Carnegie Mellon

Orientation Distribution: Definition, Discrete Forms, Examples

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27-731 (normally, 27-750)

Texture, Microstructure & Anisotropy



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.
- Show qualitative explanation of the effect of symmetry on the OD.

In Class Questions: 1

- 1. Why does an orientation distribution (OD) require three parameters? For the straightforward reason that an orientation requires 3 parameters therefore a distribution must also be 3-dimensional.
- 2. What are the similarities and differences between an OD and a probability density function? An OD can thought of as a PDF in 3D. However, the scaling is different, i.e., it is *not* unit volume but scaled such that a uniform distribution (everywhere the same probability of finding a given component) is unity.
- 3. What is the practical value of an OD (as compared to pole figures, e.g.)? For quantifying textures and essential for computing the anisotropy of a material.
- 4. Does an OD have to be parameterized with Euler angles? Any suitable parameterization of rotations is acceptable; Rodrigues vectors is a common alternative especially for grain boundaries.
- 5. Against which Euler angles are ODs typically sectioned? For fcc metals, phi-2; for bcc metals, phi-1.

In Class Questions: 2

- 1. What distribution of intensity do we expect to see for a rolled fcc metal? See the example: most intensity is found along the beta fiber.
- 2. What is meant by the "beta fiber"? This is a line of intensity between the Brass and Copper components.
- 3. Where are standard texture components of rolled fcc metals located in the space? Cube, Goss, Brass, S and Copper.
- 4. What are some differences between discrete forms of ODs and series expansion forms? For example, a series expansion provides a functional form with weighting coefficients that allows an intensity to be calculated for any orientation. In the discrete form, the intensity is only defined for each cell.
- 5. What is the size of the volume element in orientation space? This depends on the measure used: for Euler angles given in degrees but see the notes for details.

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). In effect, projection along phi-1 removes variations about that angle so it makes a map of the variation in the crystal-Z w.r.t. the sample frame. And vice versa for the phi-2 projection.
- 2. What are generalized spherical harmonic (functions)? These are the 3D polynomial functions that allow any 3D polar/spherical information to be fitted.
- 3. How do pole figures relate to the OD? Any pole figure is a projection of the 3D texture information (in the OD) onto the sample frame, based on a specific choice of (hkl).
- 4. How do *volume fractions* (of texture components) relate to intensity values in the OD? A volume fraction is obtained by *integrating* the intensity in the OD over a region surrounding the selected texture component.

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 $f \ge 0$ (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).

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

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.

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.

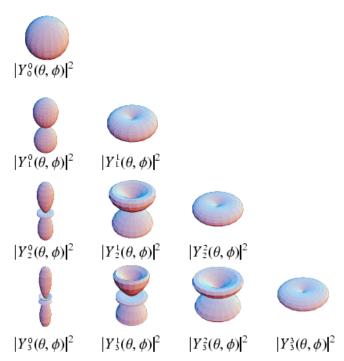
*R. J. Roe: *J. Appl. Phys.* **36**, (1965), p. 2024.

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.

Another website:

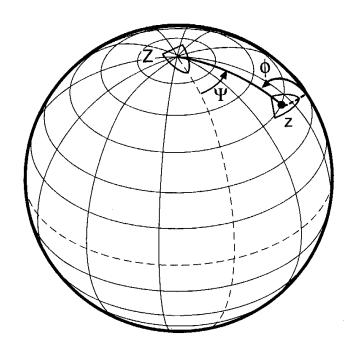
http://wwwudc.ig.utexas.edu/external/becke r/teaching-sh.html



Look for visualization as: spherical_harmonics.mpeg

Euler Angles, Ship Analogy

- Analogy: position and the heading of a boat with respect to the globe. Latitude or colatitude (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]

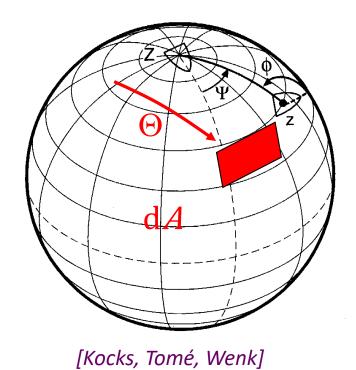
Area Element, Volume Element

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

```
dA = \sin\Theta d\Theta d\psi
Volume element = dV = dA d\phi = \sin\Theta d\Theta d\psi d\phi.
(Kocks angles)
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Bunge Euler angles:

Volume element = dV = dA d\phi_2 = \sin \Phi d\Phi d\phi_1 d\phi_2.
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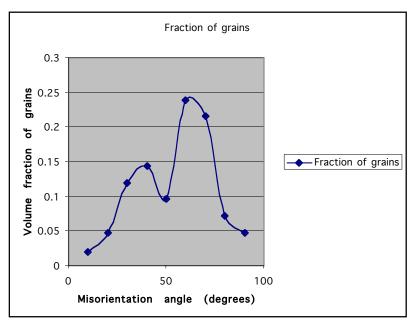
Concept Params. Euler Normalize Vol. Frac. Cartesian Polar Components

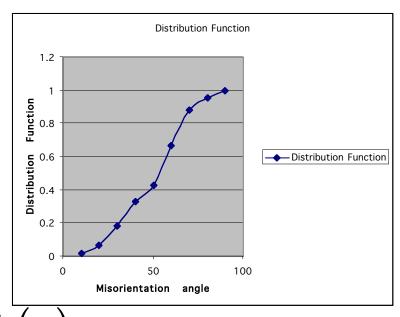
Description of Probability

• 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.



Courtesy of Prof. H. Garmestani





$$f(x) \ge 0, \quad \forall x$$

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

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

$$\frac{differentiate}{}$$

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).
- Sin(Φ) corrects for volume of the element (previous slide). The integral of Sin(Φ) on $[0,\pi)$ 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 $360^{\circ}*2^*360^{\circ} = 259,200$ (°²).

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

Example of random orientation distribution in Euler space

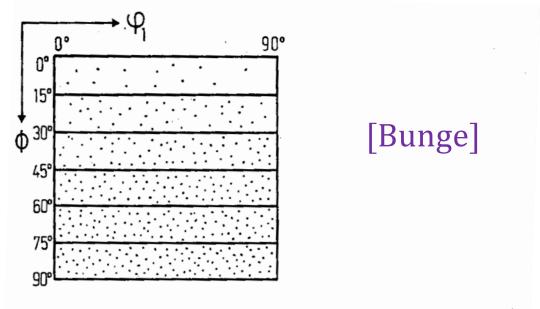


Figure 2.25 On the definition of the invariant measures by a random distribution in the Euler space $\varphi_1 \Phi \varphi_2$

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. 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).

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

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).

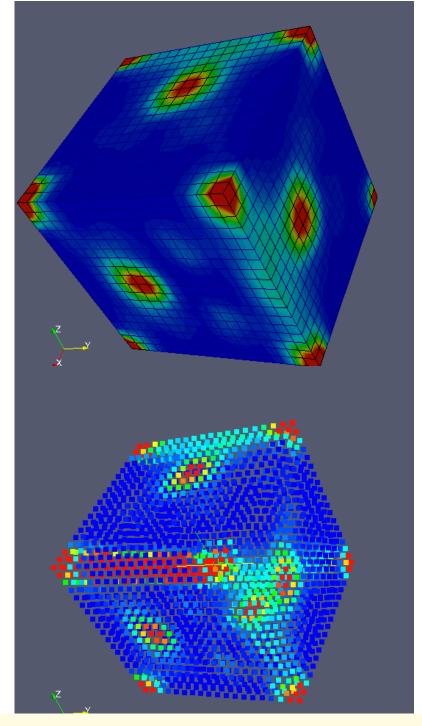
Statistics:
$$f(x) \ge 0$$
, $\forall x$ Texture: $f(x) \ge 0$, $\forall x$ $pdf \rightarrow \int_0^{\Omega} f(g)dg = 1$ ODF $\rightarrow \int_0^{\Omega} f(g)dg = \int_0^{\Omega} dg$

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.

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 clearer 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). Try thresholding the image for
 yourself.



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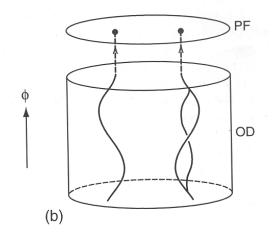
Discrete OD

- 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 $\Delta[angle] = 5^\circ$) 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*).

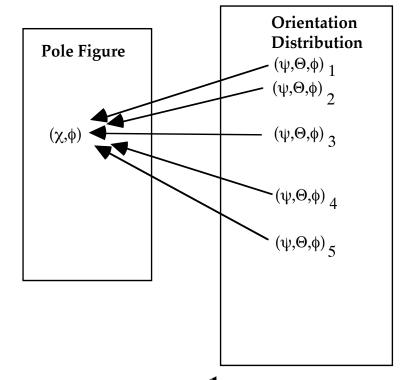
$$1 = \frac{1}{8\pi^2} \sum_{\phi_1} \sum_{\Phi} \sum_{\phi_2} f(\phi_1, \Phi_i, \phi_2) \Delta \phi_1 \Delta \phi_2 \left(\cos\left(\Phi_i - \frac{\Delta \Phi}{2}\right) - \cos\left(\Phi_i + \frac{\Delta \Phi}{2}\right) \right)$$

$PFs \rightleftarrows OD$

- 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 (defined by variable rotation about a fixed axis) 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.).



Kocks Ch. 3, fig. 1



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

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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 a true *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.

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:

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

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 Ω denotes the region around the texture component of interest. For specific ranges of Euler angles:

$$V_{f}(\varphi_{1},\Phi,\varphi_{2}) = \int_{\varphi_{1}-\Delta\varphi_{1}}^{\varphi_{1}+\Delta\varphi_{1}} \int_{\Phi-\Delta\Phi}^{\Phi_{2}+\Delta\varphi_{2}}^{\Phi_{2}} \int_{\varphi_{1}-\Delta\varphi_{1}}^{f} \int_{\Phi-\Delta\Phi}^{f} \varphi_{2} - \Delta\varphi_{2}$$

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

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, Ω is volume in orientation space, V is volume and V_f is volume fraction:

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

$$f(g) = \frac{1}{V} \frac{dV(g)}{dg} = \frac{\Delta V_f}{\Delta g} \bigg|_g$$
For a PDF, one we have $\frac{1}{V} \frac{dV(g)}{dg} = \frac{f(g)}{\int_{\Omega} dg}$

For a PDF, one would use:

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

Intensity from $V_{\mathfrak{p}}$ contd.

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

$$V_f(g) = \frac{1}{8100} \int f(g) \sin \Phi d\Phi d\phi_1 d\phi_2$$

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

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

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 (or 180°), the 1st and 3rd angles become linearly dependent.
 - At Φ =0, only ϕ_1 + ϕ_2 (or ϕ_1 - ϕ_2) is significant.

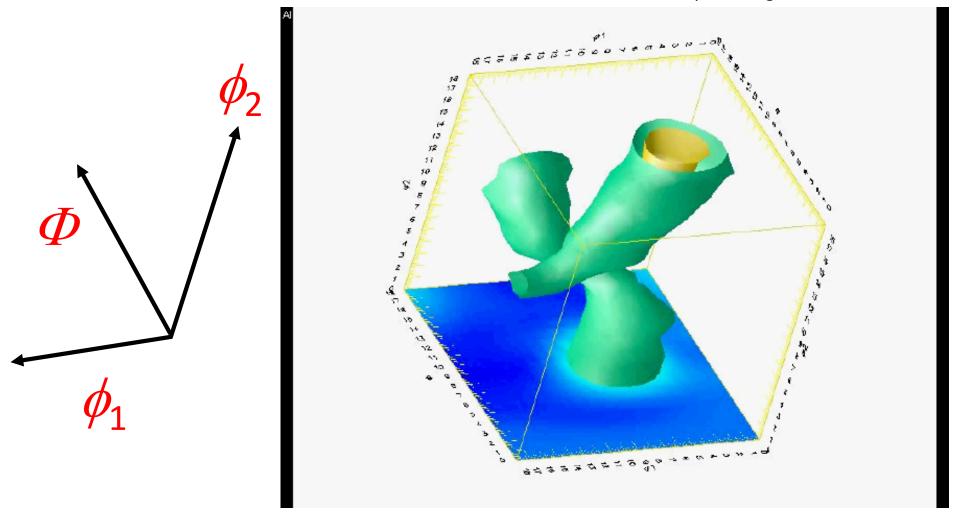
OD Example

- Example of texture in *rolled fcc* metals is presented.
- 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 .
- For *bcc* metals, it is more typical to plot sections with constant ϕ_1 .

3D Animation in Euler Space

Rolled commercial purity Al

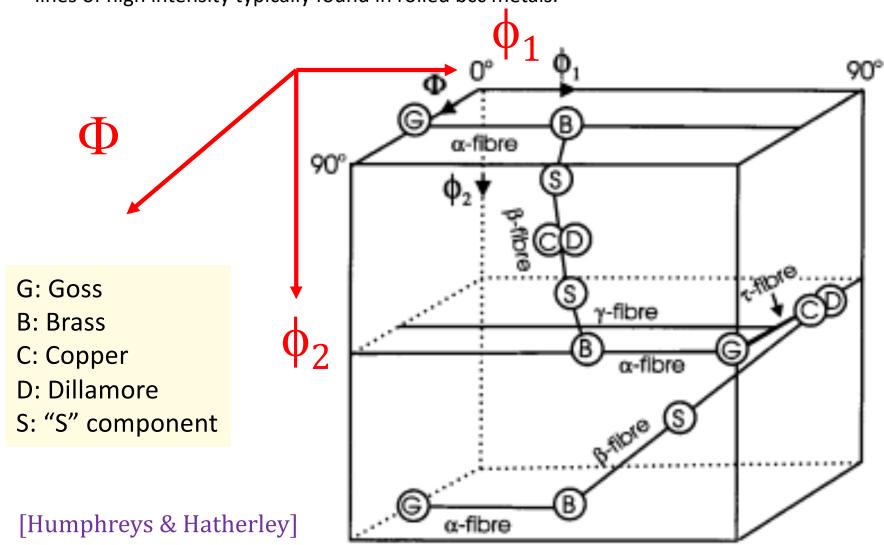
Animation made with DX - see www.opendx.org



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

Cartesian Euler Space

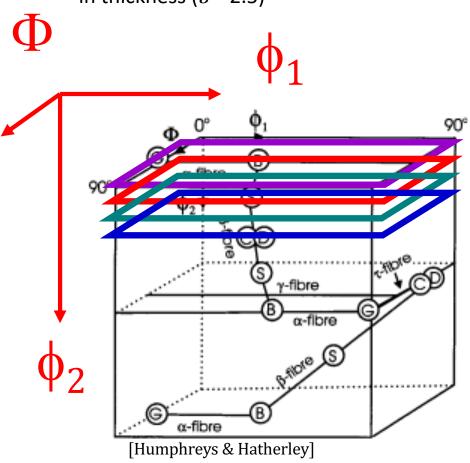
Line diagram shows a schematic of the beta-fiber typically found in an fcc rolling texture with major components labeled (see legend below). The fibers labeled "alpha" and "gamma" correspond to lines of high intensity typically found in rolled bcc metals.



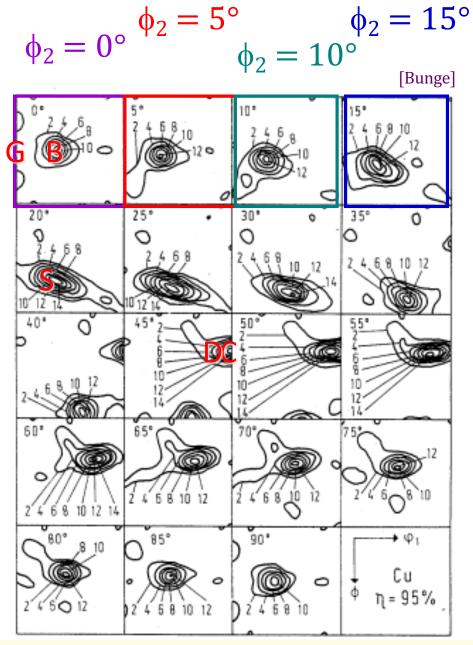
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OD Sections

Example of copper rolled to 90% reduction in thickness (ε $^{\sim}$ 2.5)



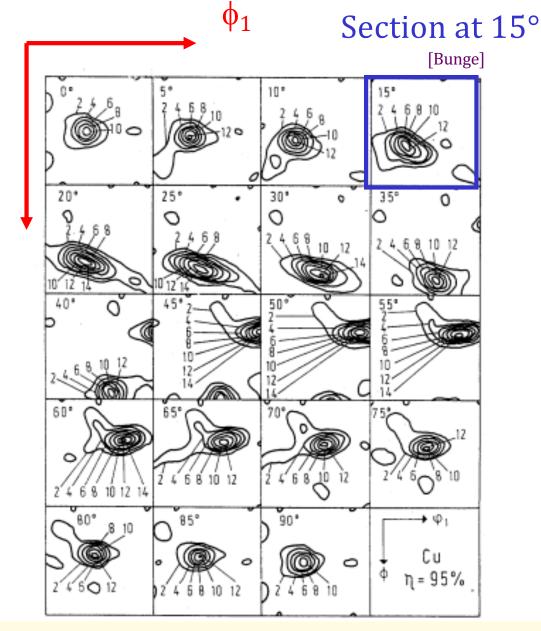
Sections are drawn as contour maps, one per value of ϕ_2 (0, 5, 10 ... 90°).



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Example of OD in Bunge Euler Space

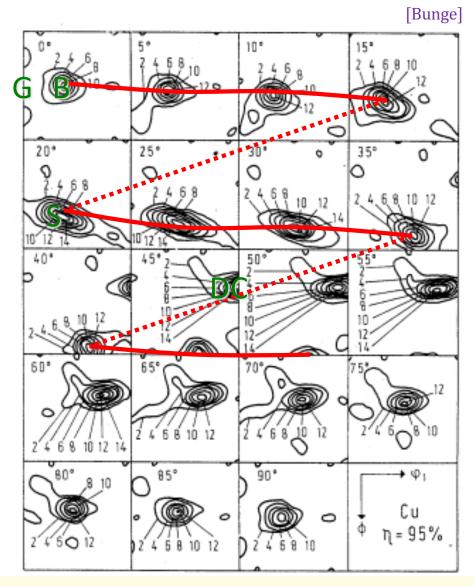
- OD is represented by a series of *sections*, i.e. one (square) box per section.
- Each section shows the variation of the OD intensity
 for a fixed value of the third angle.
- Contour plots interpolate between discrete points.
- High intensities mean that the corresponding orientation is common (occurs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

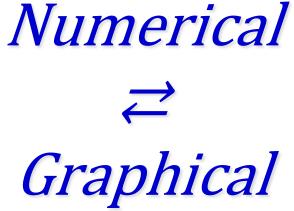


Example of OD in Bunge Euler Space, contd.

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!"

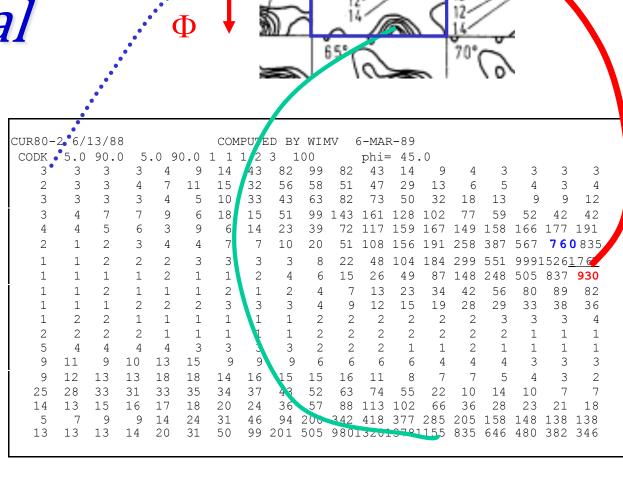
The technical name for this is the *beta fiber*.





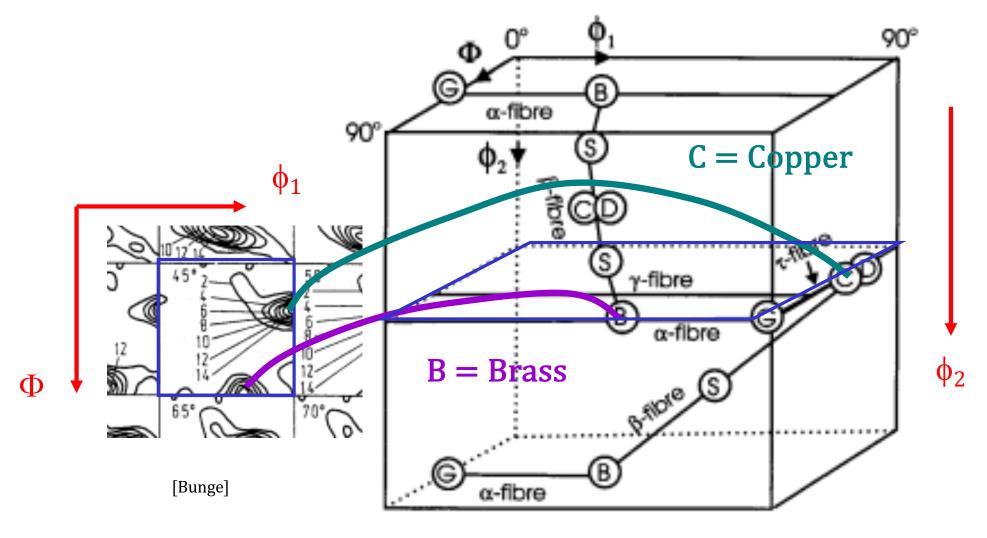
$$\phi_2 = 45^{\circ}$$

Example of a single section



[Bunge]

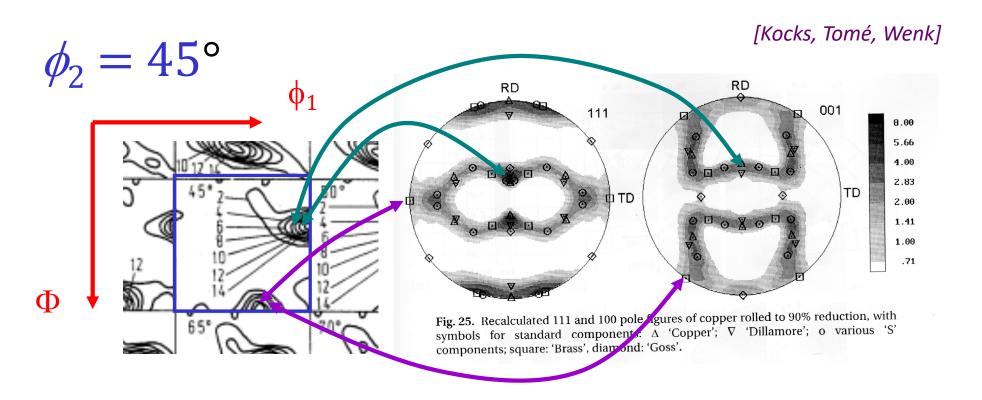
(Partial) Fibers in fcc Rolling Textures



[Humphreys & Hatherley]

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OD ≠ Pole Figure

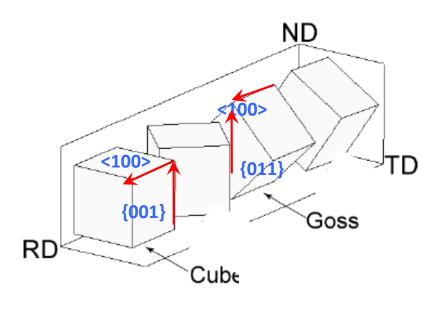


$$B = Brass$$
 $C = Copper$

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

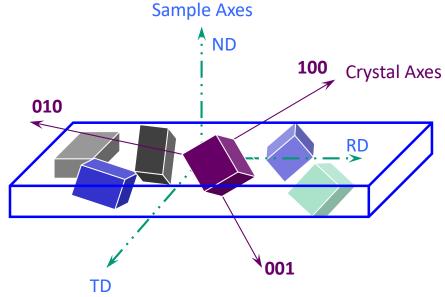
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Euler Angles: recap



Component	RD	ND
Cube	<100>	{001}
Goss	<100>	{011}
Brass	<112>	{110}
Copper	<111>	{112}

Euler Angles represent a crystal orientation with respect to sample axes

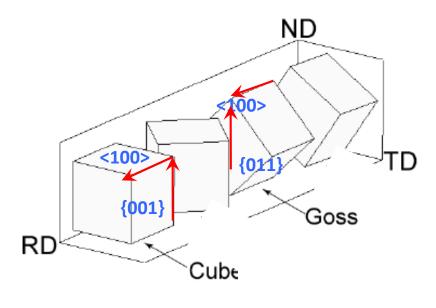


Rotation 1 (φ_1): rotate sample axes about ND

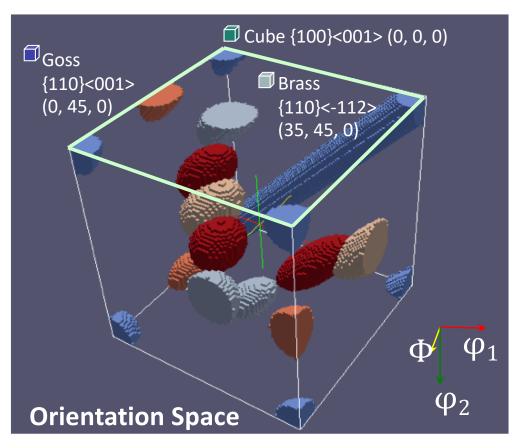
Rotation 2 (Φ): rotate sample axes about rotated RD

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

Texture Components versus Orientation Space



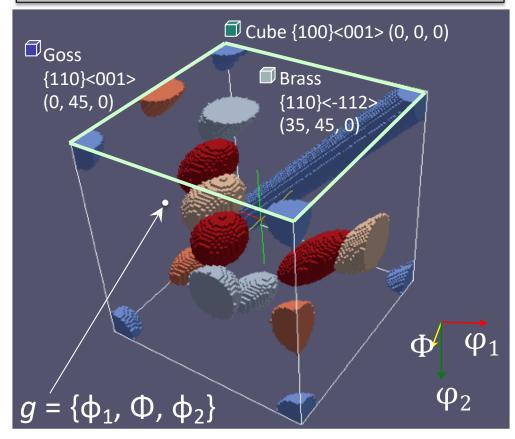
Component	Euler Angles (°)
Cube	(0, 0, 0)
Goss	(0, 45, 0)
Brass	(35, 45, 0)
Copper	(90, 45, 45)



Slide from Lin Hu [2011]

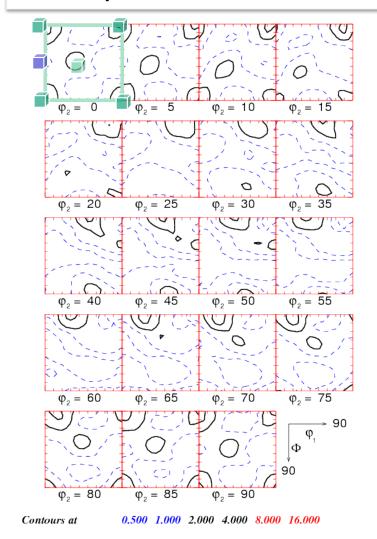
ODF: 3D vs. sections





Slide from Lin Hu [2011]

ODF gives the density of grains having a particular orientation.

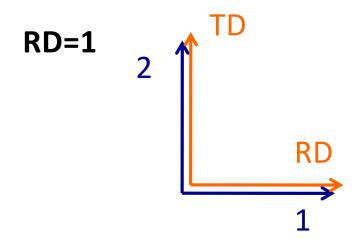


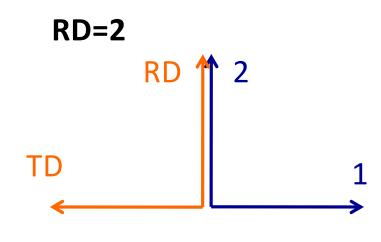
Texture Components

- 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!!

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.

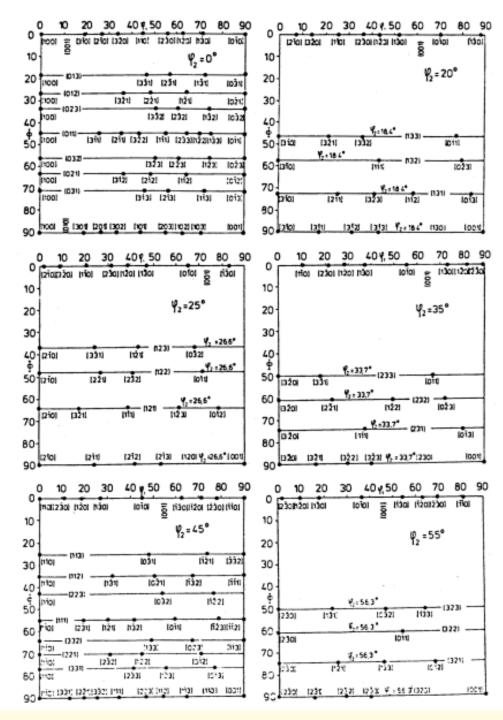


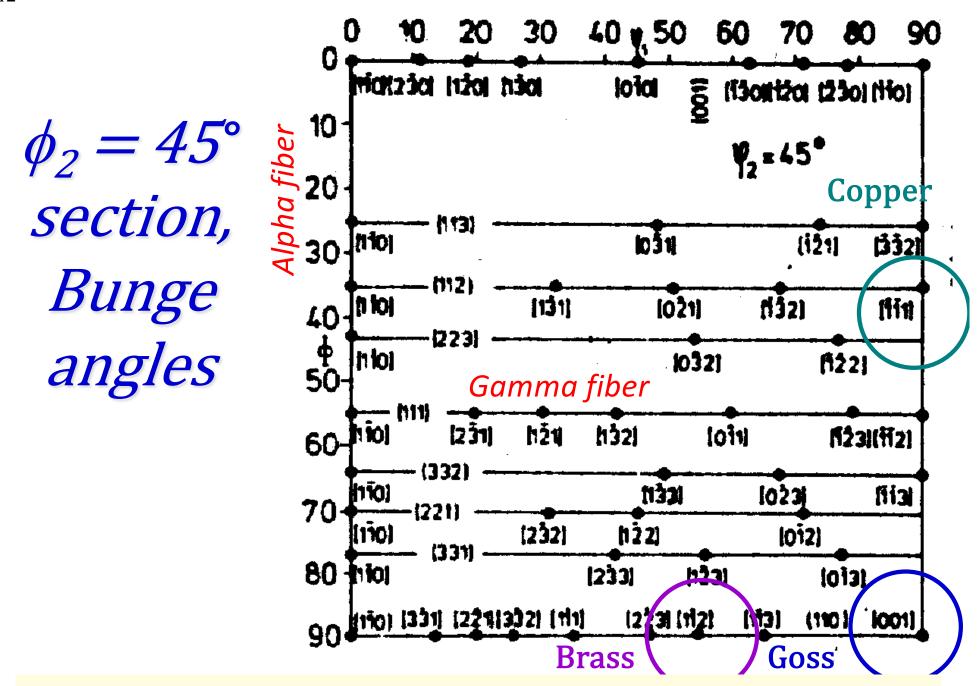


Name	Indices	Bunge	Kocks	Bunge	Kocks
Tame		$(\varphi_1,\Phi,\varphi_2)$	(ψ,Θ,ϕ)	$(\varphi_1,\Phi,\varphi_2)$	(ψ,Θ,ϕ)
		RD=1	RD=1	RD=2	RD=2
coppor/	$\{112\}\langle 11\overline{1}\rangle$	40, 65, 26	50, 65, 26	50, 65, 64	39, 66, 63
copper/	[{114}\111/	[40,03,20]	[50, 05, 20]	30,03,04	39,00,03
1 st var.	(110)/111)	00 25 45	0 25 45	0 25 45	00 25 45
copper/	$\{112\}\langle 11\overline{1}\rangle$	90, 35, 45	0, 35, 45	0, 35, 45	90, 35, 45
2 nd var.	(100)/(07)				5 0 0 5 60
S3*	$\{123\}\langle 634\rangle$	59, 37, 27	31, 37, 27	31, 37, 63	59, 37, 63
S/ 1st var.	(312)<021>	32, 58, 18	58, 58, 18	26, 37, 27	64, 37, 27
S/ 2nd var.	(312)<021>	48, 75, 34	42, 75,34	42, 75, 56	48, 75, 56
S/ 3rd var.	(312)<021>	64, 37, 63	26, 37, 63	58, 58, 72	32, 58, 72
brass/	$\{110\}\langle\bar{1}12\rangle$	35, 45, 0	55, 45, 0	55, 45, 0	35, 45, 0
1 st var.			, ,	, ,	, ,
brass/	$\{110\}\langle\overline{1}12\rangle$	55, 90, 45	35, 90, 45	35, 90, 45	55, 90, 45
2 nd var.	()(/		, , , , , ,	, , , , , , ,	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
brass/	$\{110\}\langle \overline{1}12\rangle$	35, 45, 90	55, 45, 90	55, 45, 90	35, 45, 90
3^{rd} var.	(110)(112/				22, 12, 70
Taylor	$\{4\ 4\ 11\}\langle 11\ 11\ 8\rangle$	42, 71, 20	48, 71, 20	48, 71, 70	42, 71, 70
Taylor/	$\{4411\}\langle 1111\bar{8}\rangle$	90, 27, 45	0, 27, 45	0, 27, 45	90, 27, 45
2nd var.	\4 4 11 \\11 11 0/	00,27,43	[0,27,43]	[0,27,43]	90,21,43
	(110)/001\	0.45.0	90, 45, 0	90, 45, 0	0.45.0
Goss/	{110}⟨001⟩	0,45,0	90,43,0	90,43,0	0,45,0
1 st var.	(110)/001	00 00 45	0.00.45	0.00.45	00 00 45
Goss/	{110}⟨001⟩	90, 90, 45	0, 90, 45	0,90,45	90, 90, 45
2 nd var.	(1.10) /06:1				
Goss/	{110}⟨001⟩	0,45,90	90, 45, 90	90, 45, 90	0, 45, 90
3 rd var.					

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Map in
Euler
Space

Bunge, p.23 et seq.





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,

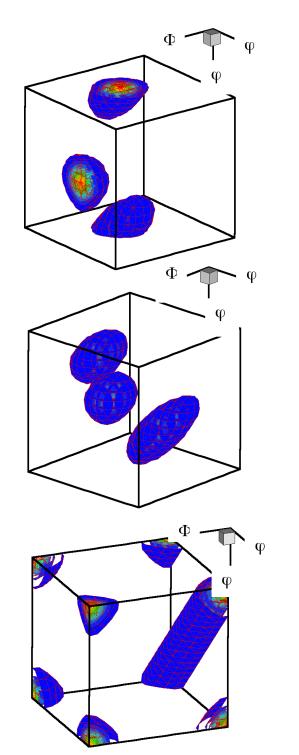
6: {27, 58, 18}, S,

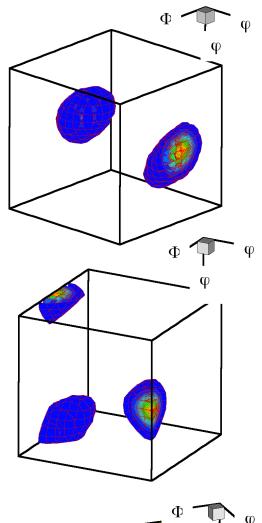
7: {53, 75, 34}, S

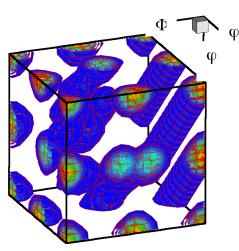
8: {90, 90, 45}, Goss

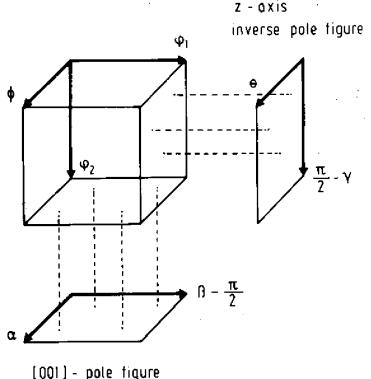
9: {0, 0, 0}, cube

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









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 3^{rd} 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.

[Kocks, Tomé, Wenk]

Section Conventions

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

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

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!

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: $\{2\pi^*RAND, acos(2*RAND-1), 2\pi^*RAND\}$.
- Note that very large numbers of points are required in order to obtain an OD with intensities close to 1, especially near Φ =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.

Polar versus Cartesian Plots

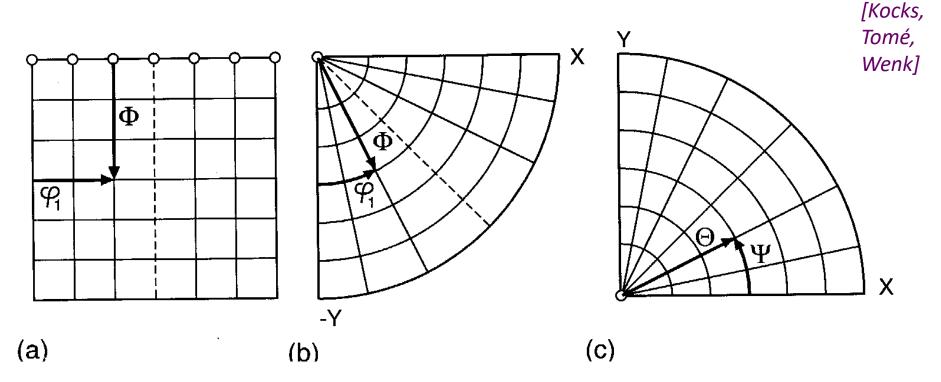
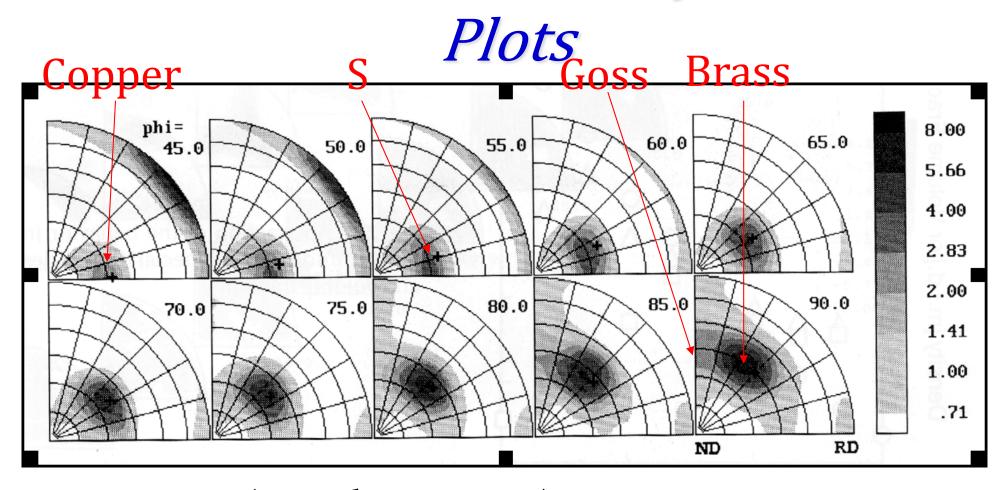


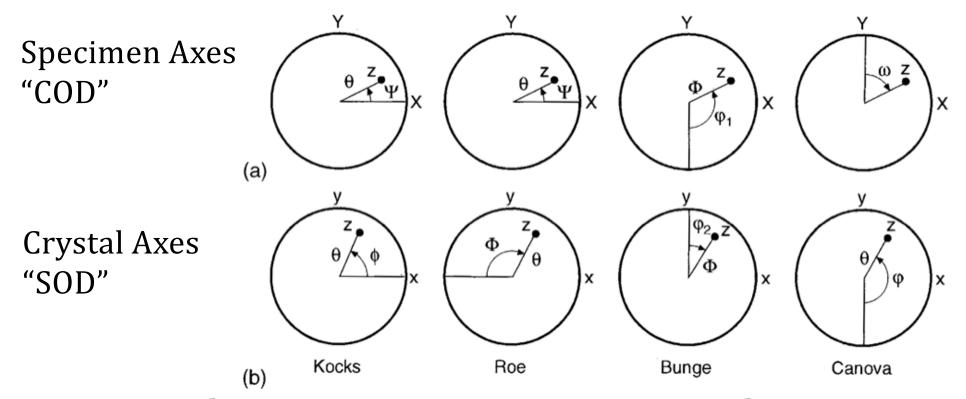
Diagram showing the relationship between coordinates in square (Cartesian) sections, polar sections with Bunge angles, and polar sections with Kocks angles.

Continuous Intensity Polar



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).

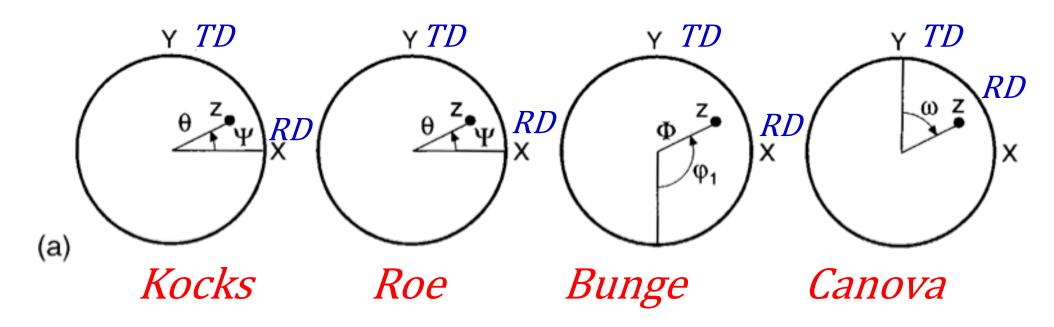
Euler Angle Conventions



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).

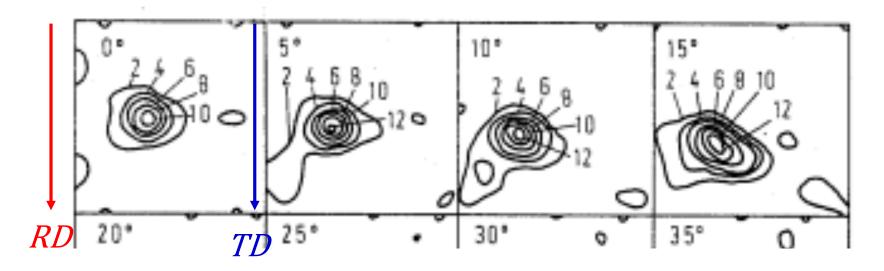
Where is the RD? (TD, ND...)

[Kocks, Tomé, Wenk]



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 ($Y=0^{\circ}$) can be thought of as being "parallel" to the RD in that its projection on the plane points towards the RD.

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



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

Miller Index Map, contd.

