0	0	0	0	0	0	0	0	0
3	3	3	7	0	9	9	9	9	9	0	0	0	0	0	0	0	0
3	3	3	7	7	9	9	9	9	9	0	0	0	0	0	0	0	0
3	3	7	7	7	7	8	8	8	8	0	0	0	0	0	0	0	0
3	7	7	7	7	7	8	8	8	8	0	0	0	0	0	0	0	0
3	3	7	7	7	7	8	8	8	8	0	0	0	0	0	0	0	0
3	3	3	7	7	9	9	9	9	9	0	0	0	0	0	0	0	0
3	3	3	7	0	9	9	9	9	9	0	0	0	0	0	0	0	0
2	2	2	0	0	0	9	9	9	0	0	0	0	0	0	0	0	5
2	2	2	0	0	0	0	0	0	0	0	0	0	0	0	5	5	5
2	2	2	0	4	0	0	0	0	0	0	0	0	0	0	5	5	5
2	2	2	4	4	4	4	0	0	0	0	4	4	4	4	5	5	5
1	1	1	4	4	4	4	0	0	0	0	4	4	4	4	1	1	1
1	1	1	4	4	4	4	0	0	0	0	4	4	4	4	1	1	1

The number in each cell indicates which component it belongs to. 0 = "random"; 8 = Brass; 1 = Cube.

# Partition Map, COD, $\phi_2 = 45^\circ$

AL 3/08/02 99 WIMV iter: 1.2%, Fon= 0 20-MAY-\*\* strength= 3.88  
 CODB 5.0 90.0 5.0 90.0 1 1 1 2 3 0 6859 Phi2= 45.0

0	0	4	4	4	4	4	1	1	1	1	1	4	4	4	4	4	0	0	
0	0	0	4	4	4	4	1	1	1	1	1	4	4	4	4	0	0	0	
0	0	0	4	4	4	4	6	6	6	6	6	4	4	4	4	0	0	0	
0	0	0	0	0	0	6	6	6	6	6	6	6	0	11	11	11	12	12	12
0	0	0	0	0	0	0	6	6	6	6	6	0	11	11	11	11	12	12	12
0	0	0	0	0	0	0	6	6	6	6	6	0	11	11	11	11	12	12	12
0	0	0	0	0	0	0	0	0	6	0	0	0	11	11	11	11	12	12	12
0	0	0	0	0	0	0	0	0	0	0	0	0	11	11	11	11	12	12	12
0	0	0	0	0	0	0	0	0	0	0	0	0	0	11	11	11	12	12	12
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	10	10	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	10	10	10	10	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	9	9	9	9	9	7	7	7	7	7	3
0	0	0	0	0	0	0	0	0	8	8	8	8	7	7	7	7	7	7	3
0	0	0	0	0	0	0	0	0	8	8	8	8	7	7	7	7	7	7	3

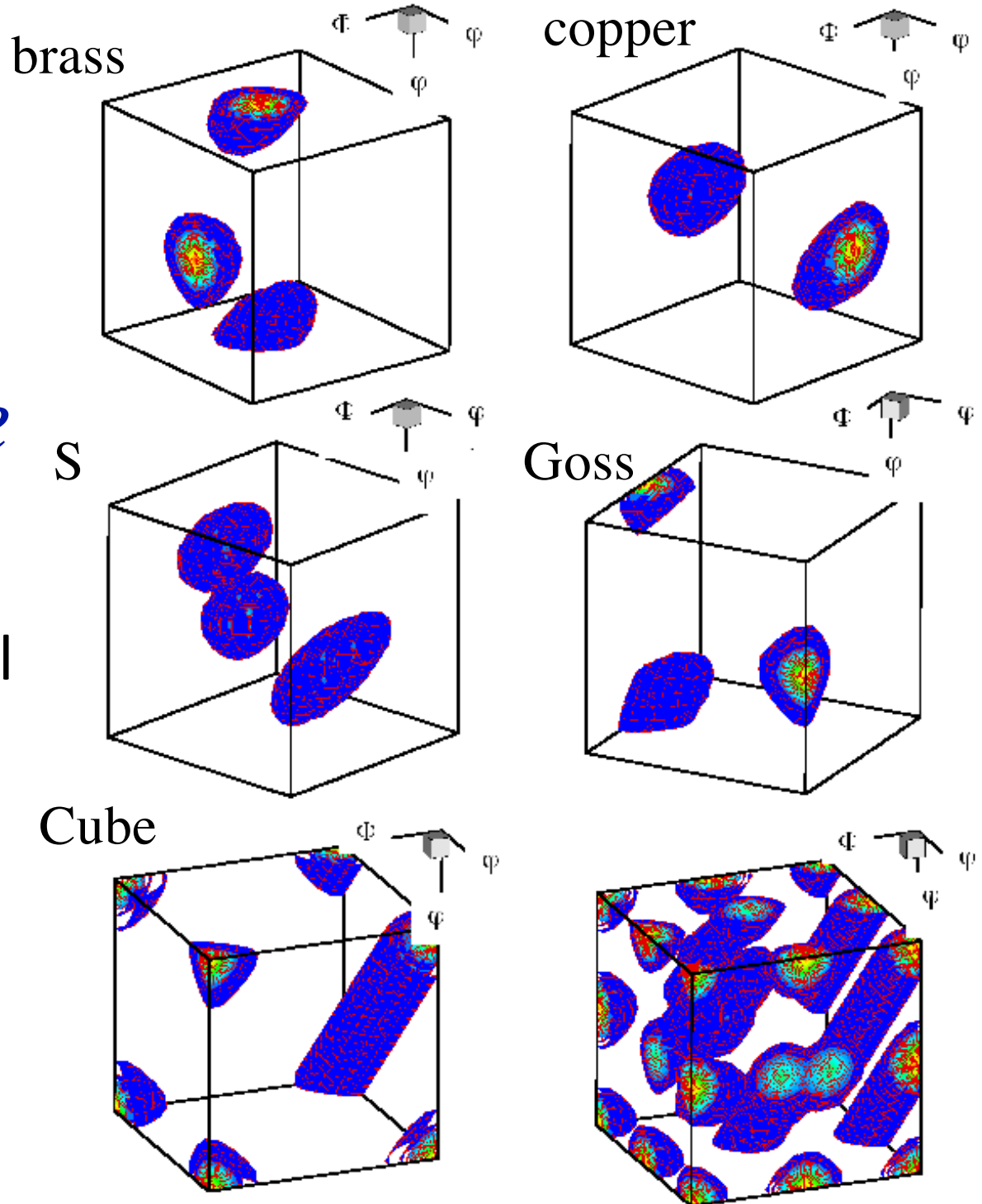
Copper

Brass

Component numbers: 0:=random; 8:=Brass; 11:= Dillamore; 12:=Copper.

# Component Volumes: fcc rolling texture

- These contour maps of individual components in Euler space are drawn for an acceptance angle of  $\sim 12^\circ$ .





## *How to calculate misorientation?*

- The next set of slides describe how to calculate misorientations, how to deal with crystal symmetry and sample symmetry, and some of the pitfalls that can arise.
- For *orientation distance*, only the magnitude of the difference in orientation needs to be calculated. Therefore some of the details that follow go beyond what you need for volume fraction. Nevertheless, you need to be aware of these issues so that you do not become confused in subsequent exercises.
- This misorientation calculation is *not* available in popLA but *is* available in TSL/HKL software. It is completely reliable but does not allow you to control the application of symmetry.

# *Objective*

- To make clear how it is possible to express a misorientation in more than (physically) equivalent fashion.
- To allow researchers to apply symmetry correctly; mistakes are easy to make!
- It is *essential* to know how a rotation/orientation/texture component is expressed in order to know how to apply symmetry operations.

## Worked Example

- In this example, we take a pair of orientations that were chosen to have a  $60^\circ \langle 111 \rangle$  misorientation between them (rotation axis expressed in crystal coordinates). In fact the pair of orientations are the two sample symmetry related variants of the Copper component. The Copper component can be written with Miller indices as  $(112)[11\bar{1}]$ .
- We calculate the 3x3 Rotation matrix for each orientation,  $g_A$  and  $g_B$ , and then form the **misorientation** matrix,  $\Delta g = g_B g_A^{-1}$ .
- From the misorientation matrix, we calculate the angle,  $= \cos^{-1}(\text{trace}(\Delta g) - 1)/2$ , and the rotation axis.
- In order to find the smallest possible misorientation angle, we have to apply crystal symmetry operators,  $O$ , to the misorientation matrix,  $O\Delta g$ , and recalculate the angle and axis.
- First, let's examine the result....

# Worked Example

```
angles..    90.  35.2599983  45.
angles..    270. 35.2599983  45.
```

```
1st Grain: Euler angles:  90.  35.2599983  45.
2nd Grain: Euler angles: 270.  35.2599983  45.
```

1st matrix:

```
[ -0.577  0.707  0.408 ]
[ -0.577 -0.707  0.408 ]
[  0.577  0.000  0.817 ]
```

2nd matrix:

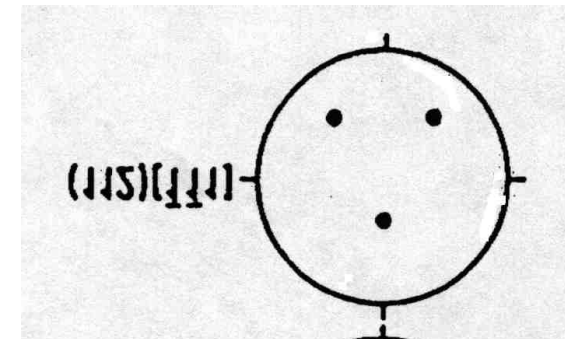
```
[  0.577 -0.707  0.408 ]
[  0.577  0.707  0.408 ]
[ -0.577  0.000  0.817 ]
```

Product matrix for  $g_A \times g_B^{-1}$ :

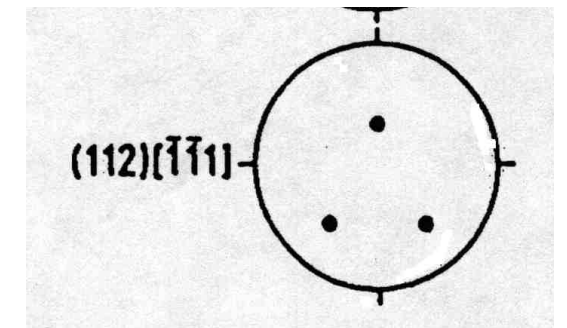
```
[ -0.667  0.333  0.667 ]
[  0.333 -0.667  0.667 ]
[  0.667  0.667  0.333 ]
```

MISORI: angle= 60. axis= 1 1 -1

{100} pole figures



+



As it happens, the result is  $60^\circ[11-1]$ , which looks reasonable, but is it, in fact, the smallest angle?

# Output with Symmetry Applied

1st matrix:  

$$\begin{bmatrix} -0.691 & 0.596 & 0.408 \\ -0.446 & -0.797 & 0.408 \\ 0.569 & 0.100 & 0.817 \end{bmatrix}$$

2nd matrix:  

$$\begin{bmatrix} 0.691 & -0.596 & 0.408 \\ 0.446 & 0.797 & 0.408 \\ -0.569 & -0.100 & 0.817 \end{bmatrix}$$

Symmetry operator number 1  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.667 & 0.333 & 0.667 \\ 0.333 & -0.667 & 0.667 \\ 0.667 & 0.667 & 0.333 \end{bmatrix}$$
  
 Trace = -1.  
 angle = 180.

Symmetry operator number 2  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.667 & 0.333 & 0.667 \\ -0.667 & -0.667 & -0.333 \\ 0.333 & -0.667 & 0.667 \end{bmatrix}$$
  
 Trace = -0.666738808  
 angle = 146.446426

Symmetry operator number 3  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.667 & 0.333 & 0.667 \\ -0.333 & 0.667 & -0.667 \\ -0.667 & -0.667 & -0.333 \end{bmatrix}$$
  
 Trace = -0.333477736  
 angle = 131.815857

Symmetry operator number 4  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.667 & 0.333 & 0.667 \\ 0.667 & 0.667 & 0.333 \\ -0.333 & 0.667 & -0.667 \end{bmatrix}$$
  
 Trace = -0.666738927  
 angle = 146.446442

Symmetry operator number 5  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.667 & -0.667 & -0.333 \\ 0.333 & -0.667 & 0.667 \\ -0.667 & 0.333 & 0.667 \end{bmatrix}$$
  
 Trace = -0.666738987  
 angle = 146.446442

Symmetry operator number 6  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.667 & 0.667 & 0.333 \\ 0.333 & -0.667 & 0.667 \\ 0.667 & -0.333 & -0.667 \end{bmatrix}$$
  
 Trace = -0.666738987  
 angle = 146.446442

Symmetry operator number 7  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.667 & -0.333 & -0.667 \\ 0.333 & -0.667 & 0.667 \\ -0.667 & -0.667 & -0.333 \end{bmatrix}$$
  
 Trace = -0.333477974  
 angle = 131.815872

Symmetry operator number 8  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.667 & -0.333 & -0.667 \\ -0.333 & 0.667 & -0.667 \\ 0.667 & 0.667 & 0.333 \end{bmatrix}$$
  
 Trace = 1.66695571  
 angle = 70.5199966

Symmetry operator number 9  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.333 & -0.667 & 0.667 \\ 0.667 & -0.333 & -0.667 \\ 0.667 & 0.667 & 0.333 \end{bmatrix}$$
  
 Trace = 0.333477855  
 angle = 109.46682

Symmetry operator number 10  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.333 & 0.667 & -0.667 \\ -0.667 & 0.333 & 0.667 \\ 0.667 & 0.667 & 0.333 \end{bmatrix}$$
  
 Trace = 0.333477855  
 angle = 109.46682

Symmetry operator number 11  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.333 & 0.667 & -0.667 \\ 0.667 & 0.667 & 0.333 \\ 0.667 & -0.333 & -0.667 \end{bmatrix}$$
  
 Trace = -0.333261013  
 angle = 131.807526

Symmetry operator number 12  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.667 & 0.667 & 0.333 \\ 0.667 & -0.333 & -0.667 \\ -0.333 & 0.667 & -0.667 \end{bmatrix}$$
  
 Trace = -0.333261073  
 angle = 131.807526

Symmetry operator number 13  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.333 & 0.667 & -0.667 \\ -0.667 & -0.667 & -0.333 \\ -0.667 & 0.333 & 0.667 \end{bmatrix}$$
  
 Trace = -0.333261013  
 angle = 131.807526

Symmetry operator number 14  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.667 & -0.667 & -0.333 \\ -0.667 & 0.333 & 0.667 \\ -0.333 & 0.667 & -0.667 \end{bmatrix}$$
  
 Trace = -1.  
 angle = 180.

Symmetry operator number 15  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.333 & -0.667 & 0.667 \\ -0.667 & -0.667 & -0.333 \\ 0.667 & -0.333 & -0.667 \end{bmatrix}$$
  
 Trace = -1.  
 angle = 180.

Symmetry operator number 16  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.667 & -0.667 & -0.333 \\ 0.667 & -0.333 & -0.667 \\ 0.333 & -0.667 & 0.667 \end{bmatrix}$$
  
 Trace = -0.333260953  
 angle = 131.807526

Symmetry operator number 17  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.333 & -0.667 & 0.667 \\ 0.667 & 0.667 & 0.333 \\ -0.667 & 0.333 & 0.667 \end{bmatrix}$$
  
 Trace = 1.66652203  
 angle = 70.533165

Symmetry operator number 18  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.667 & 0.667 & 0.333 \\ -0.667 & 0.333 & 0.667 \\ 0.333 & -0.667 & 0.667 \end{bmatrix}$$
  
 Trace = 1.66652203  
 angle = 70.533165

Symmetry operator number 19  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.333 & -0.667 & 0.667 \\ -0.667 & 0.333 & 0.667 \\ -0.667 & -0.667 & -0.333 \end{bmatrix}$$
  
 Trace = 0.333044171  
 angle = 109.480003

Symmetry operator number 20  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.667 & -0.333 & -0.667 \\ 0.667 & 0.667 & 0.333 \\ 0.333 & -0.667 & 0.667 \end{bmatrix}$$
  
 Trace = 2.  
 angle = 60.

Symmetry operator number 21  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.667 & 0.667 & 0.333 \\ -0.333 & 0.667 & -0.667 \\ -0.667 & 0.333 & 0.667 \end{bmatrix}$$
  
 Trace = 2.  
 angle = 60.

Symmetry operator number 22  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} 0.667 & -0.333 & -0.667 \\ -0.667 & -0.667 & -0.333 \\ -0.333 & 0.667 & -0.667 \end{bmatrix}$$
  
 Trace = -0.666522205  
 angle = 146.435211

Symmetry operator number 23  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.667 & -0.667 & -0.333 \\ -0.333 & 0.667 & -0.667 \\ 0.667 & -0.333 & -0.667 \end{bmatrix}$$
  
 Trace = -0.666522026  
 angle = 146.435196

Symmetry operator number 24  
 Product matrix for  $gA \times gB^{-1}$ :  

$$\begin{bmatrix} -0.333 & 0.667 & -0.667 \\ 0.667 & -0.333 & -0.667 \\ -0.667 & -0.667 & -0.333 \end{bmatrix}$$
  
 Trace = -0.999999881  
 angle = 179.980209

MISORI: angle= 60. axis= 1 1

MISORI: angle= 60. axis= 1 1 -1-1

**This set of tables shows each successive result as a different symmetry operator is applied to  $\Delta g$ . Note how the angle and the axis varies in each case! Note that #20 is the one that gives a 60° angle.**

# Misorientations

- Misorientations:

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

transform from crystal axes of grain A back to the reference axes, and then transform *to* the axes of grain B.

- Note that this use of “g” is based on the standard Bunge definition (transformation of axes)

# Notation

- In some texts, misorientation formed from axis transformations is written with a tilde.

$$\Delta\tilde{g}$$

- Standard A->B transformation is expressed in *crystal* axes. The reason for this is that we generally want to know the common axis between the two crystals in terms of crystal coordinates.

# *Misorientation + Symmetry*

- $\Delta g =$   
 $(O_c g_B)(O_c g_A)^{-1}$   
 $= O_c g_B g_A^{-1} O_c^{-1}.$
- Note the presence of symmetry operators pre- & post-multiplying
- Note that removing the parentheses from the term with the inverse swaps the order of the two matrices.



# *Symmetry: how many equivalent representations of misorientation?*

- Axis transformations:  
24 independent operators (for cubic) present on either side of the misorientation. Two equivalents from switching symmetry, i.e. the fact that there is no (physical) difference between passing from grain A to grain B, versus passing from grain B to grain A.
- Number of equivalents =  $24 \times 24 \times 2 = 1152$ .

## *When to include Sample Symmetry?*

- Answer: only for volume fractions
- The rule is simple:
- For calculating orientation distances for the purpose of partitioning orientation space, you *do* include sample symmetry. You only have to apply the sample symmetry, however, to either the component or the cell being tested but not both.
- For calculating misorientations for the purpose of characterizing grain boundaries, you do *not* include sample symmetry.

## *Practical Help with Volume Fractions*

- To calculate volume fractions directly from popLA .SOD files (orientation distributions in popLA format), use `sod2vf.f` (a Fortran 77 code)
- To calculate volume fractions from a list of discrete orientations in .WTS format, use `wts2pop[-latest_revision_date].f`, which also bins the orientations into an SOD as well as pole figures and inverse pole figures. Look at any .WTS file to learn about the format (or read the popLA manual). You can find these programs at **[pajarito.materials.cmu.edu/rollett/texture\\_subroutines](http://pajarito.materials.cmu.edu/rollett/texture_subroutines)**
- If your data source is a \*.ANG orientation map (from TSL, or, a \*.CTF from HKL) then first use `OIM2WTS.f` to convert it to the .WTS format. If your material has hexagonal symmetry be very careful about how the Cartesian x-axis is aligned with the crystal axes (TSL and HKL are, typically, different).

## *Volume fractions from Random?*

- Based on a list of 20,000 random orientations and a **15°** acceptance angle, you should expect this set of volume fractions:
  - |            |           |             |         |
|------------|-----------|-------------|---------|
| {001}<100> | cube      | vol. frac.= | 2.175 % |
| {001}<110> | NDcube    | vol. frac.= | 2.144 % |
| {011}<100> | Goss      | vol. frac.= | 2.310 % |
| {110}<112> | brass     | vol. frac.= | 4.116 % |
|            | Dillamore | vol. frac.= | 3.030 % |
| {211}<111> | Copper    | vol. frac.= | 3.721 % |
| {231}<124> | S         | vol. frac.= | 8.475 % |
  - Remember that more orientations are required for greater precision (more significant figures).

# *Volume fractions from Random?*

- Based on a list of 20,000 random orientations and a **10°** acceptance angle, you should expect this set of volume fractions:

For component	cube	vol. frac.=	0.575	%
For component	NDcube	vol. frac.=	0.690	%
For component	Goss	vol. frac.=	0.715	%
For component	brass	vol. frac.=	1.310	%
For component	Dillam	vol. frac.=	1.103	%
For component	Copper	vol. frac.=	1.382	%
For component	231124	vol. frac.=	2.775	%

- Note how the volume fractions have decreased markedly with the decrease in acceptance angle.
- Eliminating the Dillamore component, which is only about 10° from Copper, the following set is found: note that Copper has increased but not by a factor of 2.

For component	cube	vol. frac.=	0.575	%
For component	NDcube	vol. frac.=	0.690	%
For component	Goss	vol. frac.=	0.715	%
For component	brass	vol. frac.=	1.310	%
For component	Copper	vol. frac.=	<b>1.710</b>	%
For component	231124	vol. frac.=	2.775	%

# *More Random/Uniform Volume Fractions by Component*

Table 1: Orientations, Multiplicities, and Volume Fractions of 5 Orientation Poles

Component	$\{hkl\}$	$\langle uvw \rangle$	$rst$	$(\phi_1, \Phi, \phi_2)$	Multiplicity	5°	1°	5°	1°
						Code A	Code A	Code B	Code B
Cube	001	100	010	(0, 0, 0)	4	0.65%	0.68%	0.54%	0.67%
Goss	011	100	01 $\bar{1}$	(0, 45, 0)	4	0.64%	0.67%	0.59%	0.67%
Brass	101	1 $\bar{2}$ 1	10 $\bar{1}$	(35.26, 45, 90)	2	1.19%	1.35%	1.19%	1.35%
$\eta$ – fiber <sub>1</sub>	012	100	02 $\bar{1}$	(0, 26.57, 0)	2	1.34%	1.35%	1.34%	1.35%
S	213	3 $\bar{6}$ 4	22 1 $\bar{7}$ 9	(58.98, 36.70, 63.43)	1	2.76%	2.70%	2.78%	2.70%

Taken from unpublished work by Kreuziger, Hu & Rollett (2010).

## *Variations in Random $V_f$*

- Why do the volume fractions vary with component location?
- Answer: mainly because of variations in how close they lie to symmetry planes in orientation space.
- Assume cubic-orthorhombic (crystal+sample) symmetry
- An orientation such as Goss lies on one edge, so despite including 3 symmetry-related locations, its volume is only about  $1/4^{\text{th}}$  of, say, the S component.
- Similarly the Copper component, only includes  $1/2^{\text{th}}$  of the space of the S component.
- The rest of the variation is related to location with respect to the second Euler angle. See the next slide for illustrations of the above points.

# 3D Views

a) Brass b) Copper c) S  
Goss e) Cube

f) combined texture

1: {35, 45, 90}, Brass,

2: {55, 90, 45}, Brass

3: {90, 35, 45}, Copper,

4: {39, 66, 27}, Copper

5: {59, 37, 63}, S,

6: {27, 58, 18}, S,

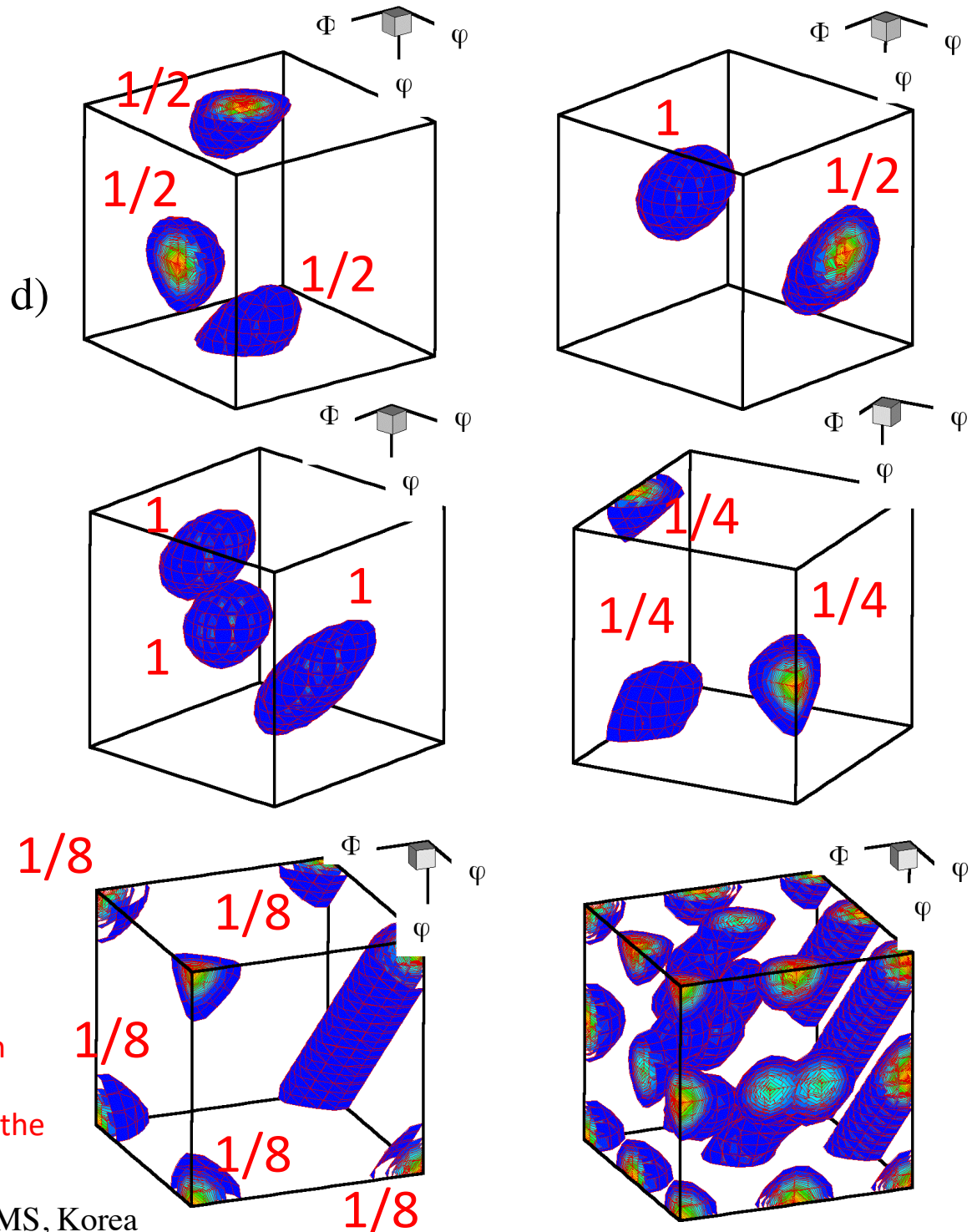
7: {53, 75, 34}, S

8: {90, 90, 45}, Goss

9: {0, 0, 0}, cube\*

10: {45, 0, 0}, rotated cube

\* Note that the cube exists as a line between (0,0,90) and (90,0,0) because of the linear dependence of the 1st and 3rd angles when the 2nd angle = 0.





## *Scaling by Random $V_f$*

- It has been argued that volume fractions are more reliable than intensities partly because they reflect the physical makeup of the material more accurately. For example, the intensity at the cube position rises to very high values once the volume fraction of orientations near cube rises much above 25%, which is not true of other orientations.
- Given that the volume fraction varies significantly with position in the space, especially for components near symmetry planes, it has also been argued that volume fractions should be reported as a multiple of the fraction associated with a random (uniform) texture.

# *Volume fractions from continuous distributions*

- Using texture components in crystal plasticity finite element simulations, D. Raabe, F. Roters, International Journal of Plasticity, 20, 339–361 (2004), doi:10.1016/S0749-6419(03)00092-5. [look in Box folder]
- The iterative series-expansion method for quantitative texture analysis. I. General outline, M. Dahms and H. J. Bunge, J. Appl. Cryst. (1989). 22, 439-447, doi:10.1107/S0021889889005261
- Discretization techniques for orientation distribution functions, LS Toth & P van Houtte, Textures & Microstructures (1992). [look in Box folder]
- Section 3.4 (p 70) in Orientations & Rotations by A. Morawiec.
- Chapter 13 in Quantitative Texture Analysis, edited by HJ Bunge and C Esling (1982).
- The first paper by Raabe & Roters is based on the concept of representing each component by a Gaussian peak in orientation space. The simplest mathematical form is this:
$$f(g) = S_0 \exp(-\omega^2/\omega_0^2)$$
- In fact, the von Mises-Fisher distribution (*q.v.* Wikipedia) is more correct for spherical parameters, which is discussed by Morawiec and others.
- If a series expansion fit for a texture is available, and the positions of a set of texture components has been identified (e.g., by inspection of the OD), then volume fractions can be obtained via a procedure that minimizes the difference between the fitted Gaussian peak and the local values of  $f(g)$ , using the coefficients of the ODF.

# Summary

- Methods for calculating volume fractions from discrete orientation distributions reviewed.
- Complementary method of calculating the OD from information on discrete orientations (e.g. OIM) provided.
- Method for calculating *orientation distance* (equivalent to *misorientation*) given, with illustrations of the importance of how to apply symmetry operators.
- For further discussion: in some cases, it is useful to compare volume fractions in a textured material to the volume fractions that would be expected in a randomly oriented material.
- Different programs may well yield different volume fraction values because of differences in the procedure (e.g. how the space is partitioned).

# *Supplemental Slides*

- The following slides illustrate what happens with misorientations if you deal with *active rotations*, instead of the standard *axis transformations* (passive rotations) used in materials science.
- This material is useful in case you have experience with solid mechanics, or you cannot get a misorientation calculation to work properly.
- Note: it does *not* matter whether you use passive or active rotations for computing the rotation angle; it only makes a difference to the rotation axis, i.e. the skew-symmetric part of the misorientation matrix.
- Caution: if you calculate the misorientation for a grain boundary with active rotations, the axis will be expressed in the sample frame. This is not what you want, generally speaking, if one is interested in the crystallographic character of the boundary.

# Passive vs. Active Rotations

These next few slides describe the differences between dealing with passive rotations (= transformations of axes) and active rotations (fixed coordinate system)

- **Passive Rotations**
- Materials Science
- $g$  describes an *axis transformation* from sample to crystal axes

Passive Rotations (Axis Transformations)

- **Active Rotations**
- Solid mechanics
- $g$  describes a *rotation* of a crystal from ref. position to its orientation.

Active (Vector) Rotations

# Matrices

$$\mathbf{g} = \mathbf{Z}_2 \mathbf{X} \mathbf{Z}_1 =$$

$$\begin{pmatrix} \cos \varphi_1 \cos \varphi_2 & \sin \varphi_1 \cos \varphi_2 & \sin \varphi_2 \sin \Phi \\ -\sin \varphi_1 \sin \varphi_2 \cos \Phi & +\cos \varphi_1 \sin \varphi_2 \cos \Phi & \cos \varphi_2 \sin \Phi \\ -\cos \varphi_1 \sin \varphi_2 & -\sin \varphi_1 \sin \varphi_2 & \cos \Phi \\ -\sin \varphi_1 \cos \varphi_2 \cos \Phi & +\cos \varphi_1 \cos \varphi_2 \cos \Phi & \cos \Phi \\ \sin \varphi_1 \sin \Phi & -\cos \varphi_1 \sin \Phi & \cos \Phi \end{pmatrix}$$

Note transpose relationship between the two matrices.

$$\mathbf{g} = \mathbf{g} \phi_{1001} \mathbf{g} \Phi_{100} \mathbf{g} \phi_{2001} =$$

$$\begin{pmatrix} \cos \varphi_1 \cos \varphi_2 & -\cos \varphi_1 \sin \varphi_2 & \sin \varphi_1 \sin \Phi \\ -\sin \varphi_1 \sin \varphi_2 \cos \Phi & -\sin \varphi_1 \cos \varphi_2 \cos \Phi & \sin \varphi_1 \sin \Phi \\ \sin \varphi_1 \cos \varphi_2 & -\sin \varphi_1 \sin \varphi_2 & -\cos \varphi_1 \sin \Phi \\ +\cos \varphi_1 \sin \varphi_2 \cos \Phi & +\cos \varphi_1 \cos \varphi_2 \cos \Phi & -\cos \varphi_1 \sin \Phi \\ \sin \varphi_2 \sin \Phi & \cos \varphi_2 \sin \Phi & \cos \Phi \end{pmatrix}$$

Passive Rotations (Axis Transformations)

Active (Vector) Rotations

# Texture + Symmetry

Symmetry Operators:

$$O_{sample} \equiv O_s$$

$$O_{crystal} \equiv O_c$$

$$g' = O_c g O_s$$

$$g' \overset{=}{\longleftrightarrow} g$$

Note that the crystal symmetry post-multiplies, and the sample symmetry pre-multiplies.

Passive Rotations (Axis Transformations)

$$g' = O_s g O_c$$

$$g' \overset{=}{\longleftrightarrow} g$$

Note the reversal in order of application of symmetry operators!

Active (Vector) Rotations

56 *Groups: Sample + Crystal Symmetry*

- $O_c \in O(432)$ ;  
proper rotations of  
the cubic point group.
- $O_s \in O(222)$ ;  
proper rotations of  
the orthorhombic  
point group.

Passive Rotations (Axis Transformations)

- Think of applying the  
symmetry operator in  
the appropriate  
frame: thus for active  
rotations, apply  
symmetry to the  
crystal *before* you  
rotate it.

Active (Vector) Rotations



# Misorientations

- Misorientations:

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

transform from crystal axes of grain A back to the reference axes, and then transform *to* the axes of grain B.

- Note that this use of “*g*” is based on the standard Bunge definition (transformation of axes)

Passive Rotations (Axis Transformations)

- Misorientations:

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

the net rotation *from* A to B is: rotate first *back from* the position of grain A and then rotate *to* the position of grain B.

- Note that this use of “*g*” is based on the a definition in terms of an active rotation (the “*g*” is the inverse, or transpose of the one on the left).

Active (Vector) Rotations

# Notation

- In some texts, misorientation formed from axis transformations is written with a tilde.

$$\Delta\tilde{g}$$

- Standard A->B transformation is expressed in *crystal* axes.

- You must verify from the context which type of misorientation is discussed in a text!
- Standard A->B rotation is expressed in *sample* axes.

# Misorientation + Symmetry

- $\Delta g =$   
 $(O_c g_B)(O_c g_A)^{-1}$   
 $= O_c g_B g_A^{-1} O_c^{-1}.$
- Note the presence of symmetry operators pre- & post-multiplying

- $\Delta g = g_B g_A^{-1};$   
 $(g_B O_c)(g_A O_c)^{-1}$   
 $= g_B O_c O_c^{-1} g_A^{-1}$   
 $= g_B O_c' g_A^{-1}.$
- Note the reduction to a single symmetry operator because the symmetry operators belong to the same group!

# *Symmetry: how many equivalent representations of misorientation?*

- Axis transformations: 24 independent operators (for cubic) present on either side of the misorientation. Two equivalents from switching symmetry.
- Number of equivalents= $24 \times 24 \times 2 = 1152$ .

Passive Rotations (Axis Transformations)

- Active rotations: Only 24 independent operators present “inside” the misorientation. 2 from switching symmetry.
- Number of equivalents= $24 \times 2 = 48$ .

Active (Vector) Rotations

# *Passive* $\leftrightarrow$ *Active*

Just as is the case for rotations, and texture components,

$$g_{\text{passive}}(\theta, \mathbf{n}) = g_{\text{active}}^T(\theta, \mathbf{n}),$$

so too for misorientations,

$$\Delta g_{\text{passive}}(\theta, \mathbf{n}) = \Delta g_{\text{active}}^T(\theta, \mathbf{n}).$$

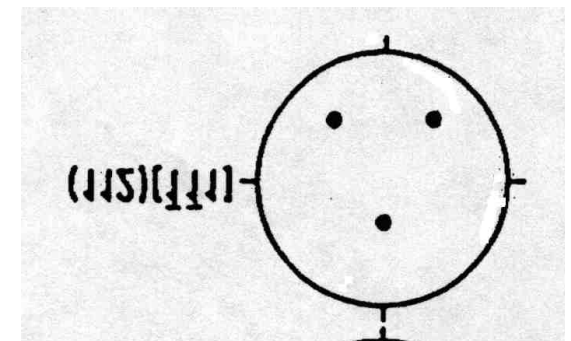
However, please be careful about the frame. The discussion given here (with the exception of the example that illustrated how the misorientation axis moved with the bi-crystal) is based on using the “local” or “crystal” frame, *not* the reference frame.

The relationship between the misorientation calculated in the local frame and the misorientation calculated in the reference frame is not at all simple. For dealing with grain boundaries, I strongly suggest that you stick to the local/crystal frame.

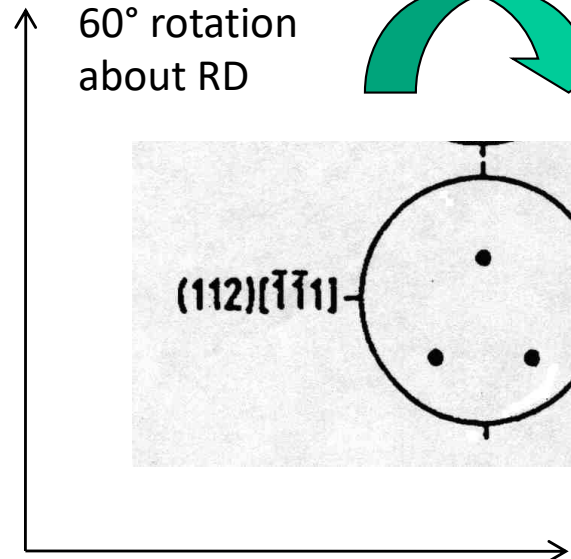
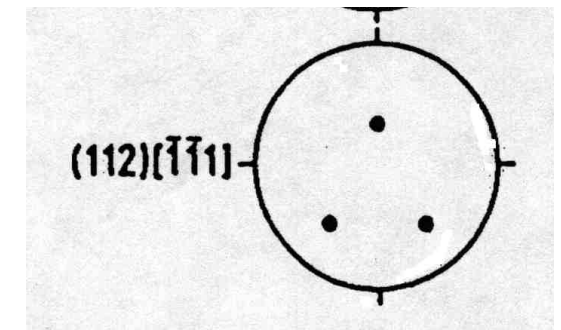
62 *Worked example: active rotations*

- So what happens when we express orientations as active rotations in the sample reference frame?
- The result is similar (same minimum rotation angle) but the axis is different!
- The rotation axis is the sample  $[100]$  axis, or  $x$ -axis, which happens to be parallel to a *crystal*  $\langle 111 \rangle$  direction because the Copper component is  $(112)[11-1]$ .

{100} pole figures

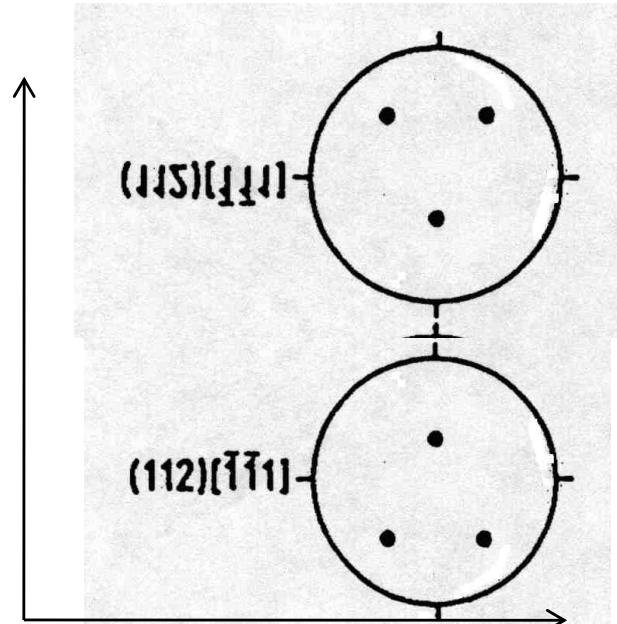


60° rotation about RD



# Active rotations example

63



```
angles.. 90. 35.2599983 45.
angles.. 270. 35.2599983 45.
```

```
1st Grain: Euler angles: 90.
                 35.2599983 45.
2nd Grain: Euler angles: 270.
                 35.2599983 45.
```

1st matrix:

```
[ -0.577  0.707  0.408 ]
[ -0.577 -0.707  0.408 ]
[  0.577  0.000  0.817 ]
```

2nd matrix:

```
[  0.577 -0.707  0.408 ]
[  0.577  0.707  0.408 ]
[ -0.577  0.000  0.817 ]
```

MISORInv: angle= 60. axis= 1 0 0

```
Symmetry operator number 1
Product matrix for gB X gA^-1:
[ -1.000  0.000  0.000 ]
[  0.000 -1.000  0.000 ]
[  0.000  0.000  1.000 ]
Trace = -1.
angle = 180.
```

```
Symmetry operator number 2
Product matrix for gB X gA^-1:
[ -0.333  0.000  0.943 ]
[  0.816 -0.500  0.289 ]
[  0.471  0.866  0.167 ]
Trace = -0.666738927
angle = 146.446442
```

```
Symmetry operator number 3
Product matrix for gB X gA^-1:
[  0.333  0.817  0.471 ]
[  0.817  0.000 -0.577 ]
[ -0.471  0.577 -0.667 ]
Trace = -0.333477914
angle = 131.815872
```

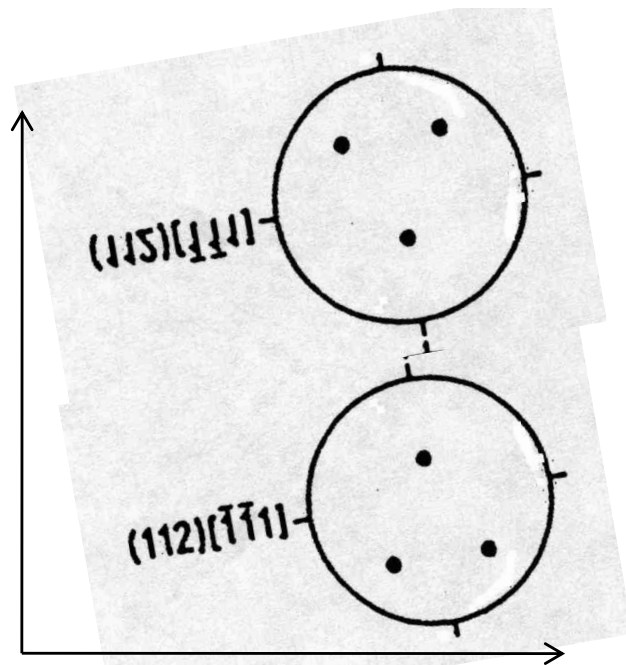
Note: same angle, different axis, now in sample frame

## *Active rotations*

- What is stranger, at first sight, is that, as you rotate the two orientations together in the sample frame, the misorientation axis moves with them, if expressed in the reference frame (active rotations).
- On the other hand, if one uses passive rotations, so that the result is in crystal coordinates, then the misorientation axis remains *unchanged*, as you rotate the pair of cr.



65



# Active rotations example

Add 10° to the first Euler angle so that  
both crystals move together:

angles.. 100. 35.2599983 45.  
angles.. 280. 35.2599983 45.

1st matrix:

```
[ -0.691  0.596  0.408 ]
[ -0.446 -0.797  0.408 ]
[  0.569  0.100  0.817 ]
```

2nd matrix:

```
[  0.691 -0.596  0.408 ]
[  0.446  0.797  0.408 ]
[ -0.569 -0.100  0.817 ]
```

MISORInv: angle= 60. axis= 6 1 0

Note the change in the misorientation axis  
from 100 to 610!

```
Symmetry operator number 1
Product matrix for gB X gA^-1:
[ -1.000  0.000  0.000 ]
[  0.000 -1.000  0.000 ]
[  0.000  0.000  1.000 ]
```

Trace = -1.

angle = 180.

```
Symmetry operator number 2
Product matrix for gB X gA^-1:
[ -0.478  0.004  0.878 ]
[  0.820 -0.355  0.448 ]
[  0.314  0.935  0.167 ]
```

Trace = -0.666738808

angle = 146.446426

```
Symmetry operator number 3
Product matrix for gB X gA^-1:
[  0.044  0.824  0.564 ]
[  0.824  0.289 -0.487 ]
[ -0.564  0.487 -0.667 ]
```

Trace = -0.333477765

angle = 131.815857

.....