Carnegie Mellon

Orientation Distribution: Definition, Discrete Forms, Examples

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27-750

Texture, Microstructure & Anisotropy

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MSE

Lecture Objectives

- Introduce the concept of the Orientation Distribution (*OD*) as the quantitative description of "preferred crystallographic orientation" a.k.a. "texture".

- Explain the motivation for using the OD as something that enables calculation of *anisotropic properties*, such as elastic compliance, yield strength, permeability, conductivity, etc.

- Illustrate discrete *OD*s and contrast them with mathematical functions that represent the OD, a.k.a. "*Orientation Distribution Function (ODF)*".

- Explain the connection between the location of components in the OD, their Euler angles and pole figure representation.

- Present an example of an *OD* for a rolled fcc metal.

- Offer preliminary (qualitative) explanation of the effect of symmetry on the *OD*.

Concept Params. Euler Normalize Vol.Frac. Cartesian Polar Components

In Class Questions: 1

1. Why does an orientation distribution (OD) require three parameters?

2. What are the similarities and differences between an OD and a probability density function?

3. What is the practical value of an OD (as compared to pole figures, e.g.)?

4. Does an OD have to be parameterized with Euler angles?

5. Against which Euler angles are ODs typically sectioned?

In Class Questions: 2

1. What distribution of intensity do we expect to see for a rolled fcc metal?

2. What is meant by the "beta fiber"?

3. Where are standard texture components of rolled fcc metals located in the space?

4. What are some differences between discrete forms of ODs and series expansion forms?

5. What is the size of the volume element in orientation space?

In Class Questions: 3

1. Explain how projecting on the first Euler angle yields an inverse pole figure (for the sample Z direction) and projecting on the 3rd Euler angle yields a pole figure (for the crystal Z direction).

2. What are generalized spherical harmonic (functions)?

3. How do pole figures relate to the OD?

4. How do *volume fractions* (of texture components) relate to intensity values in the OD?

Orientation Distribution (OD)

- The Orientation Distribution (OD) is a central concept in texture analysis and anisotropy.
- *Normalized probability* distribution*, is typically denoted by "*f*" in whatever space is used to parameterize orientation, g, i.e. as a function, $f(g)$, of three variables. Typically 3 (Bunge) Euler angles are used, hence we write the OD as $f(\phi_1, \Phi, \phi_2)$. The OD is closely related to the frequency of occurrence of any given texture component, which means that $f \geq 0$ (very important!).
- Probability density (normalized to have units of *multiples of a random density*, or *MRD*) of finding a given orientation (specified by all 3 parameters) is given by the value of the OD function, *f*. *Multiples of a uniform density*, or *MUD*, is another exactly equivalent unit.
- *OD*s can be defined mathematically in any space appropriate to a continuous description of rotations (Euler angles, axis-angle, Rodrigues vectors, unit quaternions). The Euler angle space is generally used because the series expansion representation depends on the generalized spherical harmonics.
- Remember that the space used to describe the *OD* is always periodic, although this is not always obvious (e.g. in Rodrigues vector space).
- In terms of data, think of taking measurements of orientation at individual points in an EBSD map (in the form of Euler angles) and binning them in a gridded orientation space, then normalizing the values in MRD units, then making contour plots.

*A typical OD(f) has a different normalization than a standard probability distribution; see later slides

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Meaning of an OD

- Each **point** in the orientation distribution represents a **single specific orientation** or **texture component**.

- Most properties depend on the complete orientation (all 3 Euler angles matter), therefore must have the OD to predict properties. Pole figures, for example, are not enough.

- Can use the OD information to determine presence/absence of components, volume fractions, predict anisotropic properties of polycrystals.

- Note that we *also* need the microstructure in order to predict anisotropic properties.

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Orientation Distribution Function (ODF)

- A mathematical function is always available to describe the (continuous) orientation density; this is known as an "orientation distribution function" (*ODF*). Properly speaking, any texture can be described by an OD but "ODF" should only be used if a functional form has been fitted to the data.

- From probability theory, however, remember that, strictly speaking, the term "*distribution function*" is reserved for the cumulative frequency curve (only used for volume fractions in this context) whereas the *ODF* that we shall use is actually a *probability density* but normalized in a different way so that a randomly (uniformly) oriented material exhibits a level (intensity) of unity. Such a normalization is different than that for a true probability density (i.e. such that the area under the curve is equal to one - to be discussed later).

- Historically, *ODF* was associated with the series expansion method for fitting coefficients of generalized spherical harmonics [functions] to pole figure data*. The set of harmonics+coefficients constitute a mathematical function describing the texture. Fourier transforms represent an analogous operation for 1D data.
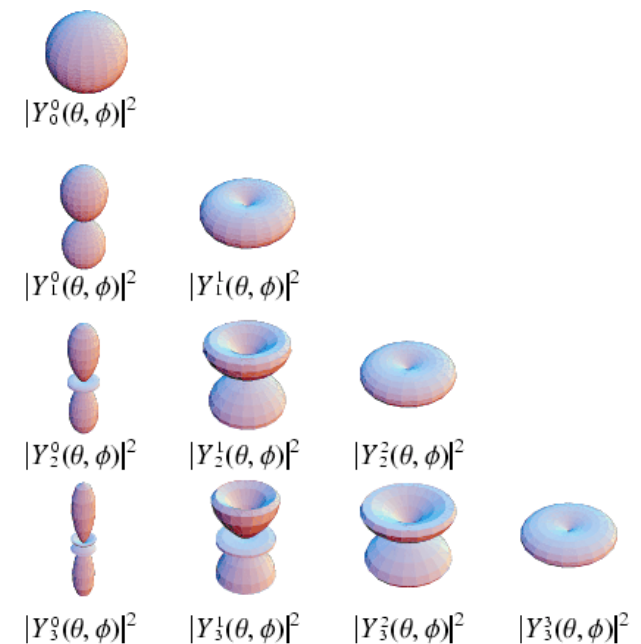
*H. J. Bunge: *Z. Metall.* **56**, (1965), p. 872.
*R. J. Roe: *J. Appl. Phys.* **36**, (1965), p. 2024.

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Orientation Space: Why Euler Angles?

- Why use Euler angles, when many other variables could be used for orientations?

- The solution of the problem of calculating ODs from pole figure data was solved by Bunge and Roe by exploiting the mathematically convenient features of the generalized spherical harmonics, which were developed with *Euler angles*. Finding the values of coefficients of the harmonic functions made it into a linear programming problem, solvable on the computers of the time.

- Generalized spherical harmonics are the same functions used to describe electron orbitals in quantum physics.

- If you are interested in a challenging mathematical problem, find a set of orthogonal functions that can be used with any of the other parameterizations (Rodrigues, quaternion etc.). See e.g. Mason, J. K. and C. A. Schuh (2008). "Hyperspherical harmonics for the representation of crystallographic texture." *Acta materialia* **56** 6141-6155.

akbar.marlboro.edu

$|Y_0^0(\theta, \phi)|^2$

$|Y_1^0(\theta, \phi)|^2$ $|Y_1^1(\theta, \phi)|^2$

$|Y_2^0(\theta, \phi)|^2$ $|Y_2^1(\theta, \phi)|^2$ $|Y_2^2(\theta, \phi)|^2$

$|Y_3^0(\theta, \phi)|^2$ $|Y_3^1(\theta, \phi)|^2$ $|Y_3^2(\theta, \phi)|^2$ $|Y_3^3(\theta, \phi)|^2$

Look for visualization as: spherical_harmonics.mpeg

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Euler Angles, Ship Analogy

- Analogy: position and the heading of a boat with respect to the globe. *Latitude* or *co-latitude* (Θ) and *longitude* (ψ) describe the position of the boat; third angle describes the *heading* (ϕ) of the boat relative to the line of longitude that connects the boat to the North Pole.

- Note the sphere always has unit radius.

[Kocks, Tomé, Wenk]

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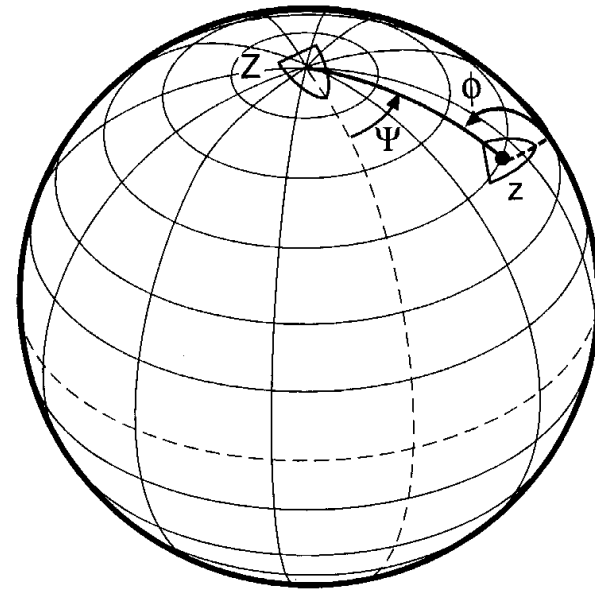
Area Element, Volume Element

- Spherical coordinates result in an area element whose magnitude depends on the declination (co-latitude):

$dA = \sin\Theta\ \mathrm{d}\Theta\ \mathrm{d}\psi$

Volume element =

$dV =$

$dA\ d\phi =$

$\sin\Theta\ \mathrm{d}\Theta\ \mathrm{d}\psi\ \mathrm{d}\phi.$

(Kocks angles)

[Kocks, Tomé, Wenk]

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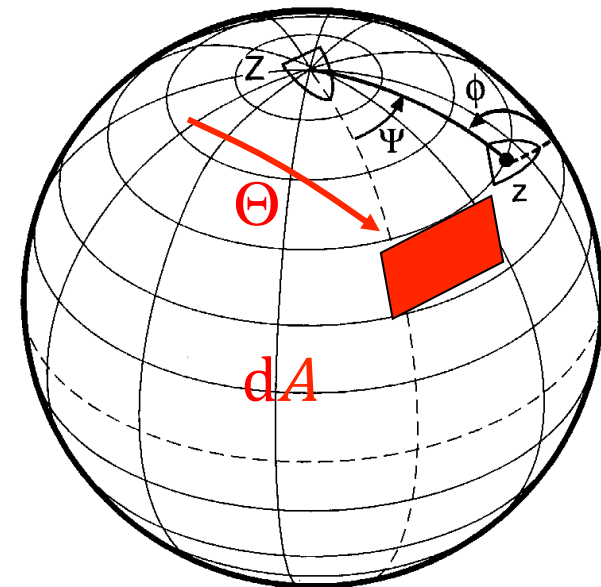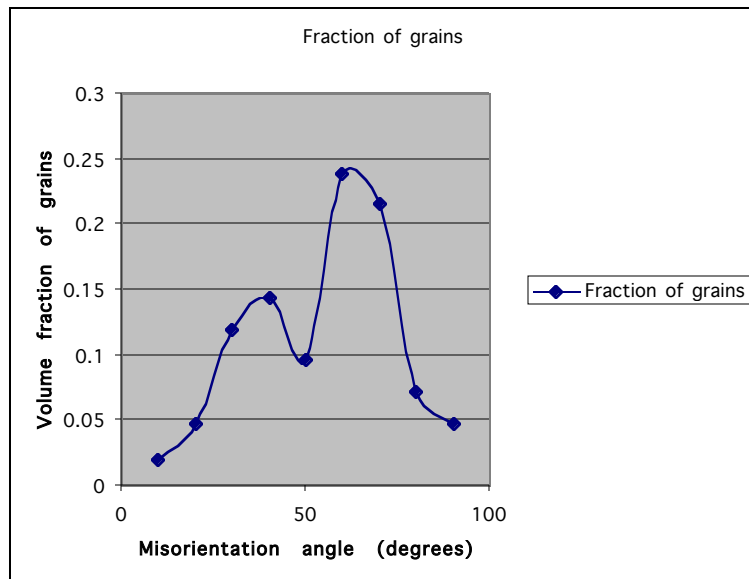
Description of Probability

- Note the difference between probability density function (pdf), *f(x)*, and the cumulative probability function (cdf), *F(x)*. The example below is that of a simple (1D) misorientation distribution in the angle.

integrate →

Fraction of grains

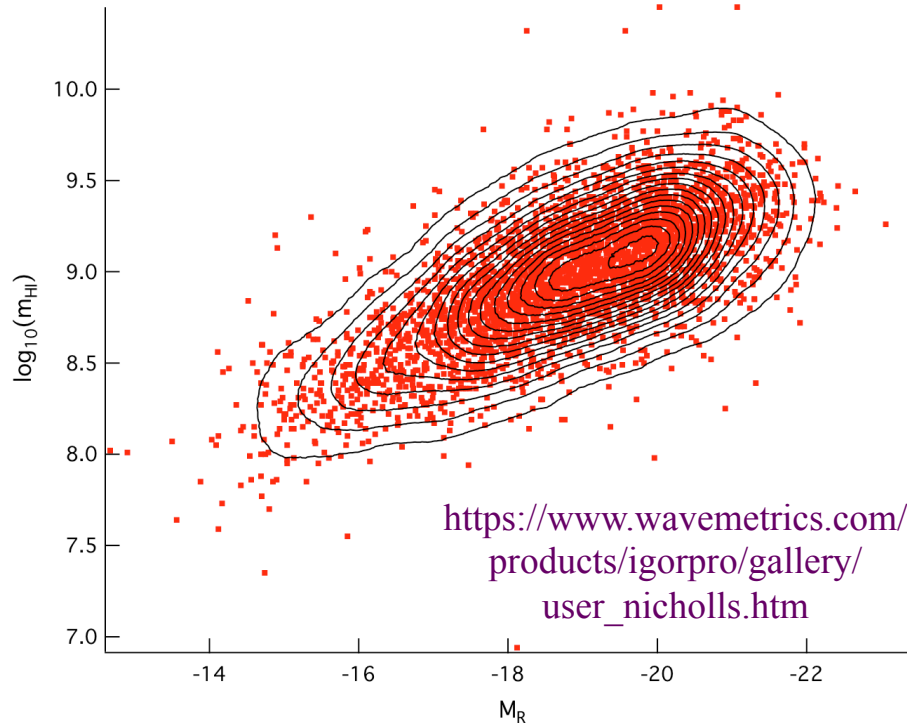Volume fraction of grains

Misorientation angle (degrees)

Fraction of grains

Distribution Function

Distribution Function

Misorientation angle

Distribution Function
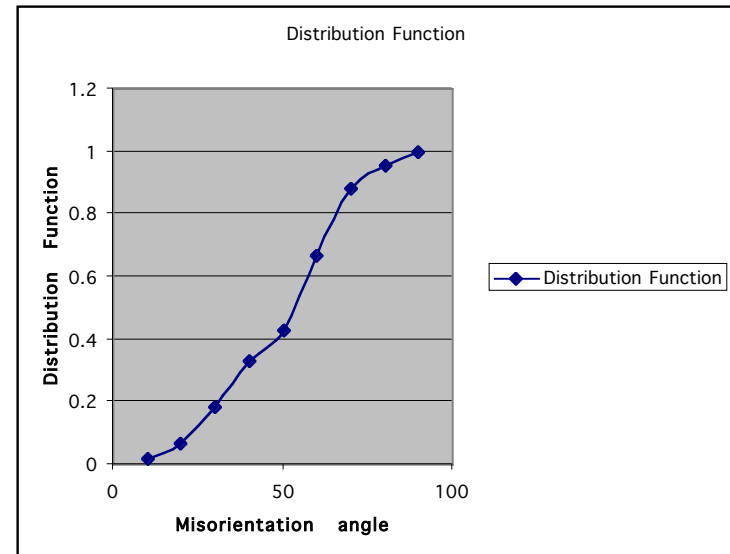
$$f(x) \geq 0, \quad \forall x$$

$$\int_0^\infty f(x)dx = 1$$

$$f(x)$$

$$f_X(x) = \frac{dF_X(x)}{dx}$$

← *differentiate*

$$F(x)$$

Binning Discrete Data Points

HOPCAT: log(HI mass) vs Absolute R-band magnitude

https://www.wavemetrics.com/
products/igorpro/gallery/
user_nicholls.htm

Below right: here, some counts were binned into hexagonal bins in a 2-D space and converted into a greyscale. Visit the page to get details.

http://www.r-bloggers.com/example-9-1-scatterplots-with-binning-for-large-datasets/

Above left: here, individual points were placed in a 2-D space. Then contours were added based on a 500^2 gridding that is not visible here. Visit the page to get details.
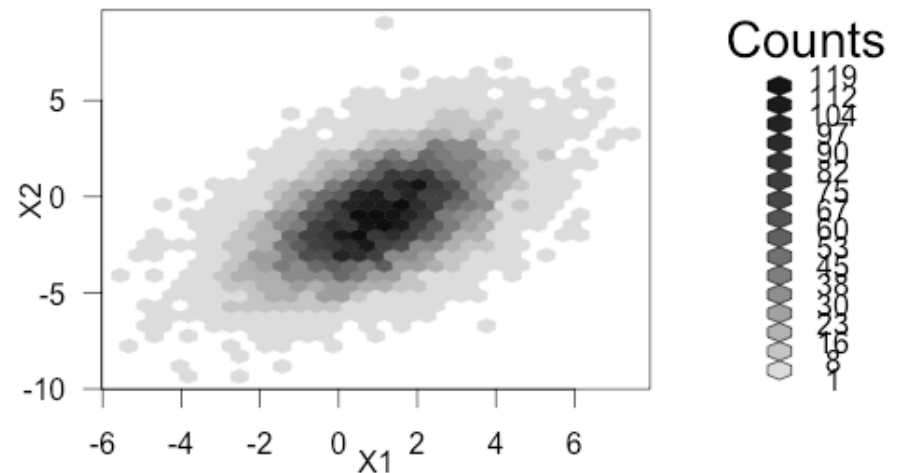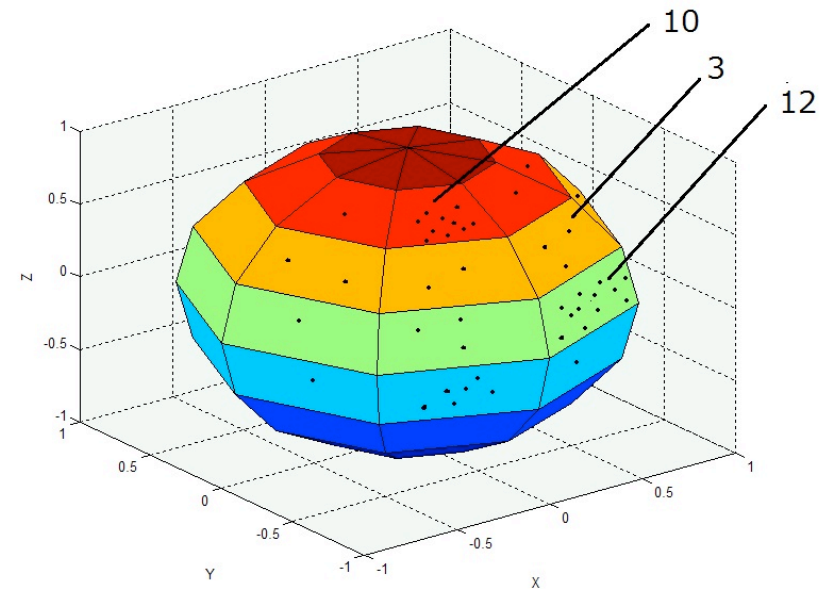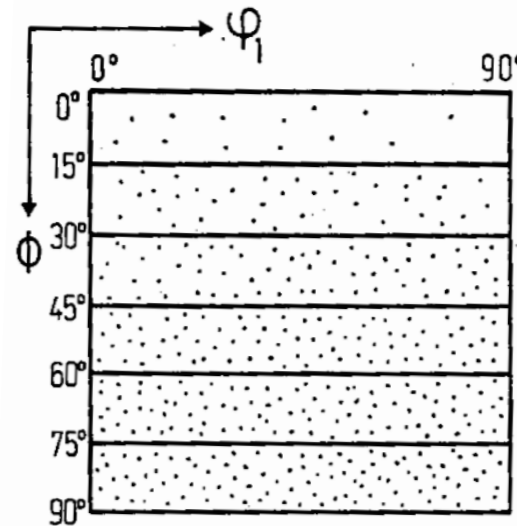
Gridding points on a Sphere
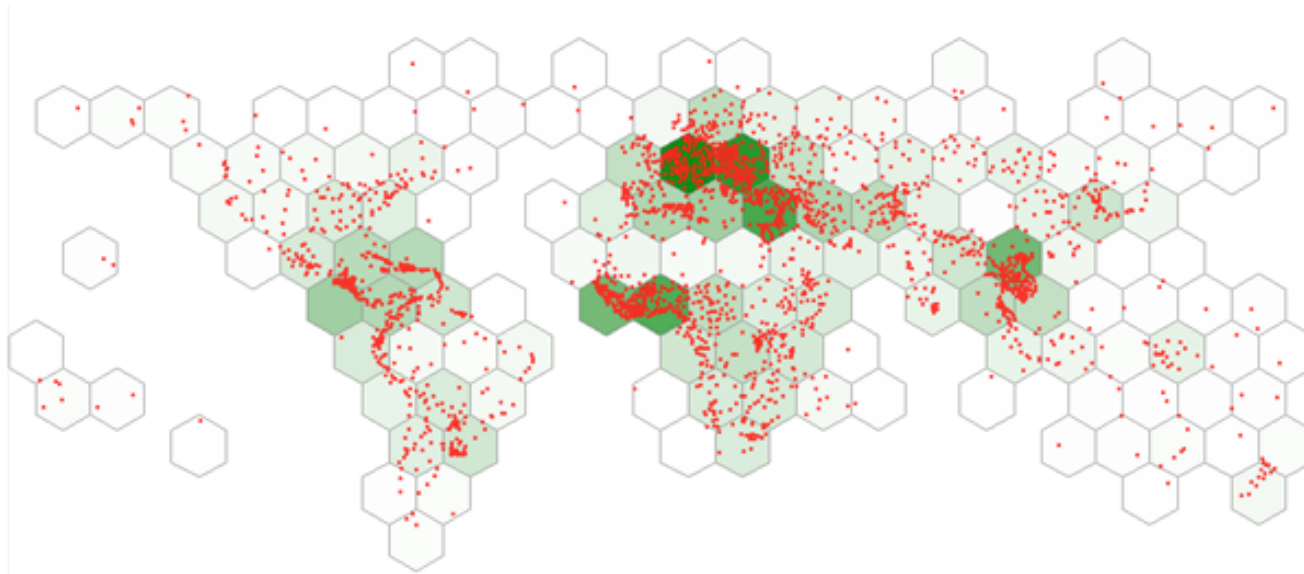
www.tatukgis.com

However, our problem with texture data is that we need to bin it on a sphere. If we use equal increments in the two angles, then the *area element* varies from small at the poles to large at the equator. Which is where the sin(Φ) comes from. **Random points give equal area density on a sphere but the number in each cell varies.**

http://stackoverflow.com/questions/26841727/
histogram-from-spherical-plots-in-matlab

10
3
12

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 $\Phi = 0°$. When converted to *intensities*, however, then the result is a uniform, constant value of the OD (because of the effect of the Cartesian grid and 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. We will investigate how to convert numbers of grains in a given region (cell) of orientation space to an intensity in a later lecture (Volume Fractions).

Normalization of OD

- If the texture is random then the OD is defined such that it has the same value of unity everywhere, i.e. 1.

- Any ODF is normalized by integrating over the space of the 3 parameters (as for pole figures).

- Sine(Φ) corrects for volume of the element (previous slide). The integral of Sin(Φ) on [0,π) is 2.

- Factor of $2\pi * 2 * 2\pi = 8\pi^2$ accounts for the volume of the space, based on using radian measure $\phi_1 = 0 - 2\pi$, $\Phi = 0 - \pi$, $\phi_2 = 0 - 2\pi$. For degrees and the equivalent ranges (360, 180, 360°), the factor is $360° * 2 * 360° = 259,200$ (°^{2}).

$$\frac{1}{8\pi^2} \iiint f(\varphi_1, \Phi, \varphi_2) \sin \Phi \, d\varphi_1 \, d\Phi \, d\varphi_2 = 1$$

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PDF versus ODF

- So, what is the difference between an ODF and a *pdf* (probability density function, as used in statistics)?

- First, remember that any orientation function is defined over a finite range of the orientation parameters (because of the periodic nature of the space).

- Note the difference in the normalization based on integrals over the whole space, where the upper limit of W signifies integration over the whole range of orientation space: integrating the PDF produces unity, regardless of the choice of parameterization, whereas the result of integrating the ODF depends on both the choice of parameters and the range used (i.e. the symmetries that are assumed) but is always equal to the volume of the space.

- Why do we use different normalization from that of a PDF? The answer is mainly one of convenience: it is much easier to compare ODFs in relation to a uniform/random material and to avoid the dependence on the choice of parameters and their range.

- Note that the periodic nature of orientation space means that definite integrals can always be performed, in contrast to many probability density functions that extend to infinity (in the independent variable).

Statistics: $f(x) \geq 0, \quad \forall\, x$

*pdf*→ $\int_0^\Omega f(g)\,dg = 1$

Texture: $f(x) \geq 0, \quad \forall\, x$

ODF→ $\int_0^\Omega f(g)\,dg = \int_0^\Omega dg$

Discrete versus Continuous Orientation Distributions

- As with any *distribution*, an OD can be described either as a continuous function (such as generalized spherical harmonics) or in a discrete form.

- Continuous form: *Pro*: for weak to moderate textures, harmonics are efficient (few numbers) and convenient for calculation of properties, automatic smoothing of experimental data; *Con*: unsuitable for strong (single crystal) textures, only available (effectively) for Euler angles.

- Discrete form: *Pro*: effective for all texture strengths, appropriate to annealed microstructures (discrete grains), available for all parameters; *Con*: less efficient for weak textures.

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Standard 5x5x5°
Discretization

- The standard discretization (in the **popLA** package, for example) is a regular 5° grid (uniformly spaced in all 3 angles) in Euler space.

- Illustrated for the texture in "demo" which is a rolled and partially recrystallized copper. *{x,y,z}* are the three Bunge Euler angles. The lower view shows individual points to make it more clear that, in a discrete OD, an intensity is defined at each point on the grid.

- 3D views with Paraview using *demo.vtk* as input (available on the 27-750 website, almost at the bottom of the page). Try thresholding the image for yourself.

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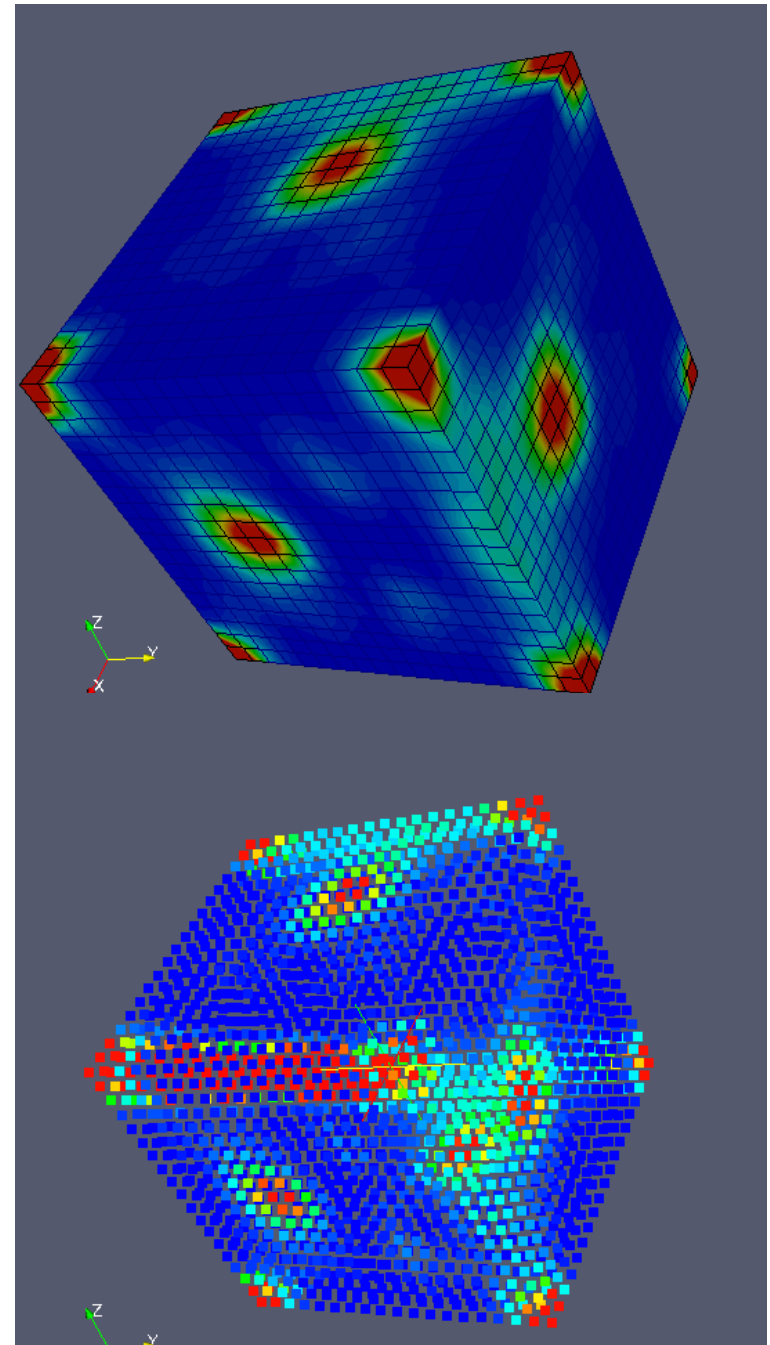
Discrete OD

- Real data is available in discrete form e.g. from *EBSD*.

- Normalization also required for discrete OD, just as it was for pole figures.

- Define a cell size (typically Δ[*angle*]= 5°) in each angle.

- Sum the intensities over all the cells in order to normalize and obtain an *intensity* (similar to a probability density, but with a different normalization in order to get units of *MRD*).

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

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$PFs \rightleftarrows OD$

(b)

- A pole figure is a *projection* of the information in the orientation distribution, i.e. many points in an ODF map onto a single point in a PF.

- Equivalently, can integrate along a line in the OD to obtain the intensity in a PF.

- The path in orientation space is, in general, a curve in Euler space. In Rodrigues space, however, it is always a straight line (which was exploited by Dawson - see N. R. Barton, D. E. Boyce, P. R. Dawson: *Textures and Microstructures* Vol. **35**, (2002), p. 113.).

$$P_{(hkl)}(\alpha, \beta) = \frac{1}{2\pi} \int f(g) \, d\Gamma$$

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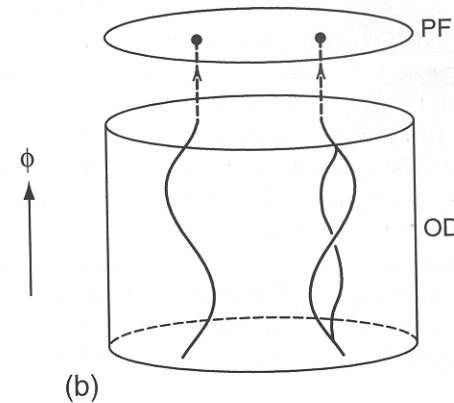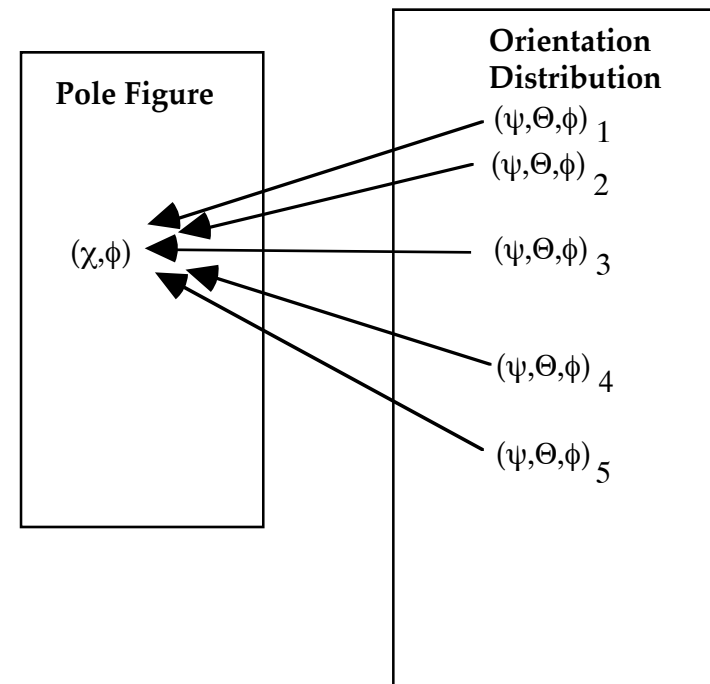
Distribution Functions and Volume Fractions

- Recall the difference between *probability density functions* and *probability distribution functions*, where the latter is the cumulative form.

- For ODs, which are like *probability densities*, integration over a range of the parameters (Euler angles, for example) gives us a *volume fraction* (equivalent to the cumulative probability function).

- Note that the typical 1-parameter Misorientation Distribution, based on just the misorientation angle, is actually a *probability density function*, perhaps because it was originally put in this form by Mackenzie (Mackenzie, J. K. (1958). "Second paper on statistics associated with the random orientation of cubes." Biometrica **45** 229-240). This is the *only* type of texture plot that is a true probability density function (as in statistics). We will discuss misorientations in later lectures.

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Grains, Orientations, and the OD

- Given a knowledge of orientations of discrete points in a body with volume *V*, OD given by:

$$\frac{dV(g)}{V} = f(g)dg$$

Given the orientations *and volumes* of the *N* (discrete) grains in a body, OD given by:

$$\frac{dN(g)}{N} = f(g)dg$$

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Volume Fractions from Intensity in the [continuous] OD

$$V_f(g) = \frac{\Delta V(g)}{V_{total}} = \frac{\int_{d\Omega} f(g)dg}{\int_{\Omega} f(g)dg}$$

where Ω denotes the entire orientation space, and $d\Omega$ denotes the region around the texture component of interest. For specific ranges of Euler angles:

$$V_f(\varphi_1, \Phi, \varphi_2) = \int_{\varphi_1 - \Delta\varphi_1}^{\varphi_1 + \Delta\varphi_1} \int_{\Phi - \Delta\Phi}^{\Phi + \Delta\Phi} \int_{\varphi_2 - \Delta\varphi_2}^{\varphi_2 + \Delta\varphi_2} f(\varphi_1, \Phi, \varphi_2)dg$$

$$V_f(\varphi_1, \Phi, \varphi_2) = \iiint f(\varphi_1, \Phi, \varphi_2)\sin\Phi \, d\varphi_1 d\Phi d\varphi_2$$

Volume fractions will be discussed in more detail in a later lecture.

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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? *Answer:* just as we differentiate a cumulative probability distribution to obtain a probability density, so we differentiate the volume fraction information:

• General relationships, where f and g have their usual meanings, V is volume and V_f is volume fraction:

$$V_f(g) = \int f(g)dg$$

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

For a PDF, one would use :

$$\frac{1}{V}\frac{dV(g)}{dg} = \frac{f(g)}{\int_\Omega dg}$$

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Intensity from V_f, contd.

- For 5°x5°x5° discretization within a 90°x90°x90° volume, we can particularize to:

$$V_f(g) = \frac{1}{8100^{°2}} \int f(g) \sin \Phi \, d\Phi \, d\varphi_1 \, d\varphi_2$$

$$f(g) = \frac{dV(g)}{dg} = \frac{\Delta V_f}{\Delta g}\bigg|_g$$

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

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Representation of the OD

- Challenging issue!
- Typical representation: Cartesian plot (orthogonal axes) of the *intensity* in Euler [angle] space.
- Standard but unfortunate choice: Euler angles, which are inherently spherical (globe analogy).
- Recall the Area/Volume element: points near the origin are distorted (too large area).
- Mathematically, as the second angle approaches zero, the 1st and 3rd angles become linearly dependent.
 At $\Phi = 0$, only $\phi_1 + \phi_2$ (or $\phi_1 - \phi_2$) is significant.

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OD Example

- Will use the example of texture in *rolled fcc* metals.

- Symmetry of the *fcc* crystal and the sample (i.e. cubic-orthorhombic) allows us to limit the space to a 90x90x90° region (see the discussion in the lecture on *symmetry*).

- Intensity is limited, approximately to lines in the space, called [partial] fibers.

- Since we dealing with intensities in a 3-parameter space, it is convenient to take *sections* through the space and make *contour maps*.

- Example has sections with constant ϕ_2.

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3D Animation in Euler Space

- Rolled commercial purity Al

Animation made with DX - see www.opendx.org

ϕ_2

Φ

ϕ_1
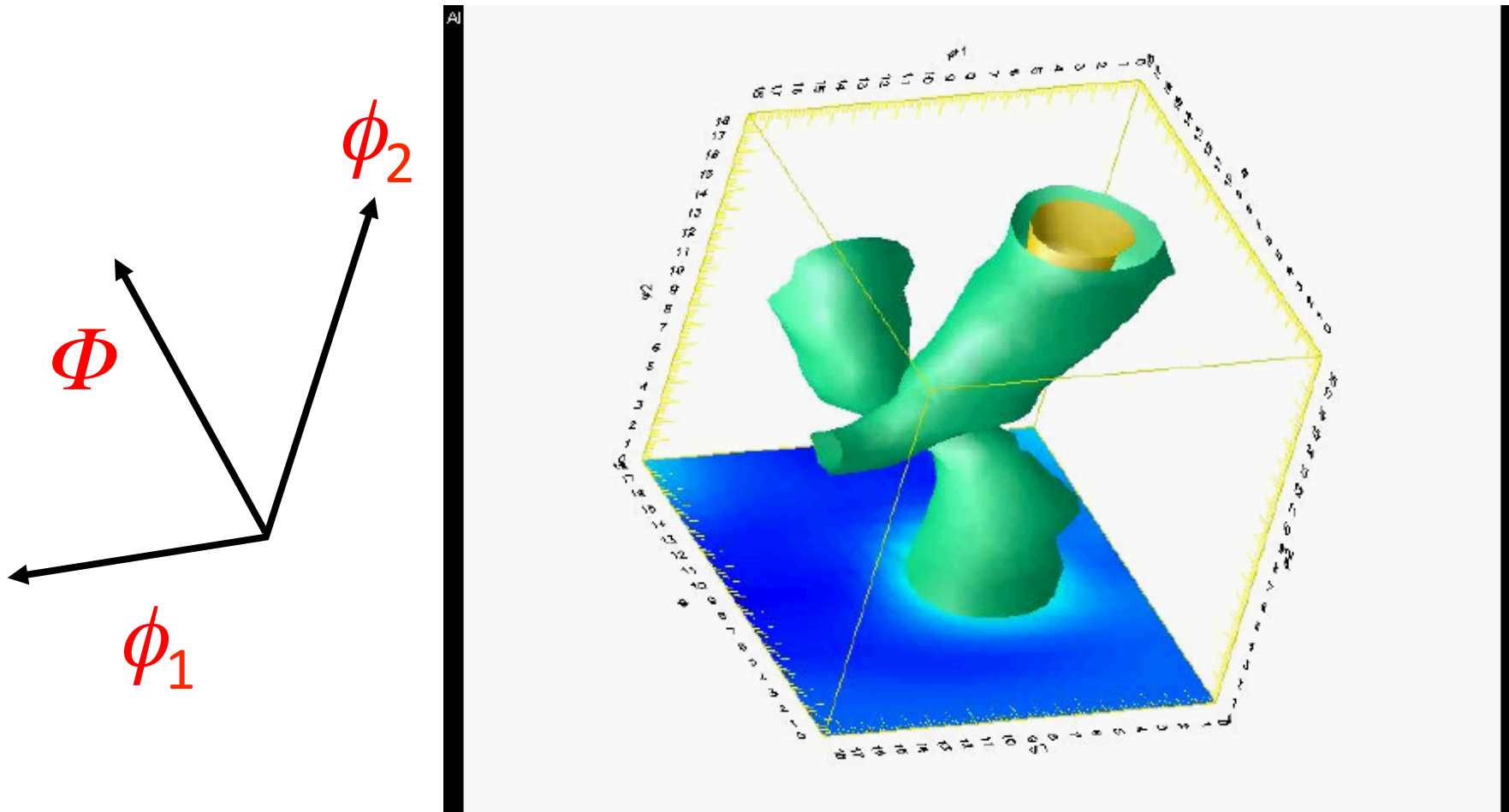
Animation shows a slice progressing up in ϕ_2; each slice is drawn at a 5° interval (slice number 18 = 90°)

Cartesian Euler Space

Line diagram shows a schematic of the beta-fiber typically found in an fcc rolling texture with major components labeled (see legend below). The fibers labeled "alpha" and "gamma" correspond to lines of high intensity typically found in rolled bcc metals.
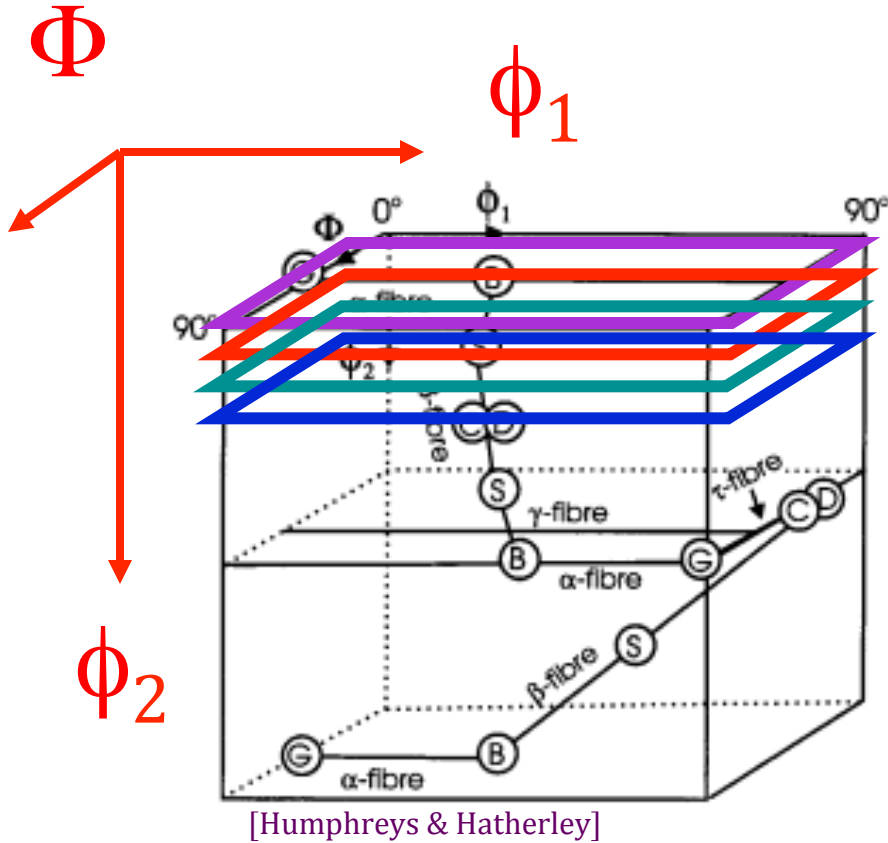

G: Goss
B: Brass
C: Copper
D: Dillamore
S: "S" component

[Humphreys & Hatherley]
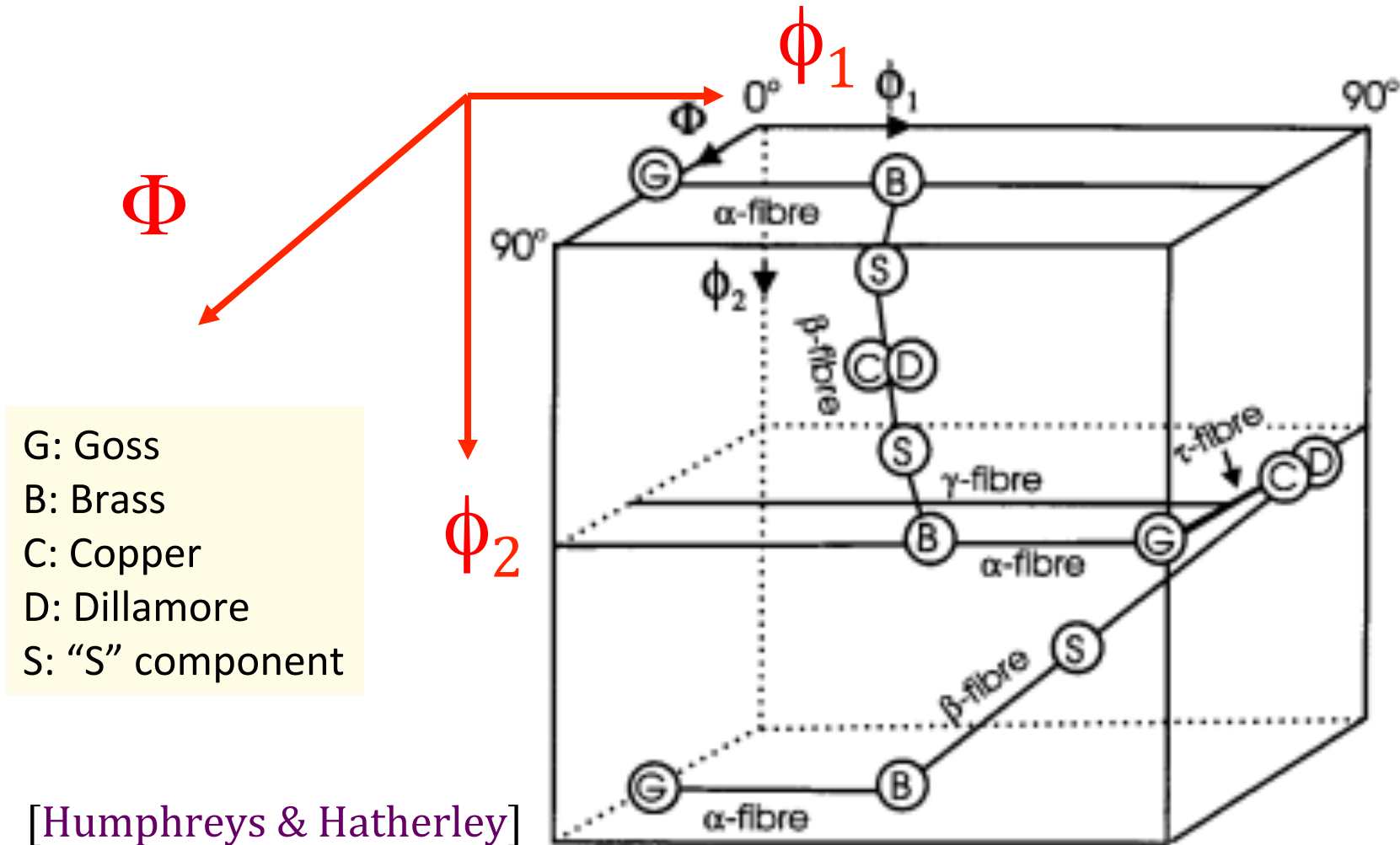
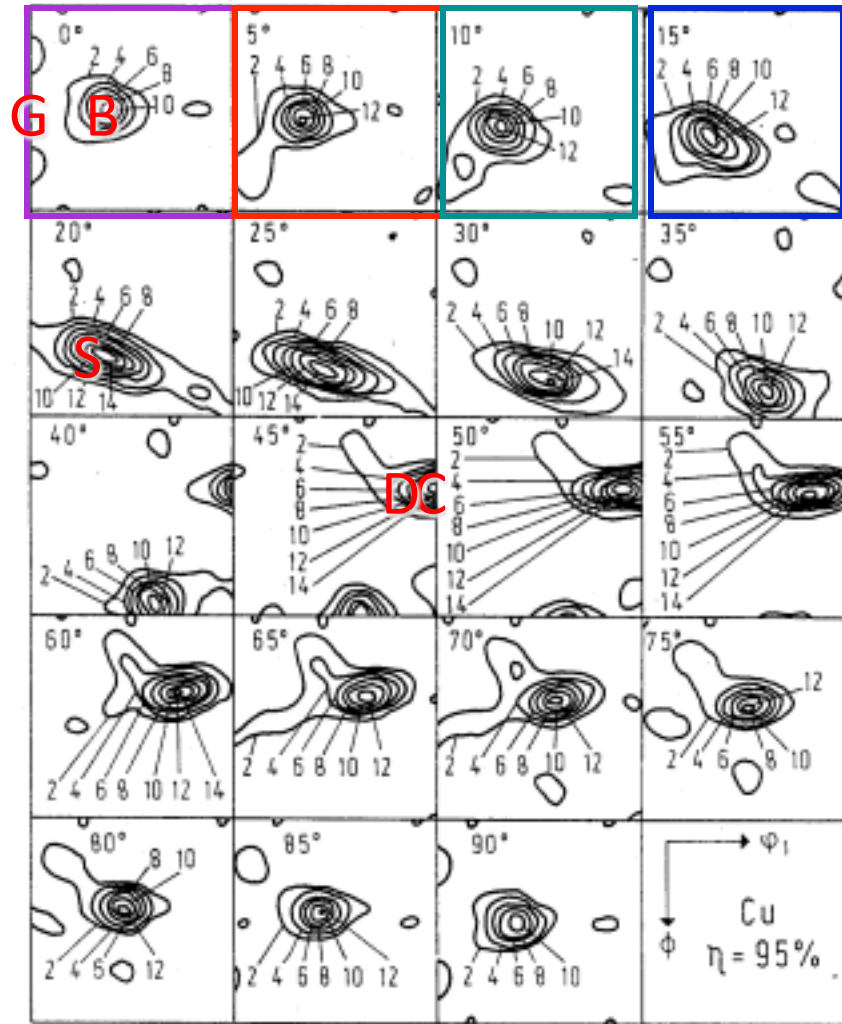Concept Params. Euler Normalize Vol.Frac. Cartesian Polar Components

OD Sections

Example of copper rolled to 90 % reduction in thickness ($\varepsilon \sim 2.5$)

$\phi_2 = 0°$ $\phi_2 = 5°$ $\phi_2 = 10°$ $\phi_2 = 15°$

[Bunge]

Φ

ϕ_1

ϕ_2

[Humphreys & Hatherley]

Sections are drawn as contour maps, one per value of ϕ_2 (0, 5, 10 ... 90°).

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Example of OD in Bunge Euler Space

ϕ_1

Section at 15°

[Bunge]

- OD is represented by a series of *sections*, i.e. one (square) box per section.
- Each section shows the variation of the OD intensity for a fixed value of the third angle.
- Contour plots interpolate between discrete points.
- High intensities mean that the corresponding orientation is common (occurs frequently).
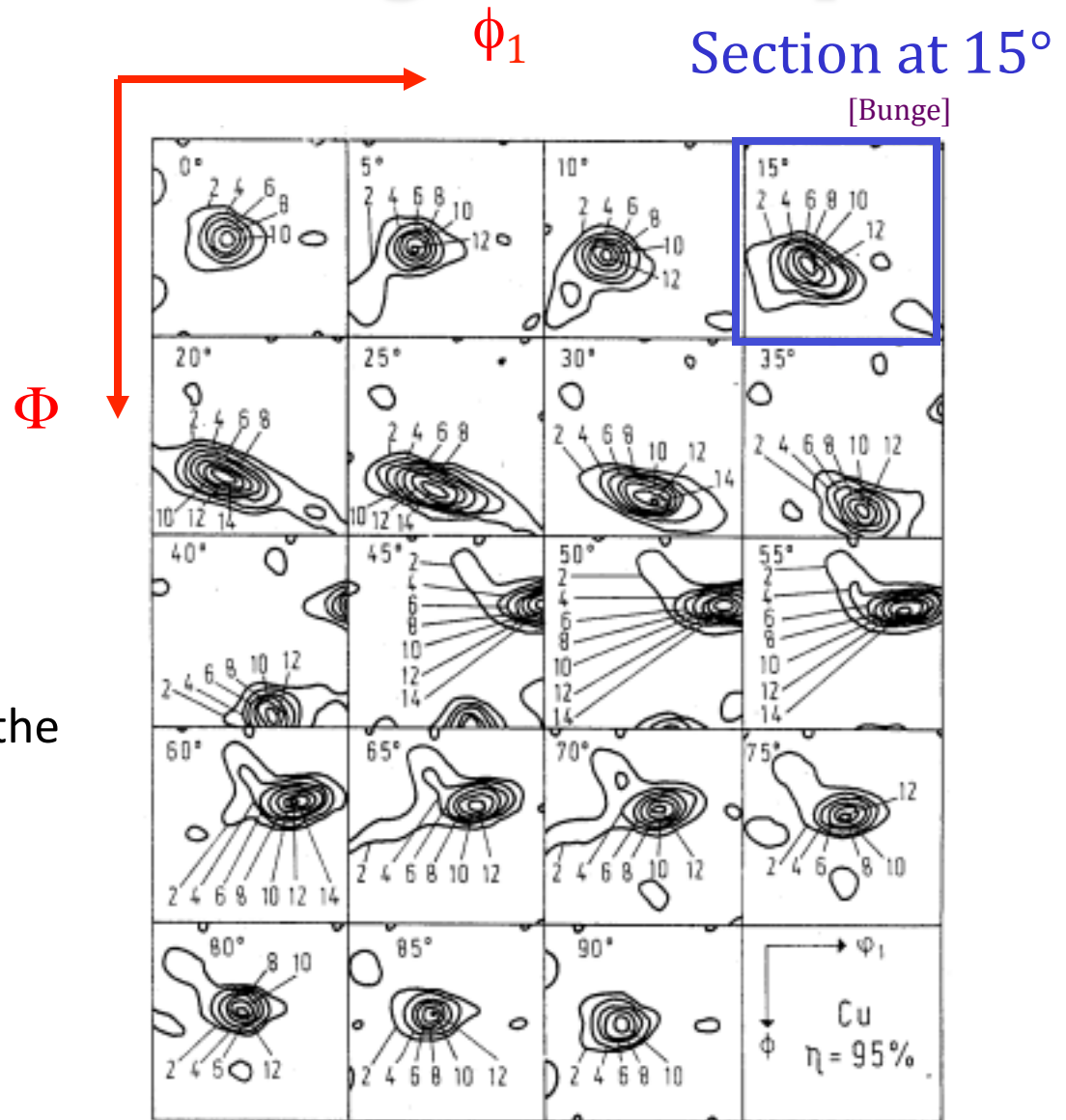
Φ

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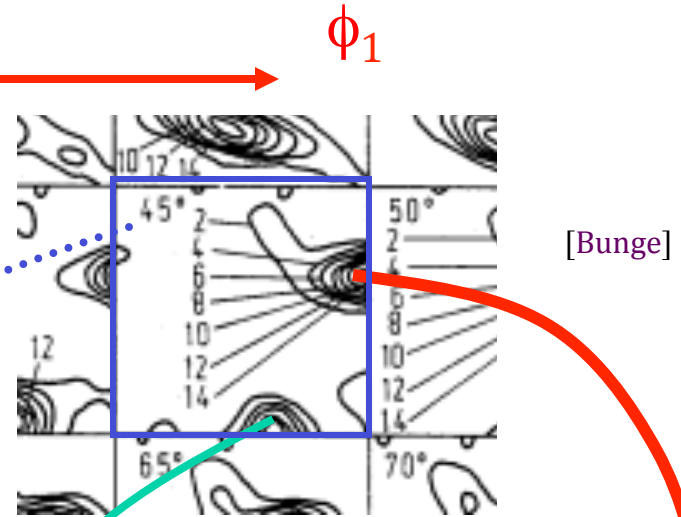# *Example of OD in Bunge Euler Space, contd.*

[Bunge]

This OD shows the texture of a cold rolled copper sheet. Most of the intensity is concentrated along a *fiber*. Think of "connect the dots!"

The technical name for this is the *beta fiber*.
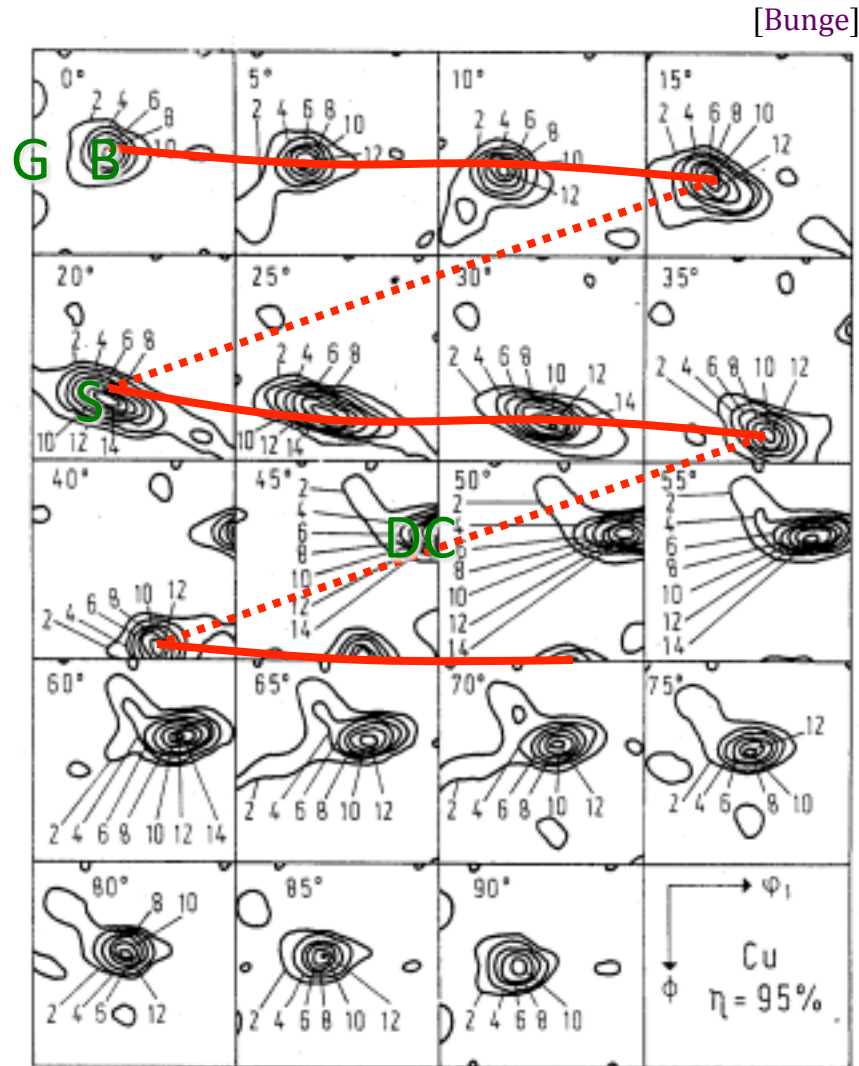
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Numerical

⇄

Graphical

ϕ_1

Φ

[Bunge]

$\phi_2 = 45°$

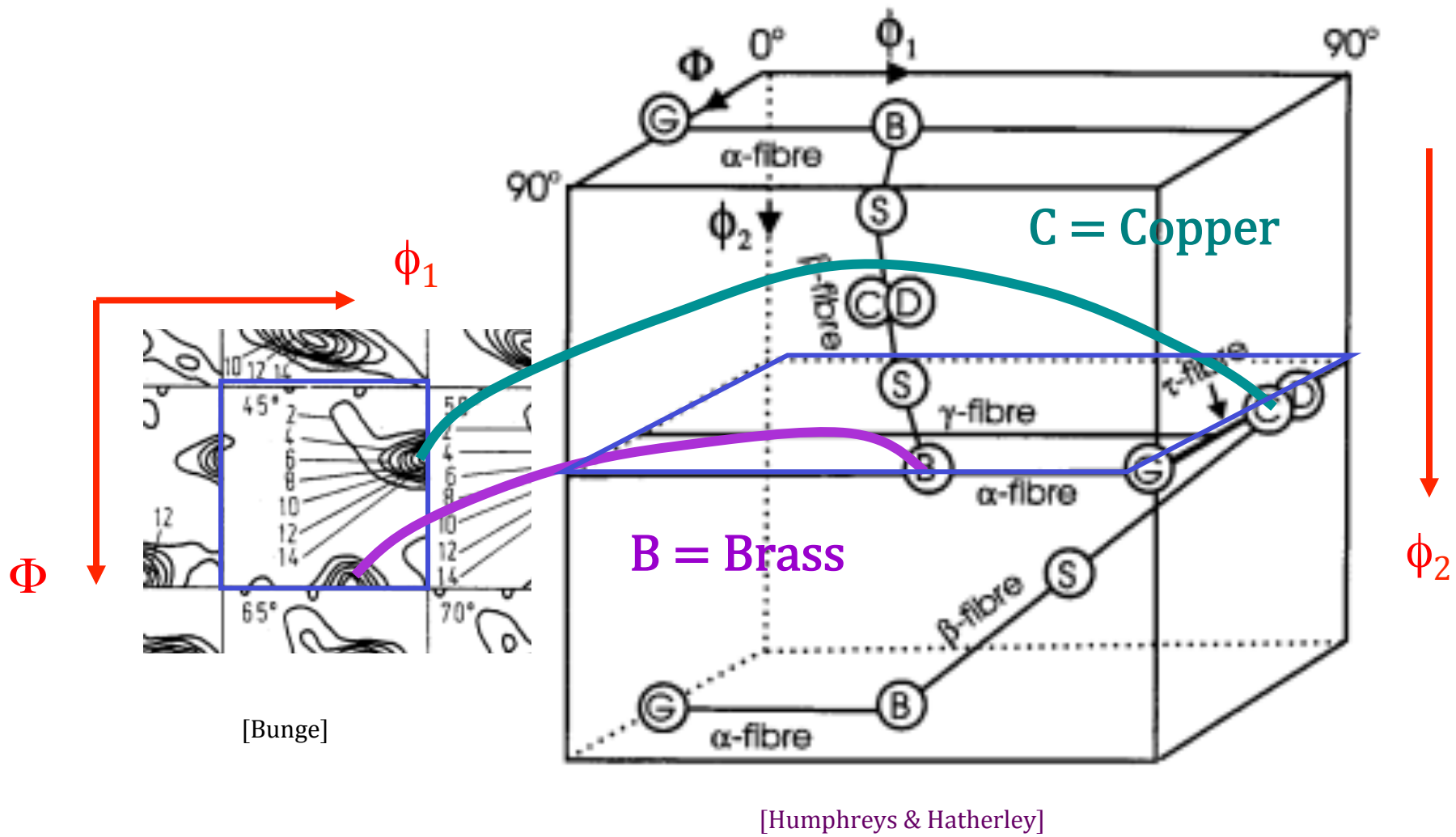Example of a
single section

```
CUR80-2 6/13/88              COMPUTED BY WIMV  6-MAR-89
 CODK   5.0  90.0   5.0  90.0 1 1 1 2 3   100        phi= 45.0
        3    3    3    3    4    9   14   43   82   99   82   43   14    9    4    3    3    3    3
        2    3    3    4    7   11   15   32   56   58   51   47   29   13    6    5    4    3    4
        3    3    3    3    4    5   10   33   43   63   82   73   50   32   18   13    9    9   12
        3    4    7    7    9    6   18   15   51   99  143  161  128  102   77   59   52   42   42
        4    4    5    6    3    9    6   14   23   39   72  117  159  167  149  158  166  177  191
        2    1    2    3    4    4    7    7   10   20   51  108  156  191  258  387  567  760 835
        1    1    2    2    2    3    3    3    8   22   48  104  184  299  551 9991526 1762
        1    1    1    1    2    1    1    2    4    6   15   26   49   87  148  248  505  837  930
        1    1    2    1    1    1    2    1    2    4    7   13   23   34   42   56   80   89   82
        1    1    1    2    2    2    3    3    3    4    9   12   15   19   28   29   33   38   36
        1    2    2    1    1    1    1    1    1    2    2    2    2    2    2    3    3    3    4
        2    2    2    2    1    1    1    1    1    2    2    2    2    2    2    2    1    1    1
        5    4    4    4    4    3    3    3    3    2    2    2    1    1    2    1    1    1    1
        9   11    9   10   13   15    9    9    9    6    6    6    6    4    4    4    3    3    3
        9   12   13   13   18   18   14   16   15   15   16   11    8    7    7    5    4    3    2
       25   28   33   31   33   35   34   37   43   52   63   74   55   22   10   14   10    7    7
       14   13   15   16   17   18   20   24   36   57   88  113  102   66   36   28   23   21   18
        5    7    9    9   14   24   31   46   94  200  342  418  377  285  205  158  148  138  138
       13   13   13   14   20   31   50   99  201  505 980132013789155  835  646  480  382  346
```
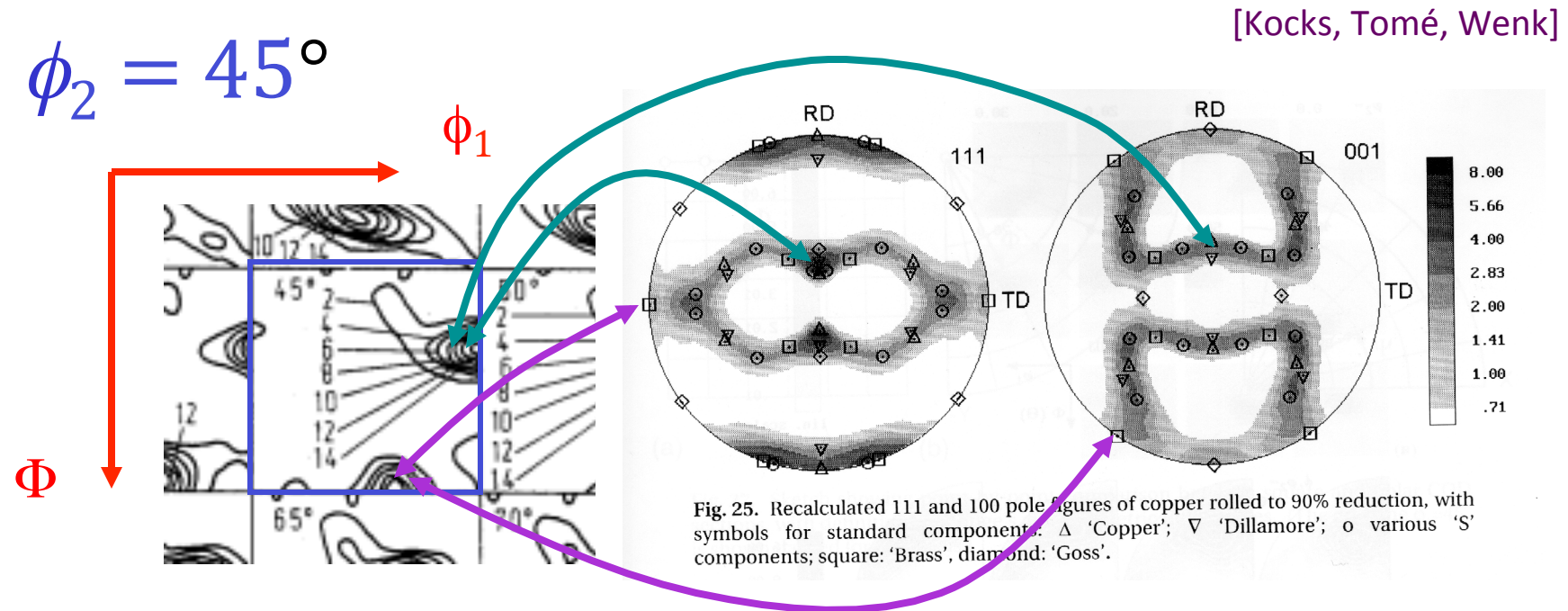
Concept Params. Euler Normalize Vol.Frac. Cartesian Polar Components

(Partial) Fibers in fcc Rolling Textures

ϕ_1

Φ

[Bunge]

C = Copper

B = Brass

ϕ_2

[Humphreys & Hatherley]

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OD ⇄ Pole Figure

$$\phi_2 = 45°$$

ϕ_1

Φ

Fig. 25. Recalculated 111 and 100 pole figures of copper rolled to 90% reduction, with symbols for standard components: Δ 'Copper'; ∇ 'Dillamore'; o various 'S' components; square: 'Brass', diamond: 'Goss'.

B = Brass   C = Copper

Note that any given component that is represented as a point in orientation space occurs in multiple locations in each pole figure.

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Euler Angles: recap

Euler Angles represent a crystal orientation with respect to sample axes
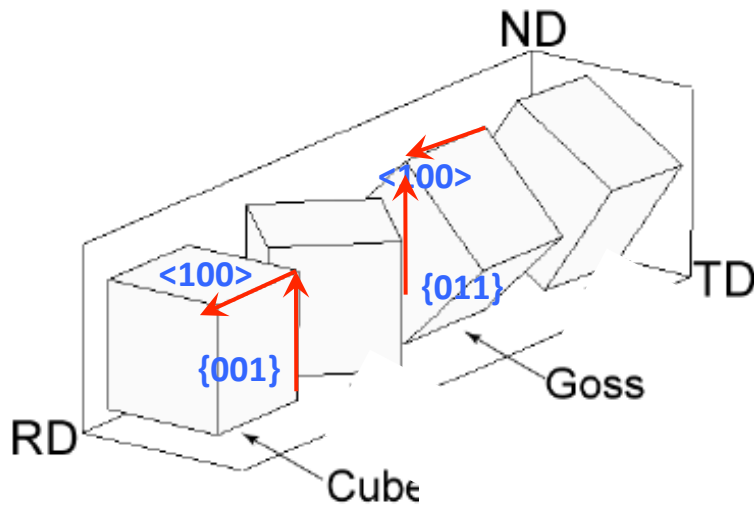
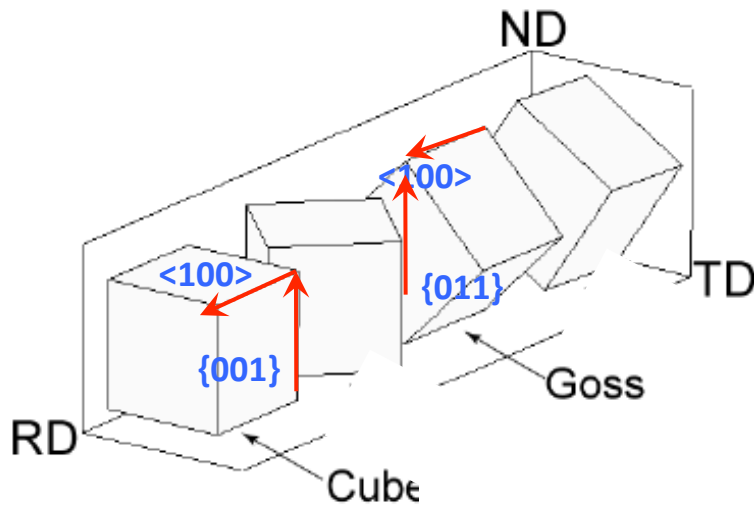| Component	RD	ND
Cube	<100>	{001}
Goss	<100>	{011}
Brass	<112>	{110}
Copper	<111>	{112}
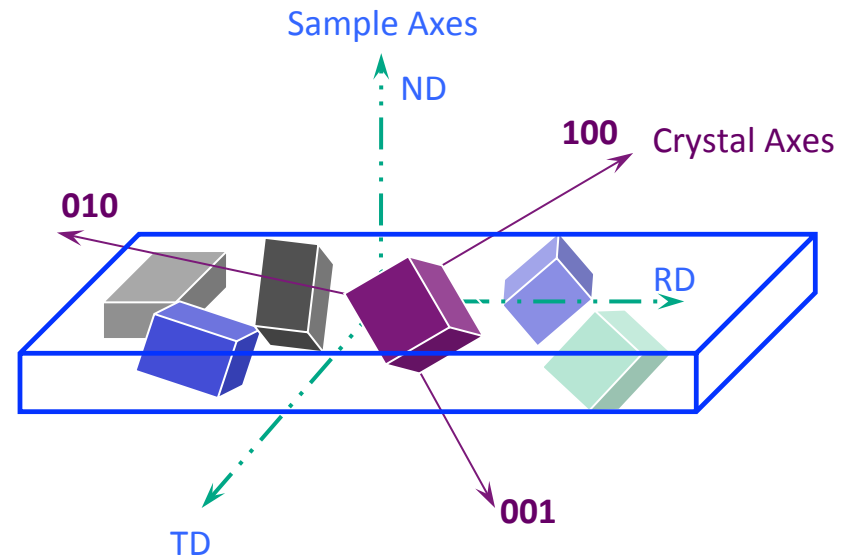
Rotation 1 (φ_1): rotate sample axes about ND

Rotation 2 (Φ): rotate sample axes about rotated RD

Rotation 3 (φ_2): rotate sample axes about rotated ND

Slide courtesy of Lin Hu [2011]

Texture Components versus Orientation Space

Component	Euler Angles (°)
Cube	(0, 0, 0)
Goss	(0, 45, 0)
Brass	(35, 45, 0)
Copper	(90, 45, 45)
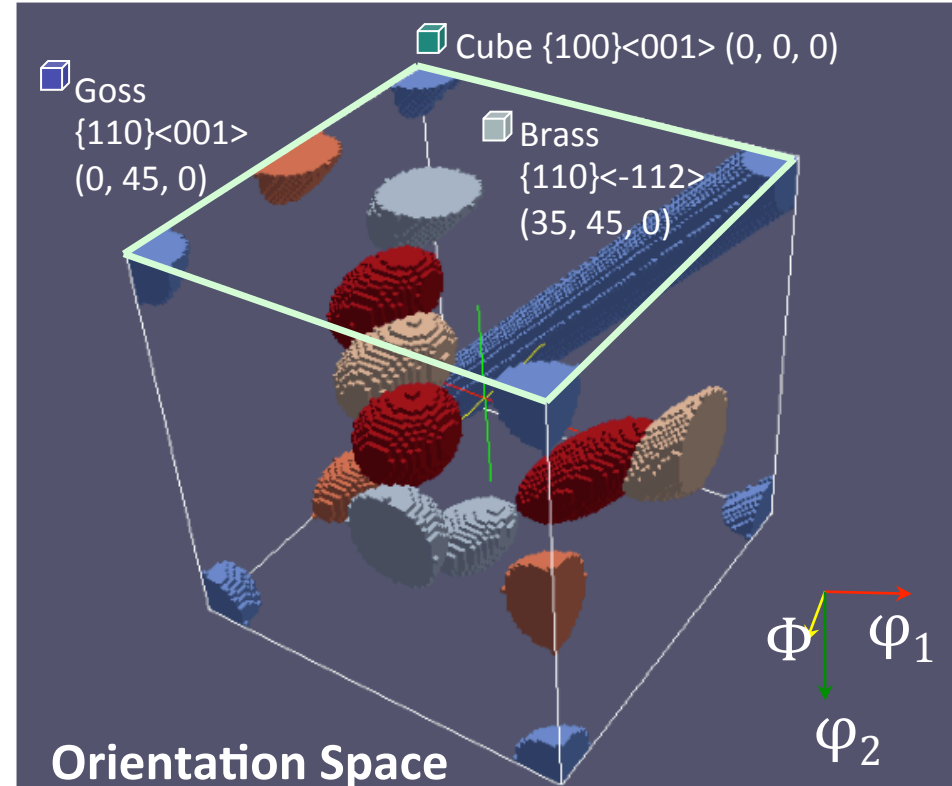
Slide courtesy of Lin Hu [2011]

ODF: 3D vs. sections

ODF
Orientation Distribution Function f (**g**)

Cube {100}<001> (0, 0, 0)

Goss
{110}<001>
(0, 45, 0)

Brass
{110}<-112>
(35, 45, 0)

Φ φ_1

φ_2

$g = \{\phi_1, \Phi, \phi_2\}$
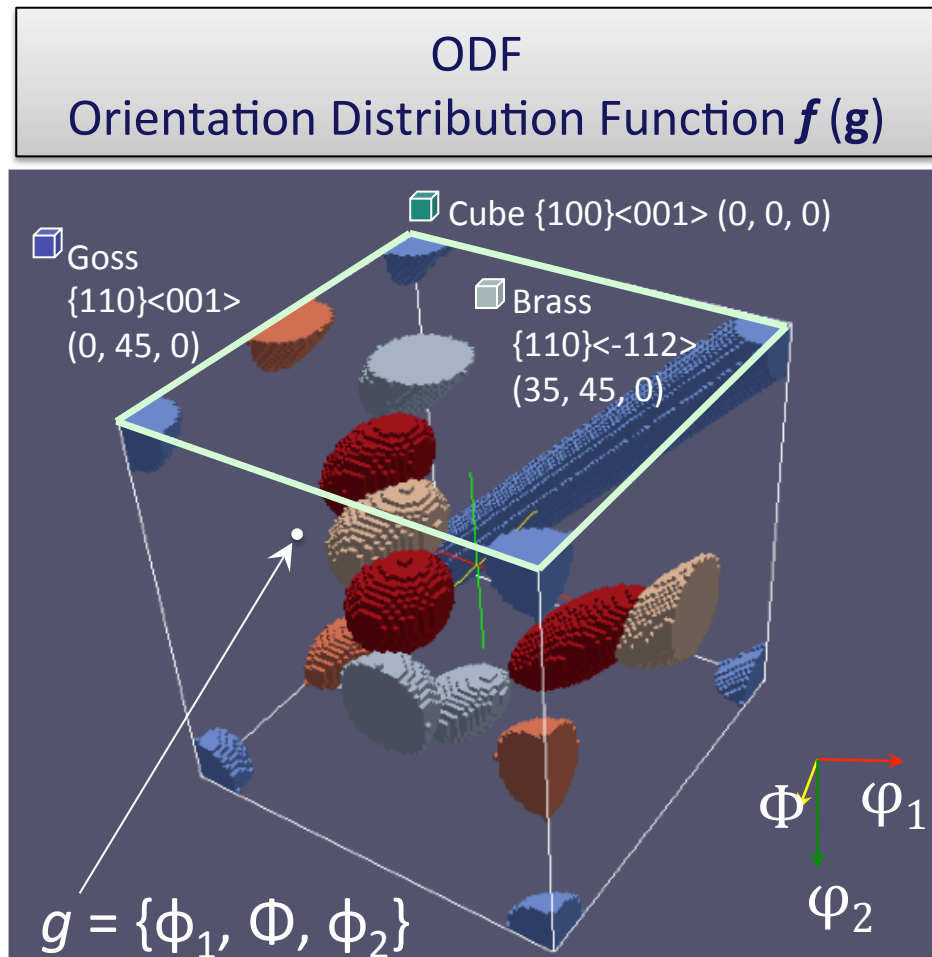
Slide courtesy of Lin Hu [2011]

ODF gives the density of grains having a particular orientation.

$\varphi_2 = 0$ $\varphi_2 = 5$ $\varphi_2 = 10$ $\varphi_2 = 15$

$\varphi_2 = 20$ $\varphi_2 = 25$ $\varphi_2 = 30$ $\varphi_2 = 35$

$\varphi_2 = 40$ $\varphi_2 = 45$ $\varphi_2 = 50$ $\varphi_2 = 55$

$\varphi_2 = 60$ $\varphi_2 = 65$ $\varphi_2 = 70$ $\varphi_2 = 75$

$\varphi_2 = 80$ $\varphi_2 = 85$ $\varphi_2 = 90$

90

φ_1

Φ

90

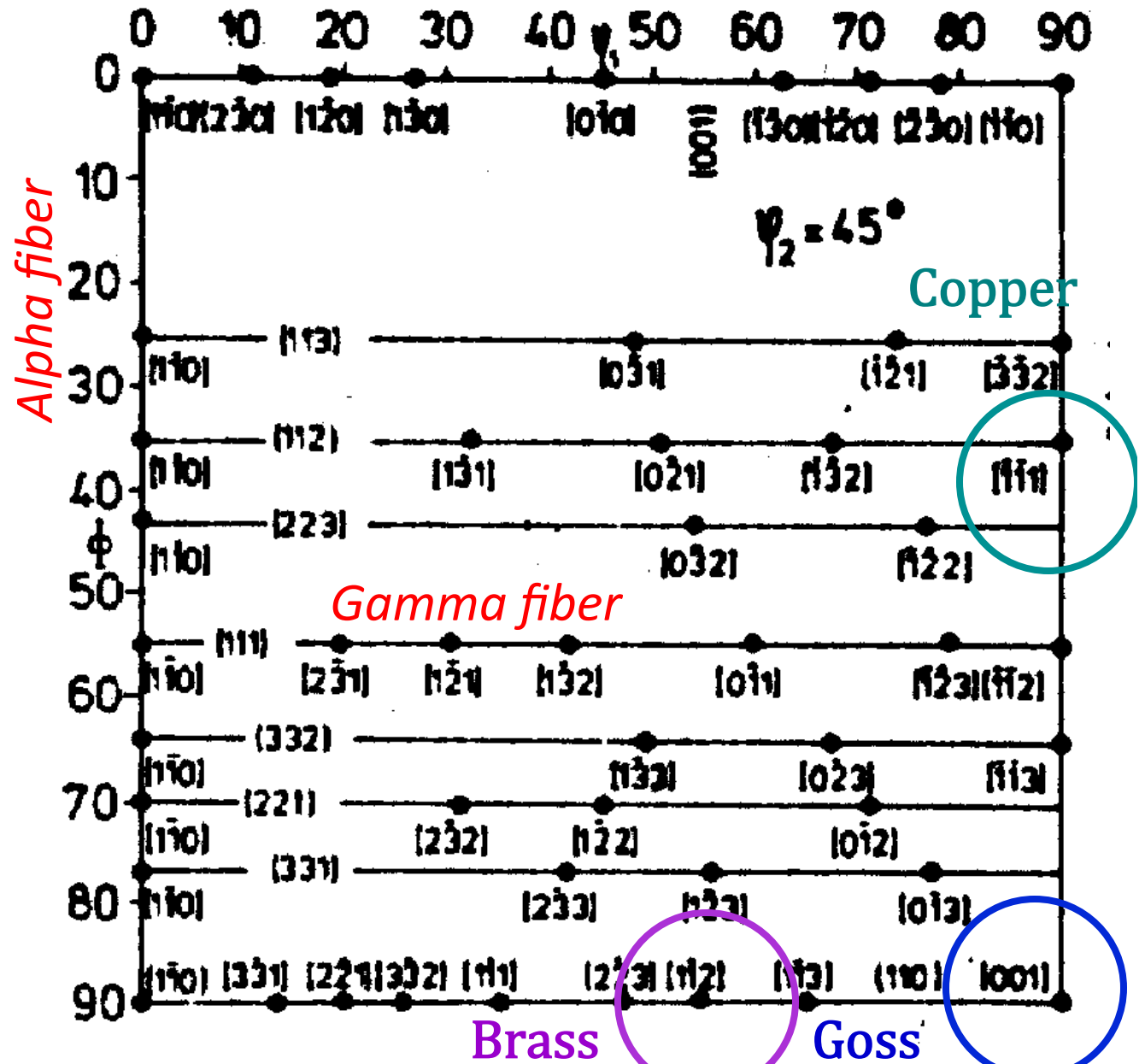*Contours at*   *0.500   1.000*   2.000   4.000   8.000   16.000
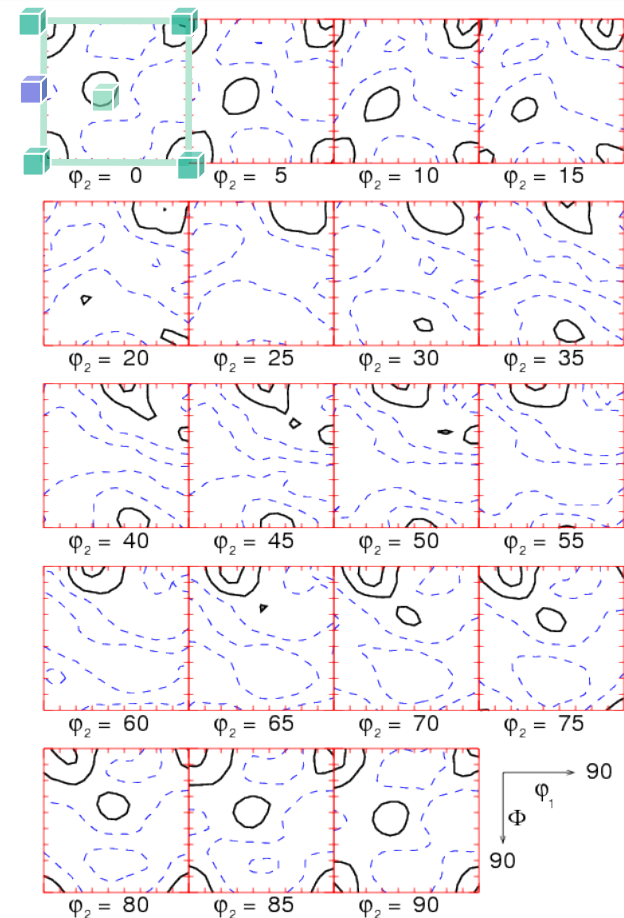
Miller Index Map in Euler Space

Bunge, p.23 *et seq*.
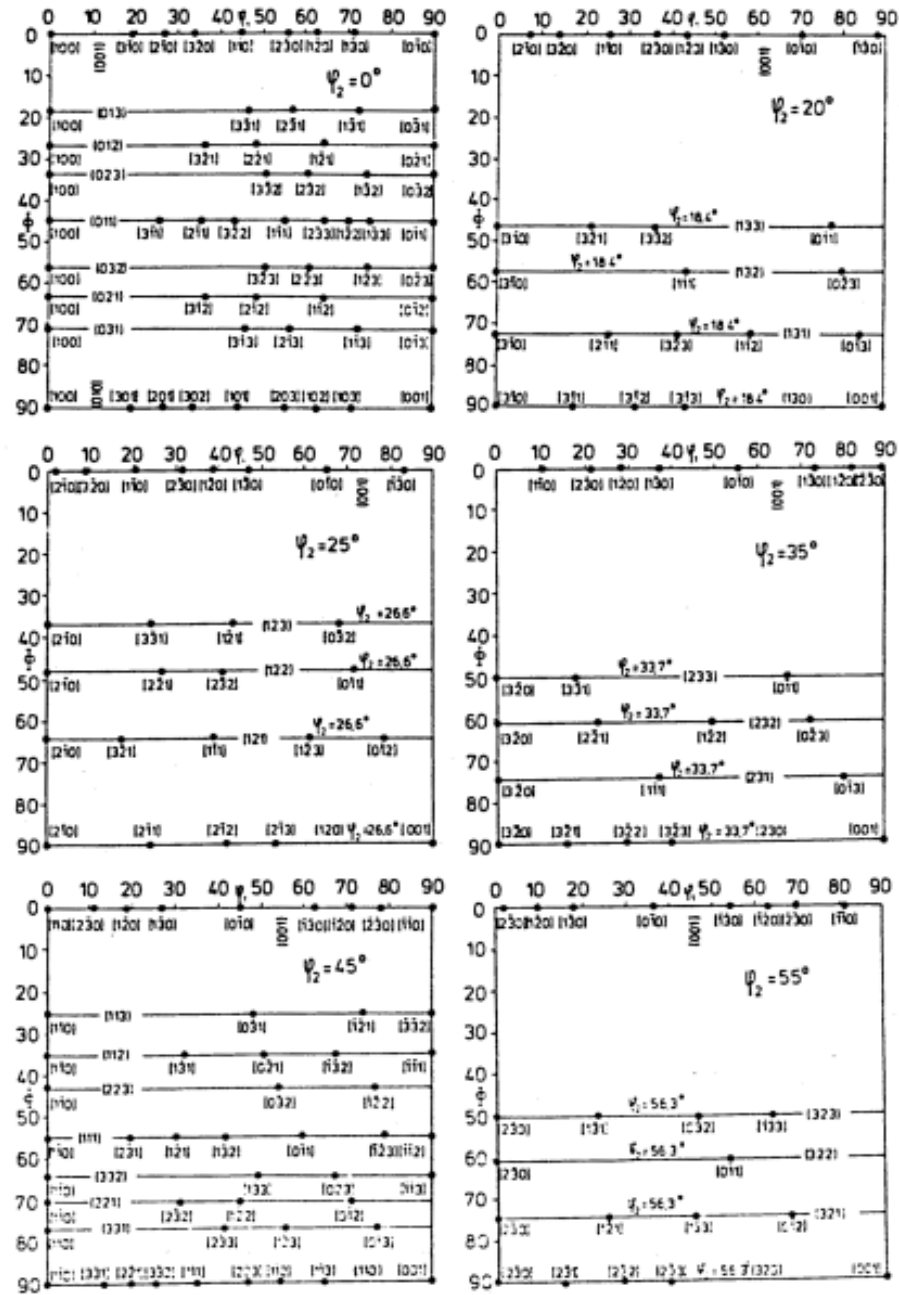
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$\phi_2 = 45°$ section, Bunge angles

3D Views

a) Brass   b) Copper   c) S
d) 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
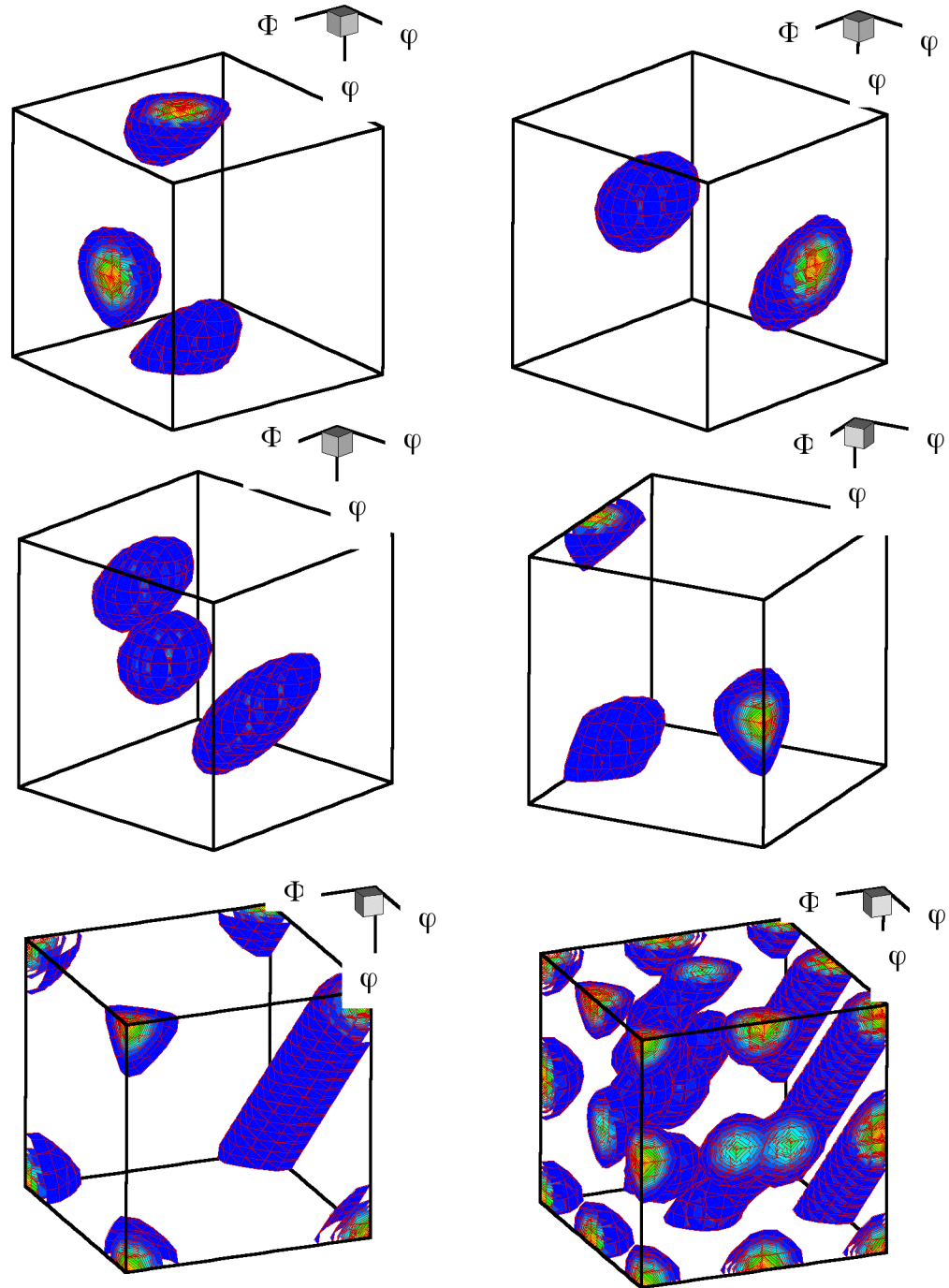8: {90, 90, 45}, Goss
9: {0, 0, 0}, cube
10: {45, 0, 0}, rotated cube

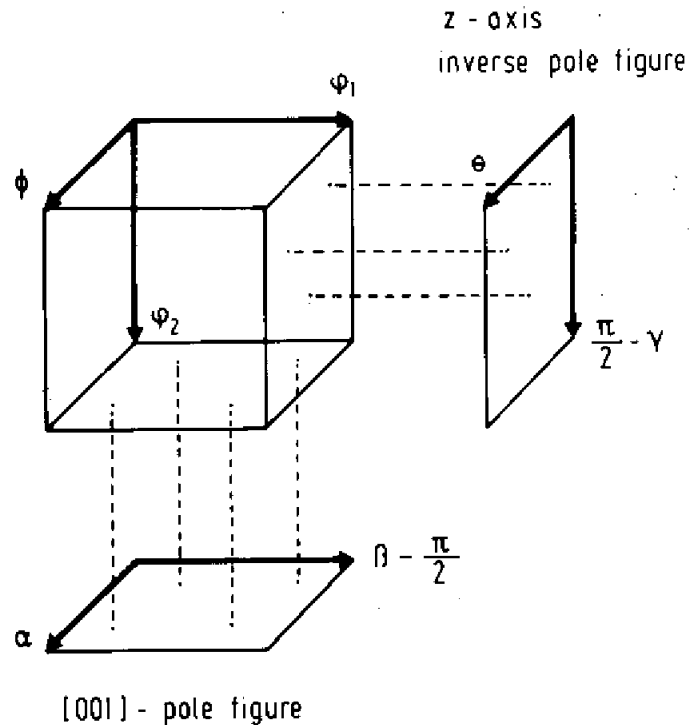Figure courtesy of Jae Hyung Cho

z - axis
inverse pole figure

SOD versus COD

- An average of the SOD made by averaging over the 1st Euler angle, ϕ_1, gives the inverse pole figure for the sample-Z (ND) direction.
- An average of the COD made by averaging over the 3rd Euler angle, ϕ_2, gives the pole figure for the crystal-Z (001) direction.

Fig. 21 The (001) pole figure and the inverse pole figure of the sample z axis (normal direction) are projections of the ODF along φ_2 and φ_1, respectively.

- One could section or slice Euler space on any of the 3 axes. By convention, only sections on the 1st or 3rd angle are used. If ϕ_1 is constant in a section, then we call it a Sample Orientation Distribution, because it displays the positions of sample directions relative to the crystal axes. Conversely, sections with ϕ_2 constant we call it a Crystal Orientation Distribution, because it displays the positions of crystal directions relative to the sample axes.

Concept Params. Euler Normalize Vol.Frac. Cartesian Polar Components

Section Conventions

Crystallite Orientation Distribution	Sample Orientation Distribution
COD	SOD
fixed third angle in each section	fixed first angle in each section
sections in $(\phi_1,\Phi)/(\Psi,\Theta)$	sections in $(\phi_2,\Phi)/(\phi,\Theta)$
ϕ_2/ϕ = constant	ϕ_1/Ψ = constant
Reference = Sample Frame	Reference = Crystal Frame
Average of sections-> (001) Pole Figure	Average of sections-> ND Inverse Pole Figure

Concept Params. Euler Normalize Vol.Frac. Cartesian Polar Components

Summary

- The concept of the orientation distribution has been explained.

- The discretization of *orientation space* has been explained.

- *Cartesian* plots have been contrasted with *polar* plots.

- An example of *rolled fcc metals* has been used to illustrate the location of components and the characteristics of an orientation distribution described as a set of intensities on a regular grid in Euler [angle] space.

- For correct interpretation of texture results in rolled materials, you **must align the RD with the X direction (sample-1)!**

- Remember that each deformation type (rolling vs. drawing vs. shear) and each crystal lattice has its own set of typical texture components.

Supplemental Slides

Texture Components

- Many components have names to aid the memory.

- Specific components in Miller index notation have corresponding *points* in Euler space, i.e. fixed values of the three angles.

- Lists of components: the *Rosetta Stone* of texture!

- Very important: each component occurs in more than one location because of the combined effects of crystal and sample symmetry!!

Concept Params. Euler Normalize Vol.Frac. Cartesian Polar Components

Texture Component Table

- In the following slide, there are four columns.

- Each component is given in Bunge and in Kocks angles.

- In addition, the values of the angles are given for two different relationships between Materials axes and Instrument axes.

- Instrument axes means the Cartesian axes to which the Euler angles are referred to. In terms of Miller indices, (hkl)//3, and [uvw]//1.

- *The difference between these two settings is not always obvious in a set of pole figures, but can cause considerable confusion with Euler angle values.*
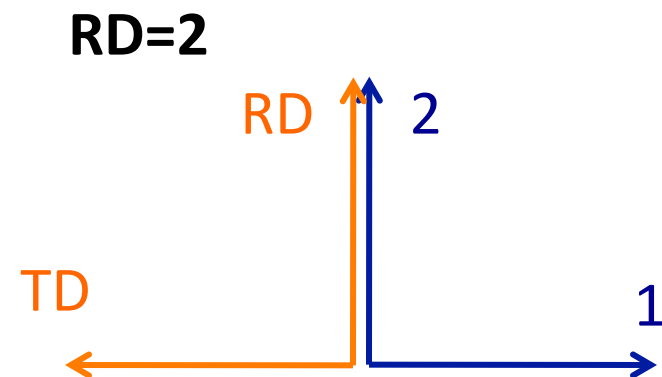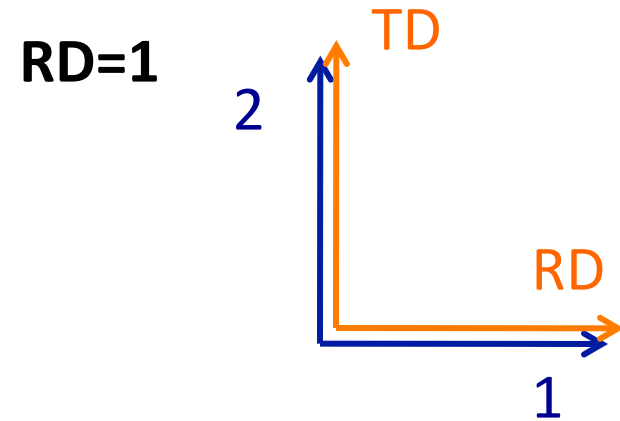
RD=1

RD=2

Table 4.F.2. <u>fcc Rolling Texture Components: Euler Angles and Indices</u>

Name	Indices	Bunge $(\varphi_1,\Phi,\varphi_2)$ RD= 1	Kocks (ψ,Θ,ϕ) RD= 1	Bunge $(\varphi_1,\Phi,\varphi_2)$ RD= 2	Kocks (ψ,Θ,ϕ) RD= 2
copper/ 1st var.	$\{112\}\langle11\bar{1}\rangle$	$40, 65, 26$	$50, 65, 26$	$50, 65, 64$	$39, 66, 63$
copper/ 2nd var.	$\{112\}\langle11\bar{1}\rangle$	$90, 35, 45$	$0, 35, 45$	$0, 35, 45$	$90, 35, 45$
S3*	$\{123\}\langle63\bar{4}\rangle$	$59, 37, 27$	$31, 37, 27$	$31, 37, 63$	$59, 37, 63$
S/ 1st var.	$(312)<0\,\bar{2}1>$	$32, 58, 18$	$58, 58, 18$	$26, 37, 27$	$64, 37, 27$
S/ 2nd var.	$(312)<0\,\bar{2}1>$	$48, 75, 34$	$42, 75, 34$	$42, 75, 56$	$48, 75, 56$
S/ 3rd var.	$(312)<0\,\bar{2}1>$	$64, 37, 63$	$26, 37, 63$	$58, 58, 72$	$32, 58, 72$
brass/ 1st var.	$\{110\}\langle\bar{1}12\rangle$	$35, 45, 0$	$55, 45, 0$	$55, 45, 0$	$35, 45, 0$
brass/ 2nd var.	$\{110\}\langle\bar{1}12\rangle$	$55, 90, 45$	$35, 90, 45$	$35, 90, 45$	$55, 90, 45$
brass/ 3rd var.	$\{110\}\langle\bar{1}12\rangle$	$35, 45, 90$	$55, 45, 90$	$55, 45, 90$	$35, 45, 90$
Taylor	$\{4\,4\,11\}\langle11\,11\,\bar{8}\rangle$	$42, 71, 20$	$48, 71, 20$	$48, 71, 70$	$42, 71, 70$
Taylor/ 2nd var.	$\{4\,4\,11\}\langle11\,11\,\bar{8}\rangle$	$90, 27, 45$	$0, 27, 45$	$0, 27, 45$	$90, 27, 45$
Goss/ 1st var.	$\{110\}\langle001\rangle$	$0, 45, 0$	$90, 45, 0$	$90, 45, 0$	$0, 45, 0$
Goss/ 2nd var.	$\{110\}\langle001\rangle$	$90, 90, 45$	$0, 90, 45$	$0, 90, 45$	$90, 90, 45$
Goss/ 3rd var.	$\{110\}\langle001\rangle$	$0, 45, 90$	$90, 45, 90$	$90, 45, 90$	$0, 45, 90$

Concept Params. Euler Normalize Vol.Frac. Cartesian Polar Components

Need for 3 Parameters

- Another way to think about orientation: rotation through θ about an arbitrary axis, **n**; this is called the axis-angle description.

- Two numbers required to define the axis, which is a *unit vector*.

- One more number required to define the magnitude of the rotation.

- Reminder! Positive rotations are anticlockwise = counterclockwise!

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Sets of Randomly Chosen Orientations

- A reasonable question to ask, or something that one needs from time to time, is how best to generate a randomly chosen set of orientations, that, when converted into an OD, yields a uniform distribution?

- We assume that the reader is familiar with how to invoke a "random number generator" on a computer (e.g. "RAND"), and that such functions are pseudo-random in the sense that they produce a sequence of values between 0 and 1 with uniform density over that interval in a sequence that has minimal regularity.

- The safest procedure is to generate random values of the Euler angles over the full range (no symmetry included). Thus: { 2π*RAND , acos(2*RAND-1) , 2π*RAND }.

- Note that very large numbers of points are required in order to obtain an OD with intensities close to 1, especially near $\Phi=0$ where the data becomes sparse.

Polar OD Plots

- As an alternative to the (conventional) Cartesian plots, Kocks & Wenk developed *polar plots* of ODs.

- Polar plots reflect the spherical nature of the Euler angles, and are similar to pole figures (and inverse pole figures).

- Caution: they are best used with angular parameters similar to Euler angles, but with sums and differences of the 1st and 3rd Euler angles.

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Polar versus Cartesian Plots

(a)   (b)   (c)
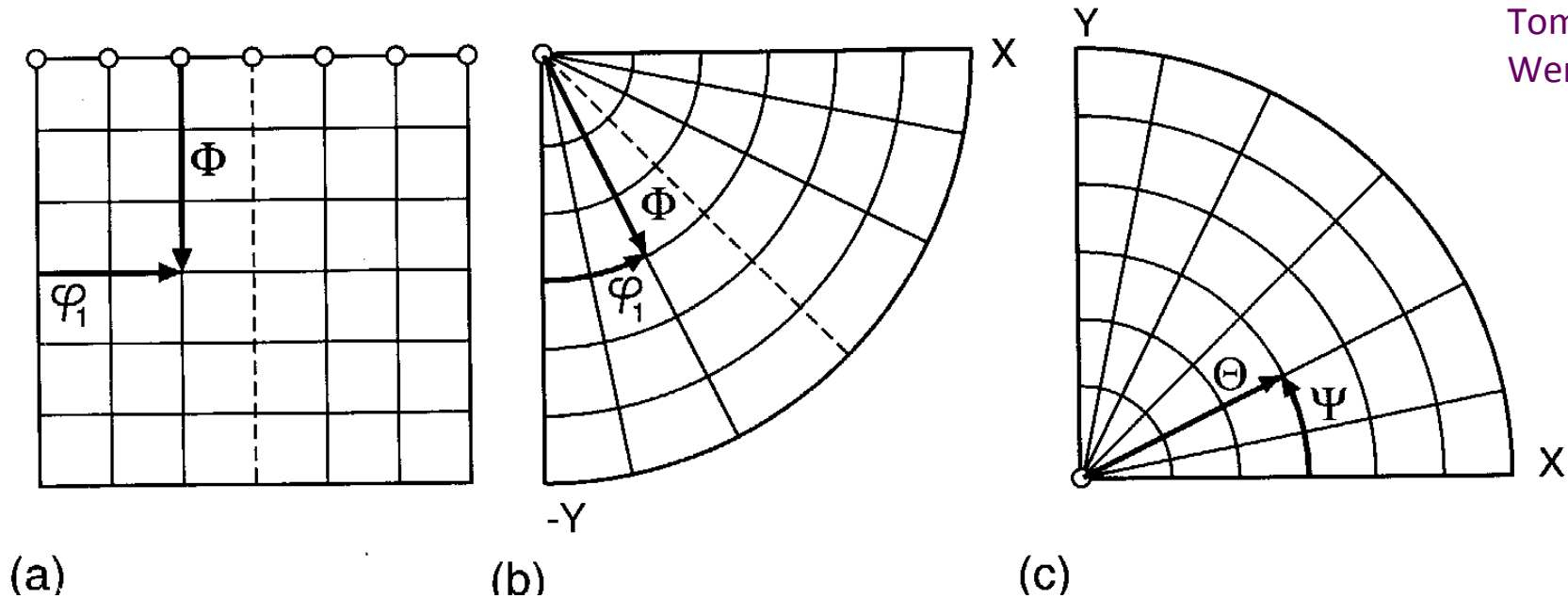
Diagram showing the relationship between coordinates in square (Cartesian) sections, polar sections with Bunge angles, and polar sections with Kocks angles.
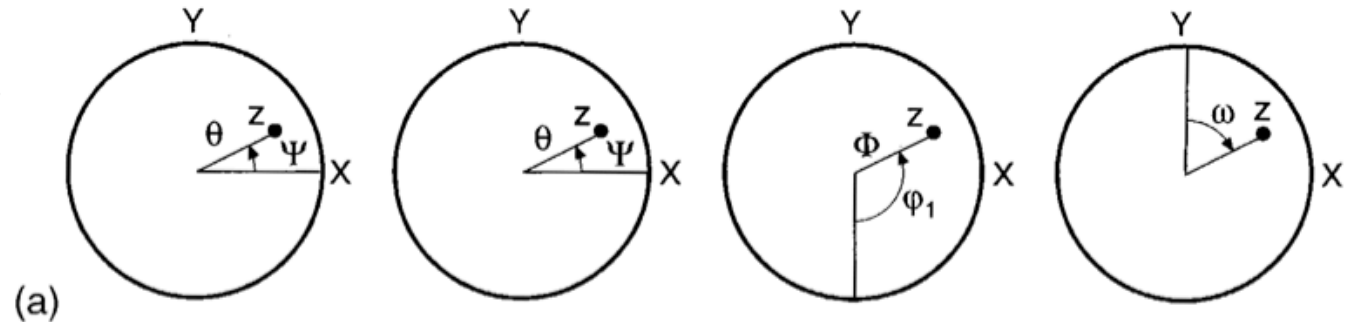
Concept Params. Euler Normalize Vol.Frac. Cartesian Polar Components

Continuous Intensity Polar Plots

Copper S Goss Brass
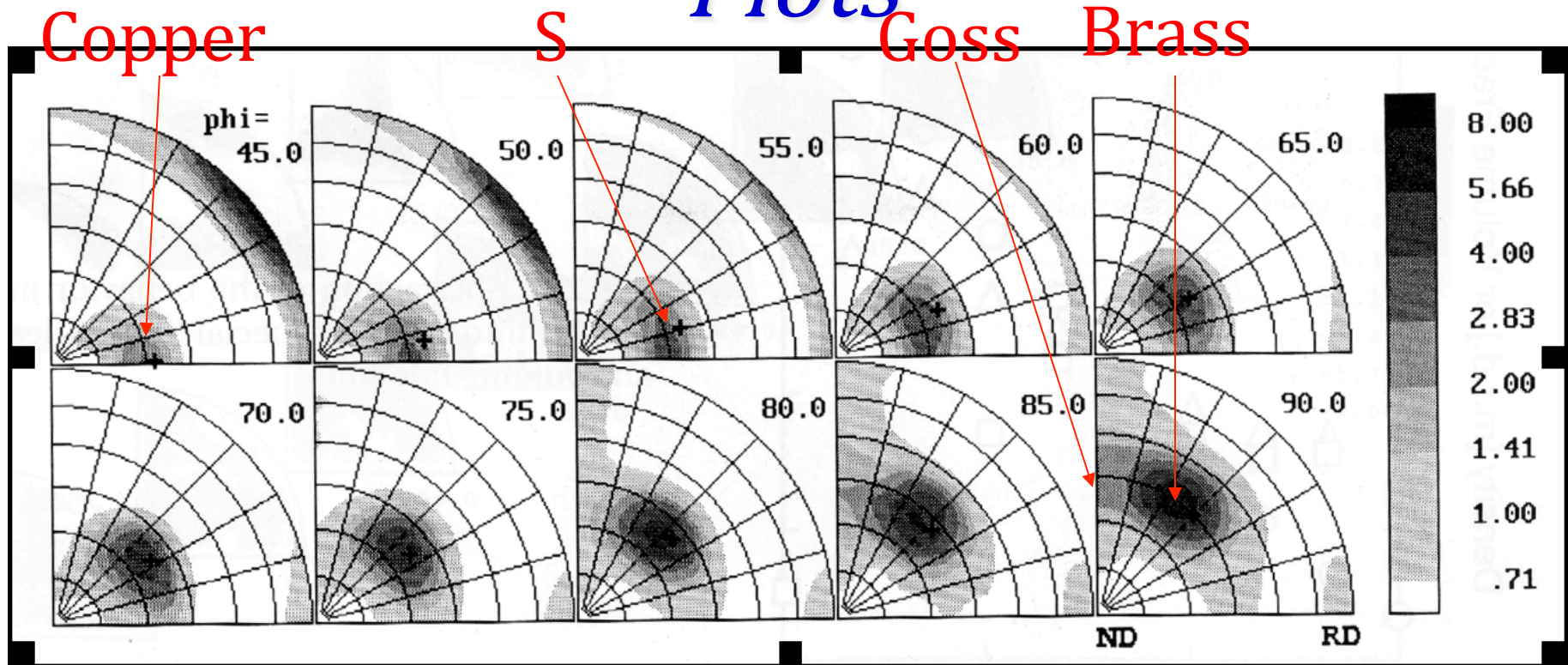
COD sections (fixed third angle, ϕ) for copper cold rolled to 58% reduction in thickness. Note that the maximum intensity in each section is well aligned with the beta fiber (denoted by a "+" symbol in each section).
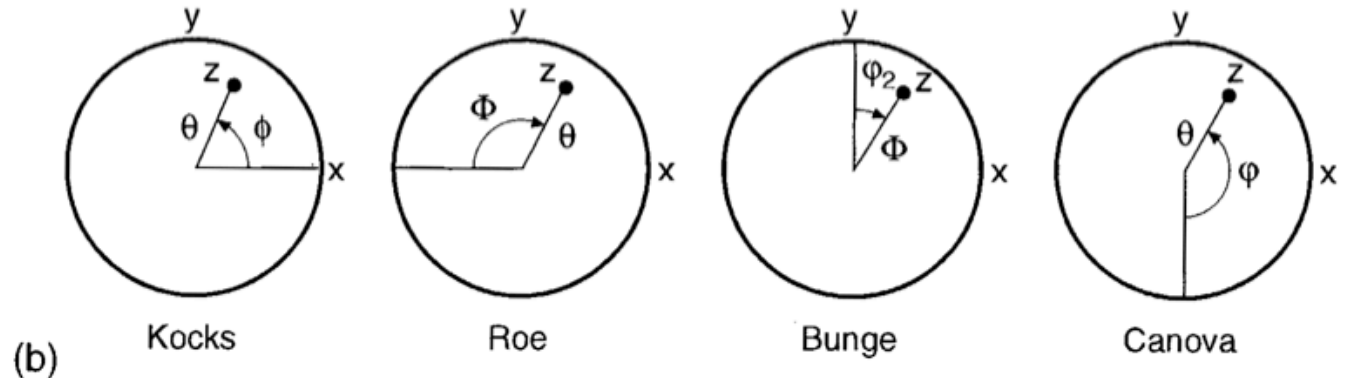
[Kocks, Tomé, Wenk]

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Euler Angle Conventions

Specimen Axes "COD"

Crystal Axes "SOD"

(a)

(b)

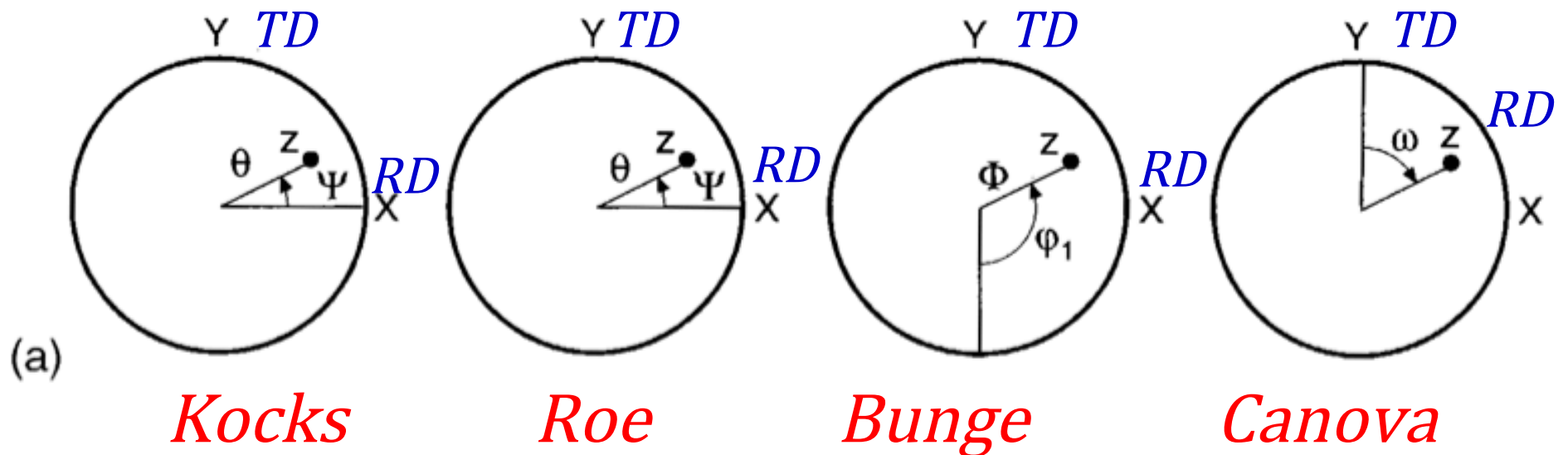Kocks   Roe   Bunge   Canova

Bunge and Canova are inverse to one another
Kocks and Roe differ by sign of third angle
Bunge and Canova rotate about x', Kocks, Roe, Matthis
 about y' (2nd angle).

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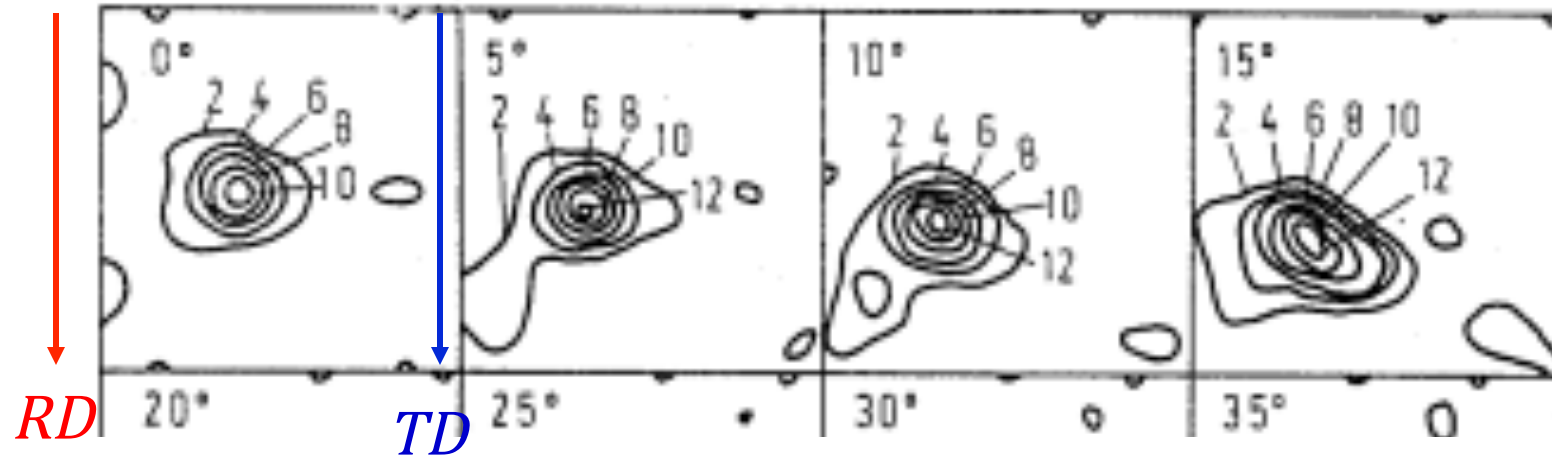
Where is the RD? (TD, ND...)

(a)

Kocks   **Roe**   **Bunge**   **Canova**

In spherical COD plots, the rolling direction is typically assigned to Sample-1 = X. Thus a point in orientation space represents the position of [001] in sample coordinates (and the value of the third angle in the section defines the rotation about that point). Care is needed with what "parallel" means: a point that lies between ND and RD (Y=0°) can be thought of as being "parallel" to the RD in that its projection on the plane points towards the RD.

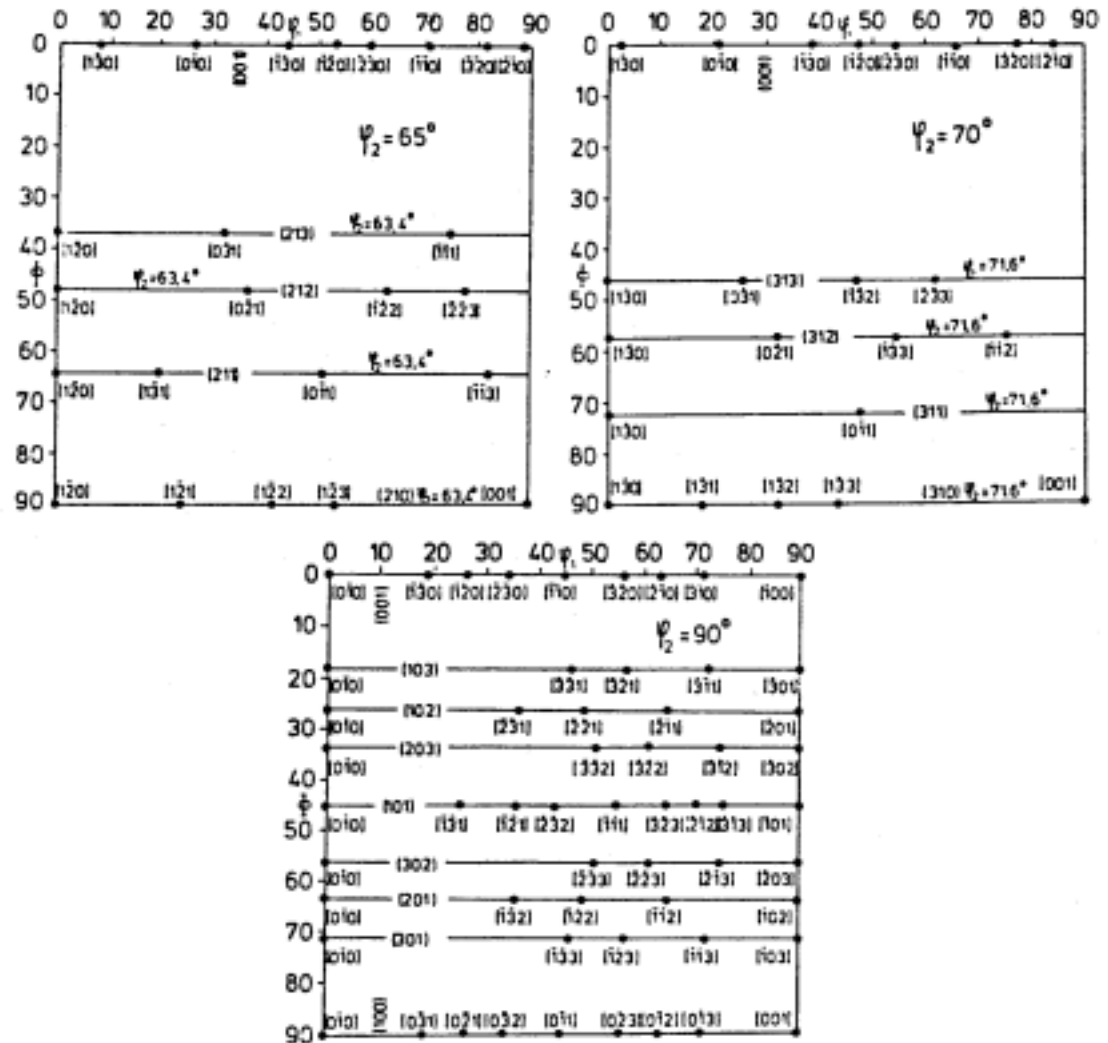Concept Params. Euler Normalize Vol.Frac. Cartesian Polar Components

Where is the RD? (TD, ND...)

RD TD

In Cartesian COD plots (ϕ_2 constant in each section), the rolling direction is typically assigned to Sample-1 = X, as before. Just as in the spherical plots, a point in orientation space represents the position of [001] in sample coordinates (and the value of the third angle in the section defines the rotation about that point). The vertical lines in the figure show where orientations "parallel" to the RD and to the TD occur. The (distorted) shape of the Cartesian plots means, however, that the two lines are parallel to one another, despite being orthogonal

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Miller Index Map, contd.