

Texture and Anisotropy

Part I:

Chapter 2. Description of Orientation

Part I: Fundamental of Orientation

- Orientation matrix
- Ideal Orientation
- Euler angles
- Angle/axis of rotation
- Rodrigues vector

Crystal systems

7 crystal
systems

↓
Lattice
types

14 Bravais
lattices

Lattice

symmetry

230 space
groups

↑
Space translation:
mirror, glide planes
and screw axis

32 point
groups

Crystal structure and symmetries

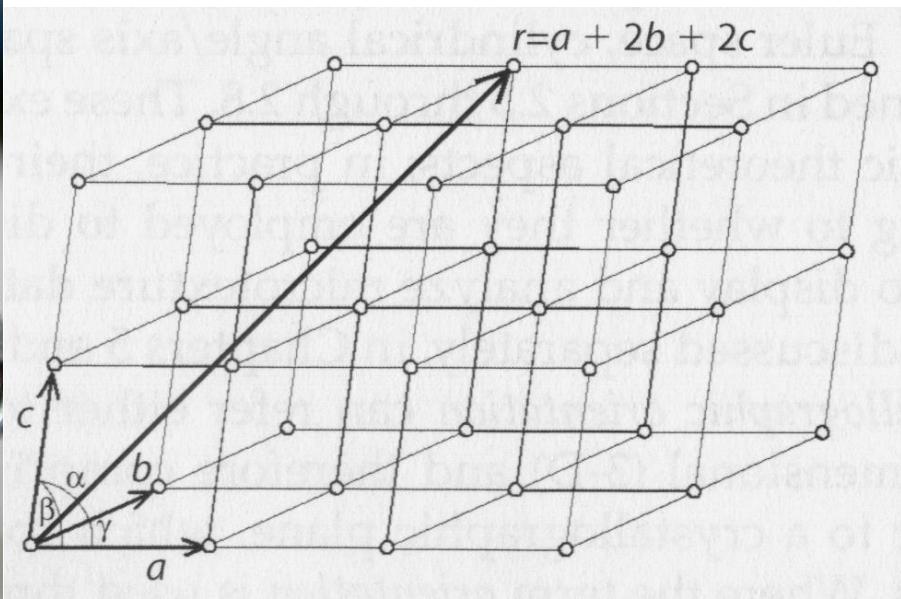
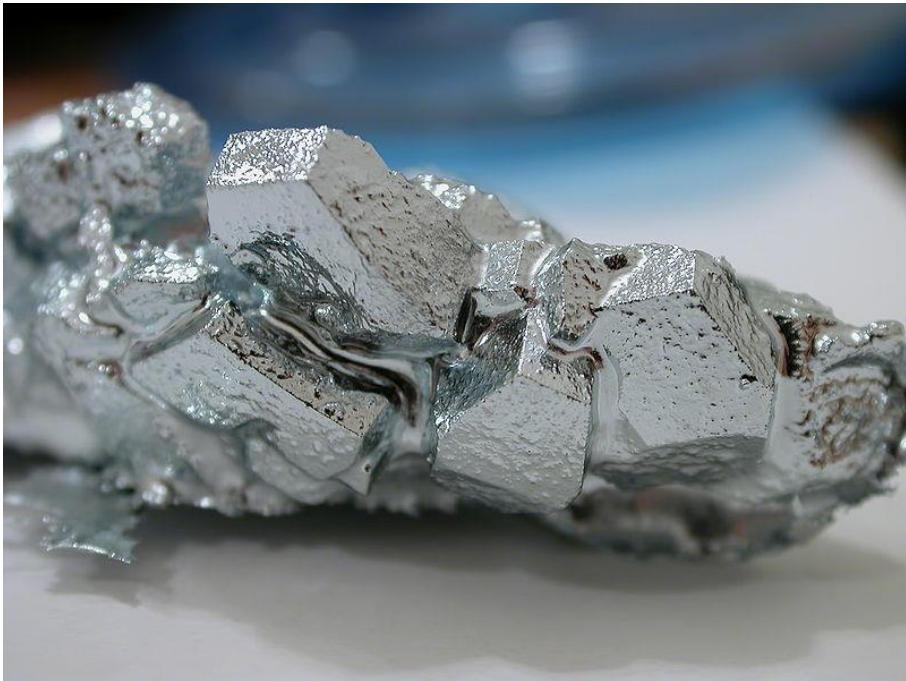
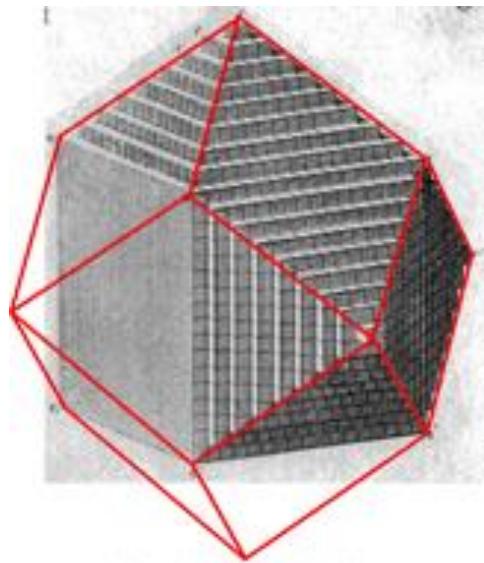


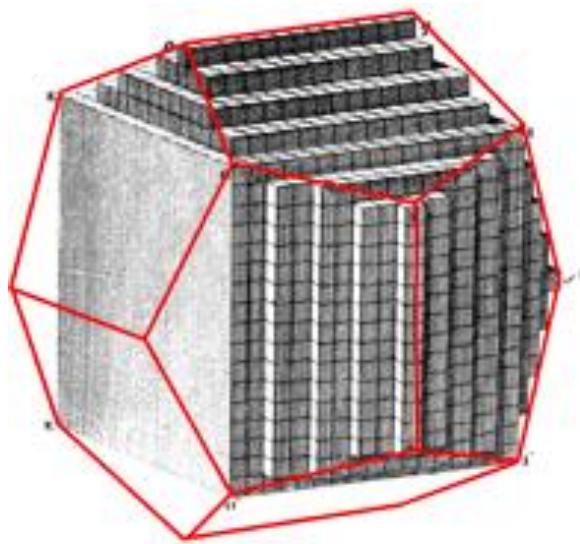
FIGURE 2.1

- (a) Centimeter-sized crystals of pure gallium. (From Wikipedia, The Free Encyclopedia, "Gallium," http://en.wikipedia.org/wiki/Image.Gallium1_640x480.jpg. With permission.);
(b) Construction of a 3-D crystal lattice based on a set of three unit vectors a , b , and c .

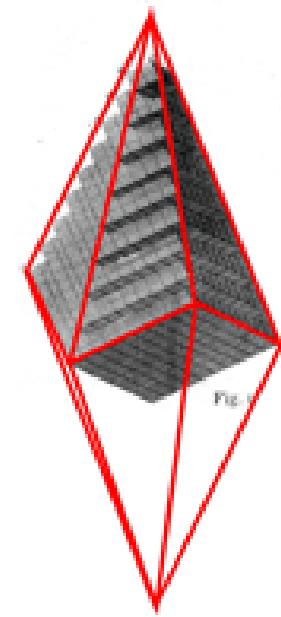
Crystal systems



Rhomb-dodecahedron



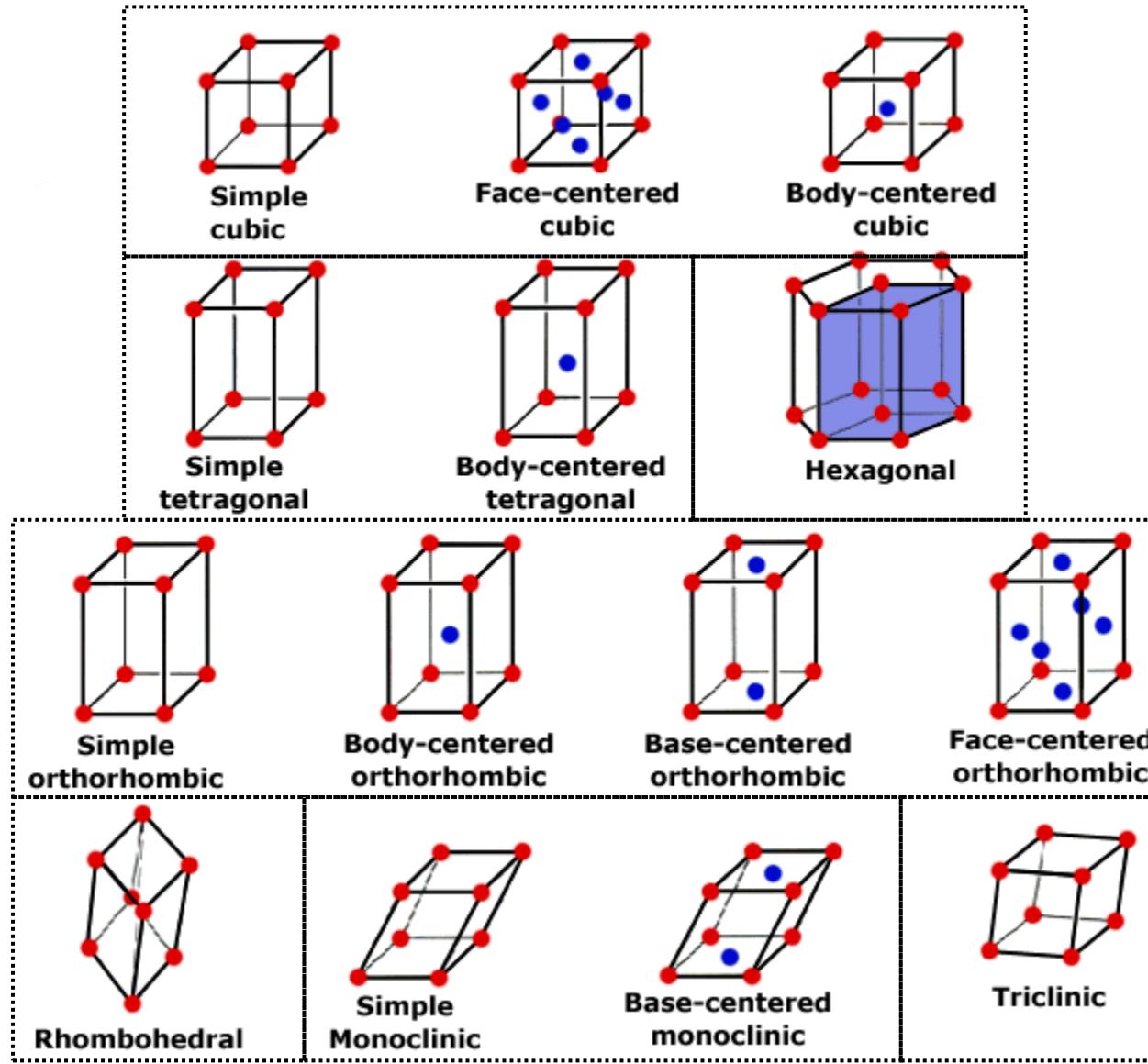
Pentagon-dodecahedron



Scalenohedron

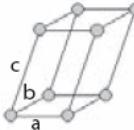
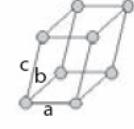
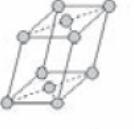
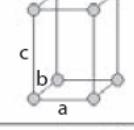
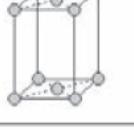
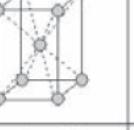
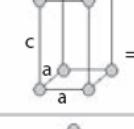
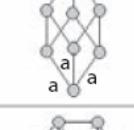
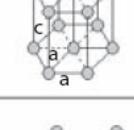
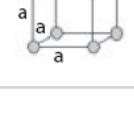
Crystalline materials are separated into 7 crystal different systems. These crystal systems are most easily identified by the constraints on the cell parameters.

7 Crystal systems



14 Bravais lattices

4 lattice types

Name	Conditions	Primitive	Base centered	Body centered	Face centered
Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$				
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90^\circ \neq \beta$				
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$				
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$				
Rhombohedral (trigonal)	$a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$				
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$				
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$				

7 crystal systems

Example of JCPD card

04-0784

Wavelength= 1.54056

	d(A)	Int	h	k	l	
Au						
Gold	2.355	100	1	1	1	
	2.039	52	2	0	0	
	1.442	32	2	2	0	
Gold, syn	1.230	36	3	1	1	
	1.177	12	2	2	2	
Rad.: CuKa1 λ : 1.54056 Filter: Ni Beta d-sp:	1.019	6	4	0	0	
Cut off:	Int.: Diffract.	I/Icor.:	.9358	23	3	3
			.912	22	4	2
Ref: Swanson, Tatge, Natl. Bur. Stand. (U.S.), Circ. 539, I, 33 (1953)	.8325	23	4	2	2	

Sys.: Cubic

S.G.: Fm $\bar{3}$ m (225)

a: 4.0786 b:

c:

A:

C:

α :

β :

γ :

Z: 4

mp: 1061.6-1063.2

Ref: Ibid.

Dx: 19.283 Dm: 19.300 SS/FOM: Fg = 129(.0078, 9)

$\epsilon\alpha$: $\eta\beta$: 0.366 $\epsilon\gamma$: Sign: 2V:

Ref: Winchell, Elements of Optical Mineralogy, 17

Color: Yellow metallic

Pattern taken at 26 C. Sample purified at NBS,
Gaithersburg, Maryland, USA and is about 99.997% Au.

CAS #: 7440-57-5. Spectrographic analysis (%): Si 0.001,
Ca 0.001, Ag 0.001(?). Opaque mineral optical data on
specimen from unspecified locality: RR2Re=71.6, Disp.=16,
VHN100=53-58, Color values=.384, .391, 72.7, Ref.: IMA
Commission on Ore Microscopy QDF. Cu type. Gold
SuperGroup, 1C-disordered Group. PSC: cF4. Optical data
reference: Winchell, Elements of Optical Mineralogy, 17.
Structural reference: Winchell, Elements of Optical
Mineralogy, 17. Mwt: 196.97. Volume[CD]: 67.85.

Space group of no. 225

Space Group Letter Symbols

Letter symbol	Lattice type	Number of lattice points per unit cell	Coordinates of lattice points
P	P	1	0,0,0
A	<i>A</i> -base centered	2	0,0,0 ; 0, $\frac{1}{2}$, $\frac{1}{2}$
B	<i>B</i> -base centered	2	0,0,0 ; $\frac{1}{2}$,0, $\frac{1}{2}$
C	<i>C</i> -base centered	2	0,0,0 ; $\frac{1}{2}$, $\frac{1}{2}$,0
I	Body centered	2	0,0,0 ; $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$
F	Face centered (all)	4	0,0,0 ; $\frac{1}{2}$, $\frac{1}{2}$,0 ; $\frac{1}{2}$,0, $\frac{1}{2}$; 0, $\frac{1}{2}$, $\frac{1}{2}$
R	Primitive (Rhombohedral axes)	1	0,0,0
	Centered (Hexagonal axes)	3	0,0,0 ; $\frac{2}{3}$, $\frac{1}{3}$, $\frac{1}{3}$; $\frac{1}{3}$, $\frac{2}{3}$, $\frac{2}{3}$ (obverse setting) 0,0,0 ; $\frac{1}{3}$, $\frac{2}{3}$, $\frac{1}{3}$; $\frac{2}{3}$, $\frac{1}{3}$, $\frac{2}{3}$ (reverse setting)
H	Centered Hexagonal	3	0,0,0 ; $\frac{2}{3}$, $\frac{1}{3}$,0 ; $\frac{1}{3}$, $\frac{2}{3}$,0

Symmetry elements in S.G. symbols

Symbol	Lattice type	Comments
m	Mirror plane	reflection
a	Axial glide plane $\perp [010], [001]$	Glide vector $a / 2$
b	Axial glide plane $\perp [001], [100]$	Glide vector $b / 2$
c	Axial glide plane $\perp [100], [010]$ $\perp [1\bar{1}0], [110]$ $\perp [100], [010], [\bar{1}\bar{1}0]$ $\perp [1\bar{1}0], [120], [\bar{2}\bar{1}0], [\bar{1}\bar{1}0]$	Glide vector $c / 2$ Glide vector $c / 2$ Glide vector $c / 2$, hexagonal axes Glide vector $c / 2$, hexagonal axes
n	Diagonal glide plane $\perp [001]; [100]; [010]$ Diagonal glide plane $\perp [1\bar{1}0]; [01\bar{1}]; [\bar{1}01]$ Diagonal glide plane $\perp [110]; [011]; [101]$	Glide vector $\frac{1}{2}(a+b); \frac{1}{2}(b+c); \frac{1}{2}(a+c)$ Glide vector $\frac{1}{2}(a+b+c); \frac{1}{2}(a+c)$ Glide vector $\frac{1}{2}(-a+b+c); \frac{1}{2}(a-b+c); \frac{1}{2}(a+b-c)$
d	Diamond glide plane $\perp [001]; [100]; [010]$ Diamond glide plane $\perp [1\bar{1}0]; [01\bar{1}]; [\bar{1}01]$ Diamond glide plane $\perp [110]; [011]; [101]$	Glide vector $\frac{1}{4}(a \pm b); \frac{1}{4}(b \pm c); \frac{1}{4}(a \pm c)$ Glide vector $\frac{1}{4}(a+b \pm c); \frac{1}{4}(\pm a+b+c); \frac{1}{4}(a \pm b+c)$ Glide vector $\frac{1}{4}(-a+b \pm c); \frac{1}{4}(\pm a-b+c); \frac{1}{4}(a \pm b-c)$
1	None	---
2, 3, 4, 6	n -fold rotation axis	A counter clockwise rotation of $360^\circ / n$
$\bar{1}$	Center of symmetry	---
$\bar{2} = m, \bar{3}, \bar{4}, \bar{6}$	\bar{n} -fold rotoinversion axis	A counter clockwise rotation of $360^\circ / n$ followed by inversion
$2_1, 3_1, 3_2, 4_1,$ $4_2, 4_3, 6_1, 6_2,$ $6_3, 6_4, 6_5$	n -fold screw axis, n_p	A counter clockwise right-handed screw rotation of $360^\circ / n$ followed by translation by $(p / n)T$

The next three symbols

Crystal System	Symmetry Direction		
	Primary	Secondary	Tertiary
Triclinic	None	- - -	- - -
Monoclinic	[010]	- - -	- - -
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	[100] / [010]	[110]
Hexagonal / Trigonal	[001]	[100] / [010]	[120] / [1(-1)0]
Cubic	[100] / [010] / [001]	[111]	[110]

Symmetry of Cubic P-lattice

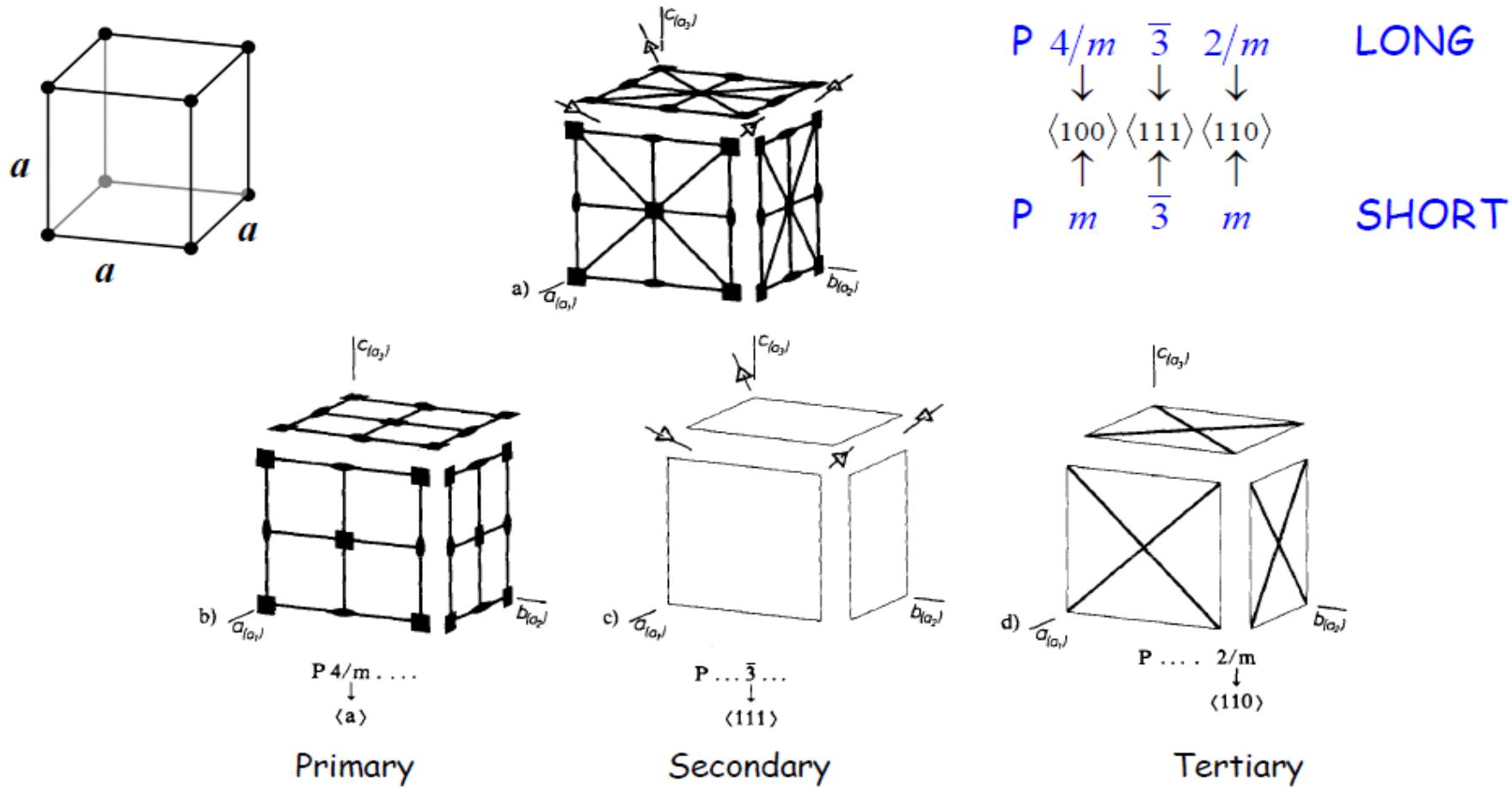


Fig. 6.24. a Space group $P\ 4/m \bar{3} 2/m$. In the other diagrams, only the symmetry elements corresponding to the symmetry directions $\langle a \rangle$, $\langle 111 \rangle$, $\langle 110 \rangle$ are shown.

b $P\ 4/m \dots \dots$, c $P \dots \bar{3} \dots \dots$, d $P \dots \dots 2/m$

$\downarrow \langle a \rangle$ $\downarrow \langle 111 \rangle$ $\downarrow \langle 110 \rangle$

Coordinate systems

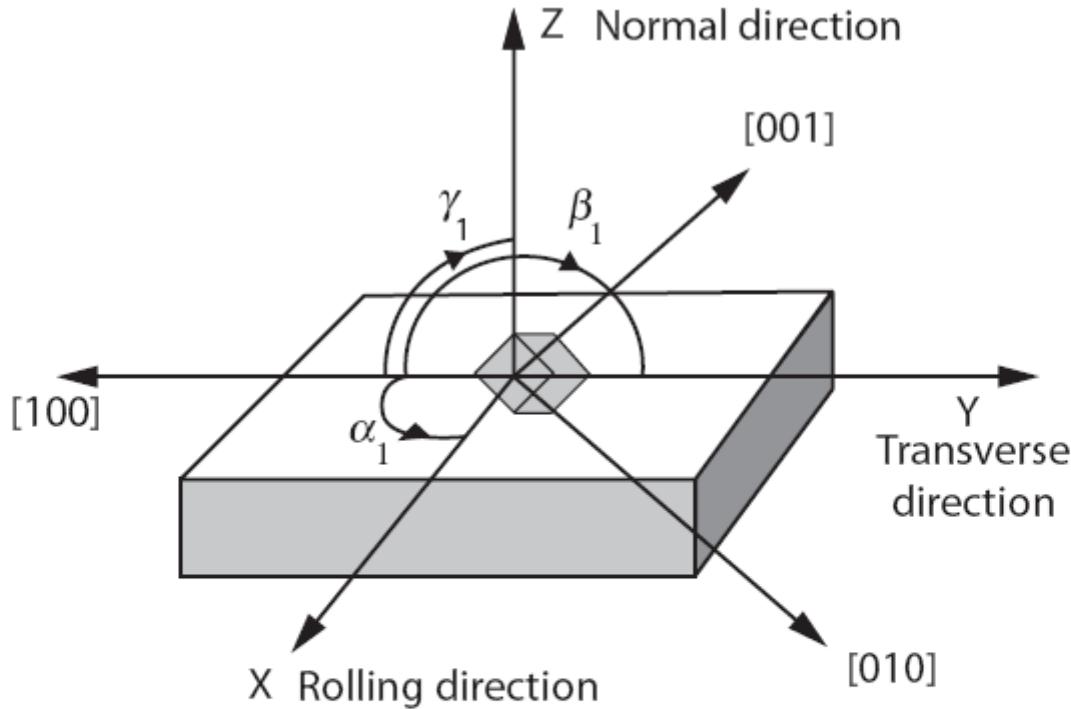


FIGURE 2.4

Relationship between the specimen coordinate system XYZ (or RD, TD, ND for a rolled product) and the crystal coordinate system 100,010,001 where the (cubic) unit cell of one crystal in the specimen is depicted. The cosines of the angles α_1 , β_1 , γ_1 give the first row of the orientation matrix (see text). (Courtesy of K. Dicks.)

Crystal and sample coordinates

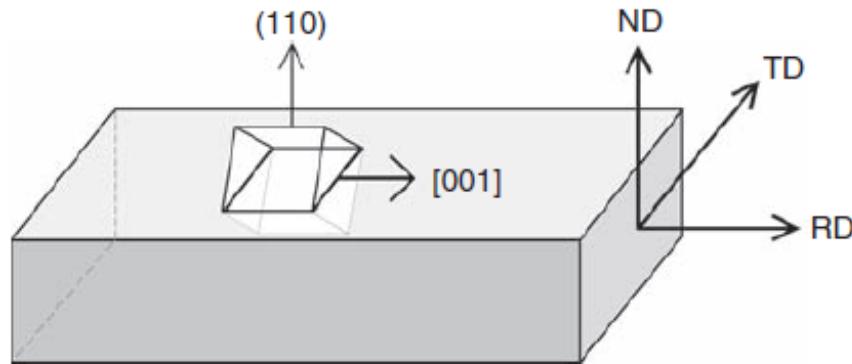


FIGURE 2.7

Schematic illustration of the relationship between the crystal and specimen axes for the (110)[001] Goss orientation, that is, the normal to (110) is parallel to the specimen ND, or Z axis and [001] is parallel to the specimen RD, or X axis.

Orientation descriptions

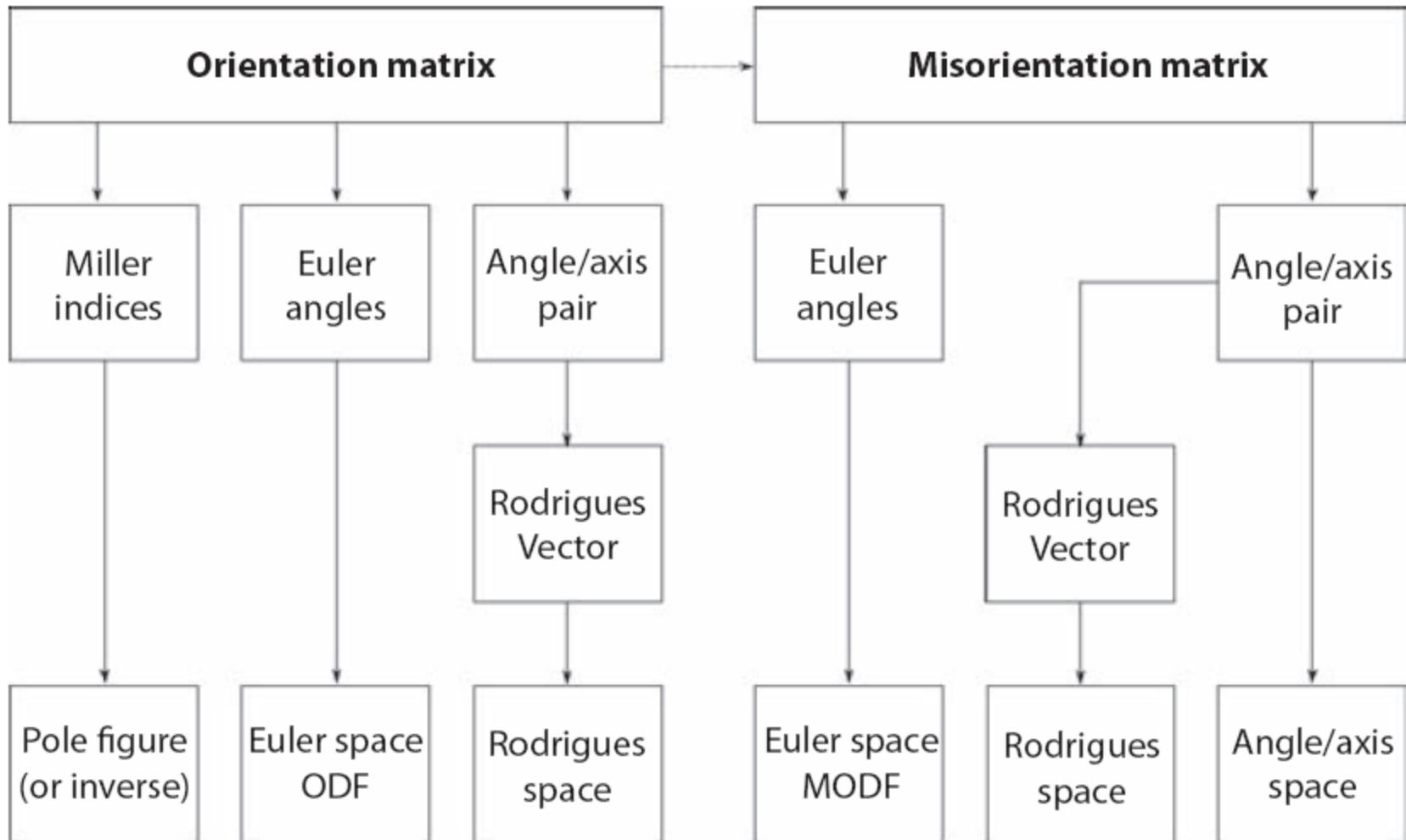
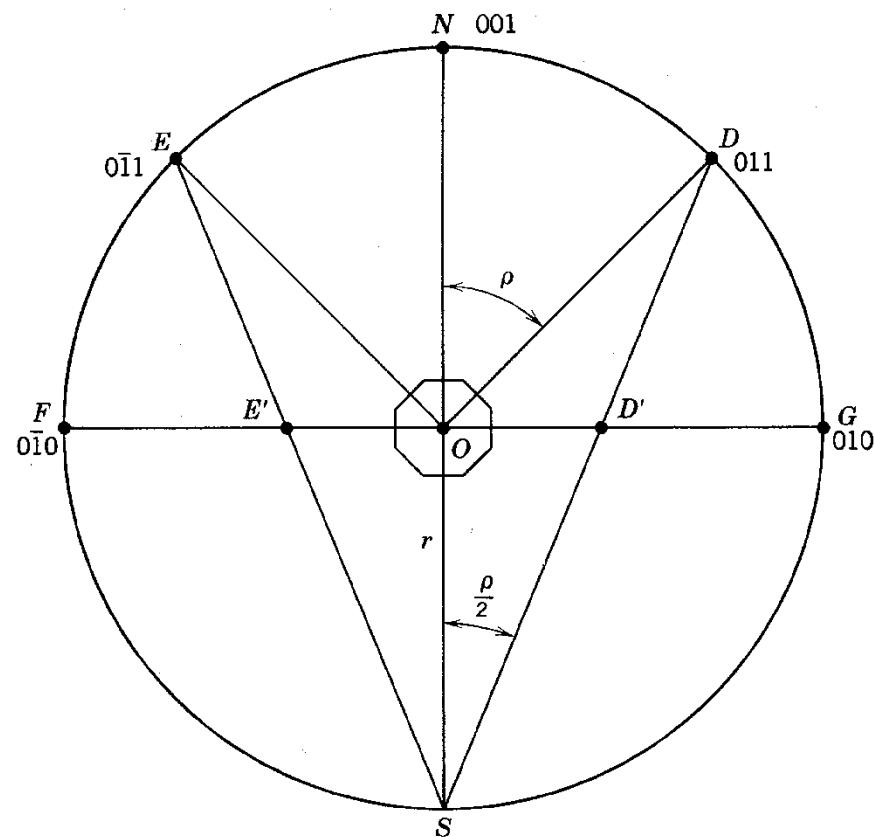


FIGURE 2.6

Relationship between the orientation matrix and the most commonly used orientation descriptors.

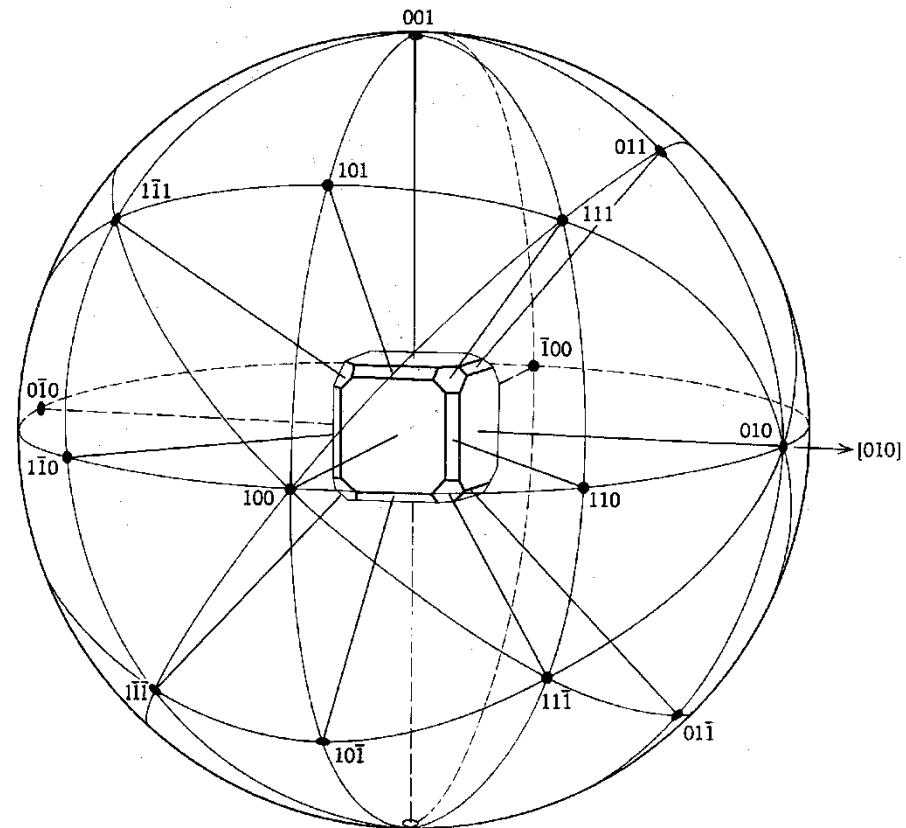
Stereographic projection



D and E are **spherical**

D' and E' are

stereographic

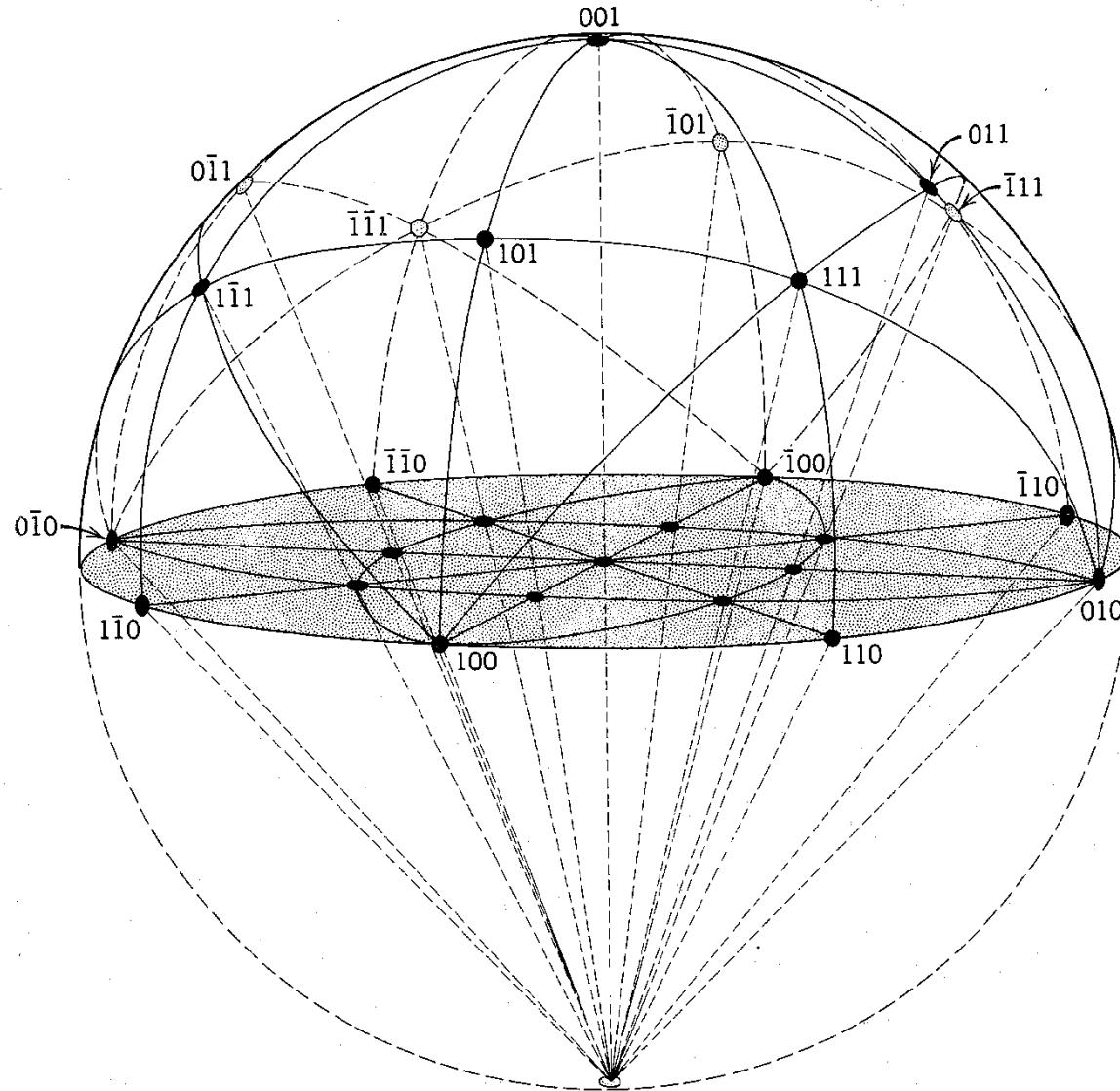


$$\text{Distance } GD' = f(\rho)$$

as $\rho \rightarrow 90^\circ$ $D' \rightarrow G$

as $\rho \rightarrow 0^\circ$ $D' \rightarrow O$

2D Stereographic projection



{100} Pole figure

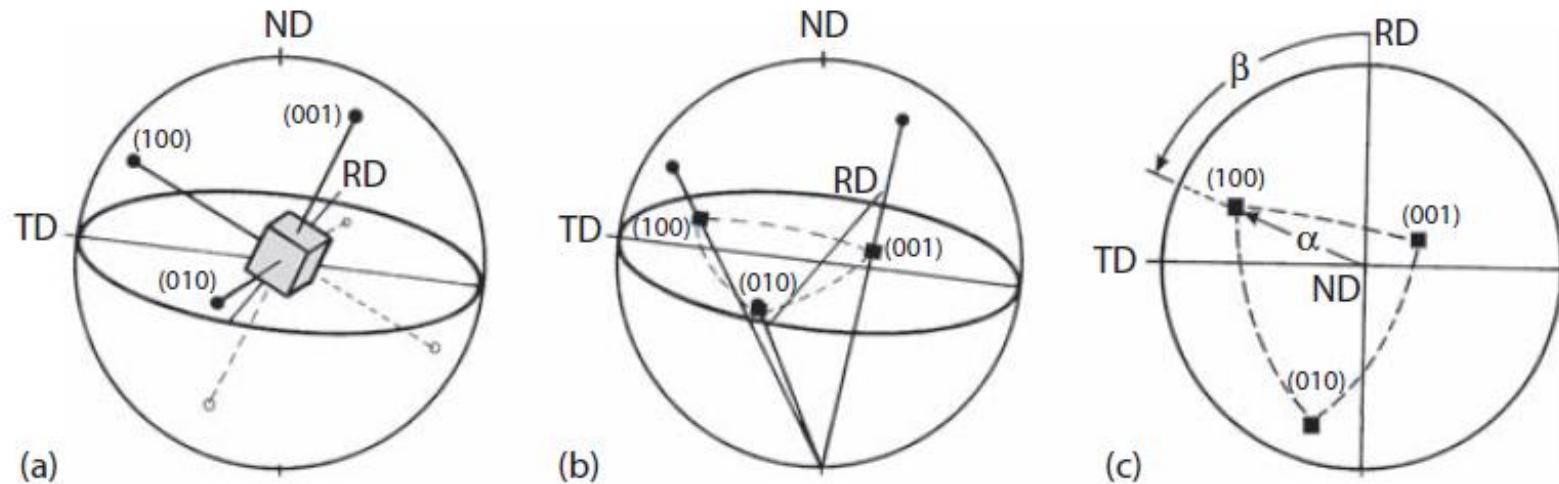
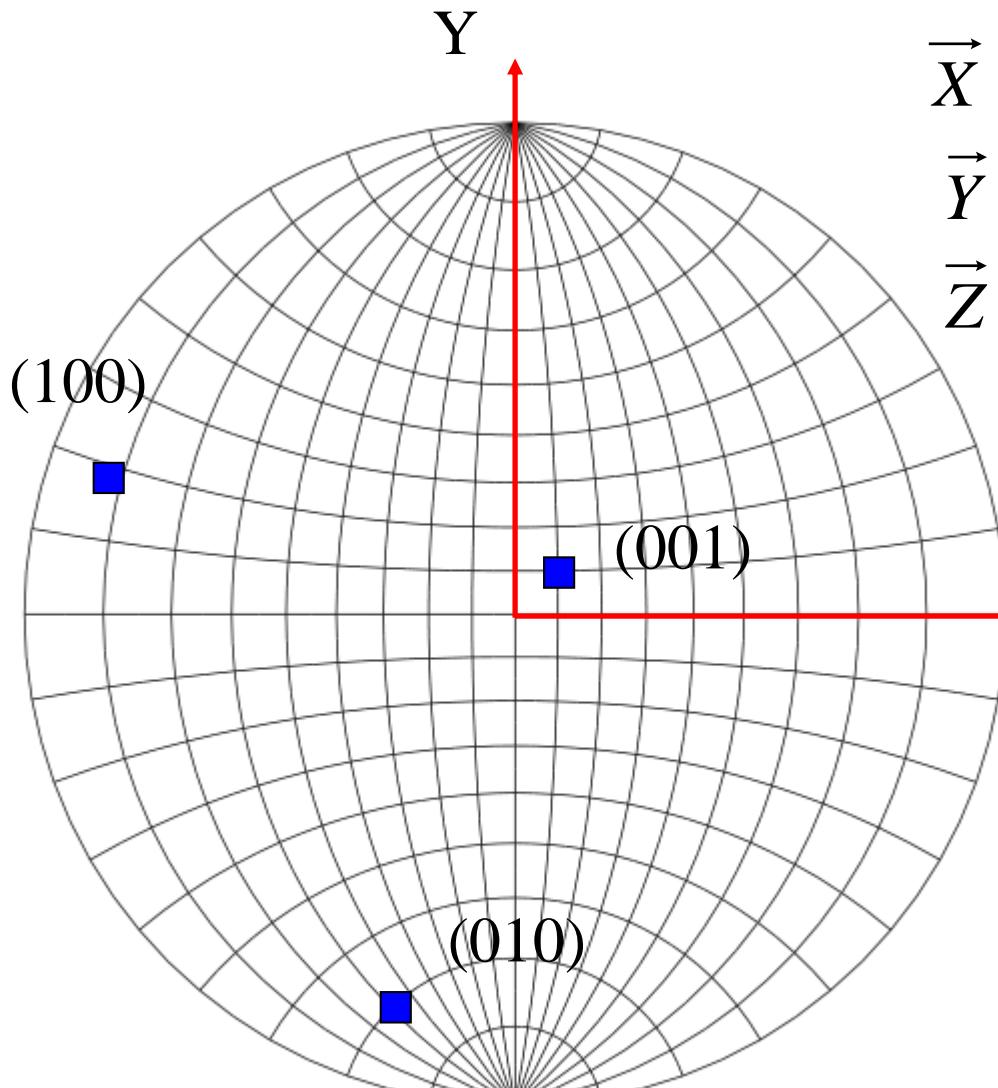


FIGURE 2.9

Presentation of the {100} poles of a cubic crystal in the stereographic projection. (a) Crystal in the unit sphere; (b) projection of the {100} poles onto the equator plane; (c) {100} pole figure and definition of the pole figure angles α and β for the (100) pole.

Indexing sample coordinates



$$\vec{X} = \cos \theta_{X_1} \vec{a} + \cos \theta_{X_2} \vec{b} + \cos \theta_{X_3} \vec{c}$$

$$\vec{Y} = \cos \theta_{Y_1} \vec{a} + \cos \theta_{Y_2} \vec{b} + \cos \theta_{Y_3} \vec{c}$$

$$\vec{Z} = \cos \theta_{Z_1} \vec{a} + \cos \theta_{Z_2} \vec{b} + \cos \theta_{Z_3} \vec{c}$$

$$\vec{Z} = (h_3, k_3, l_3) =$$

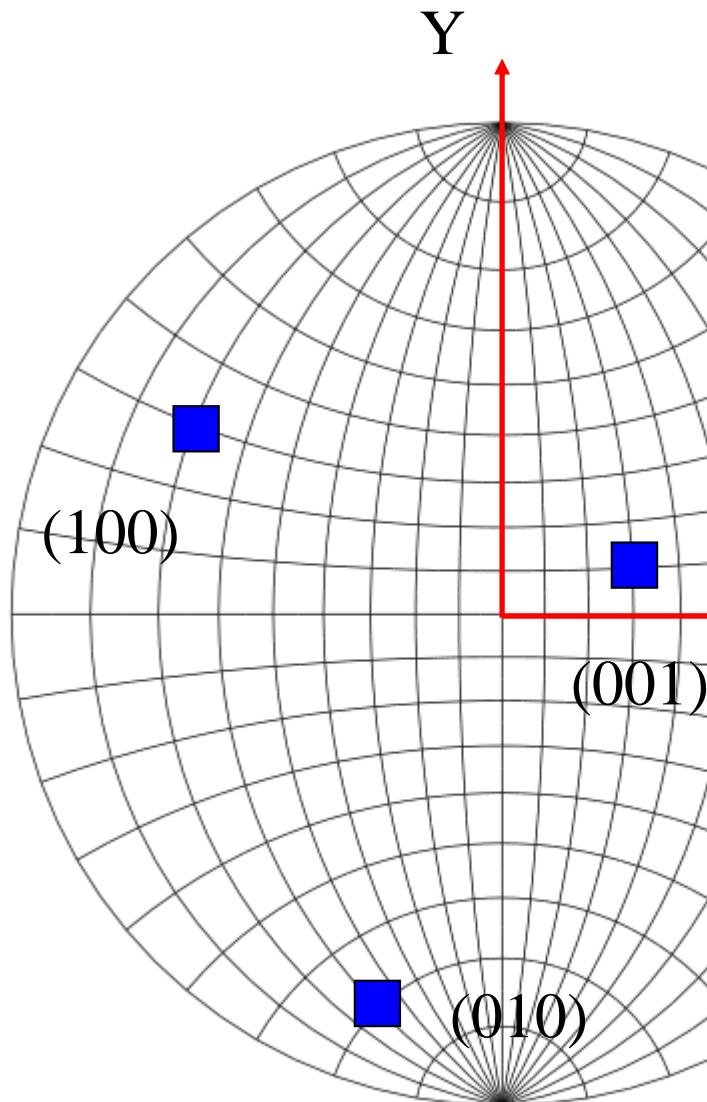
$$\vec{X} = (h_1, k_1, l_1) =$$

$$\cos \theta_{Z_1} =$$

$$\cos \theta_{Z_2} =$$

$$\cos \theta_{Z_3} =$$

Indexing sample coordinates



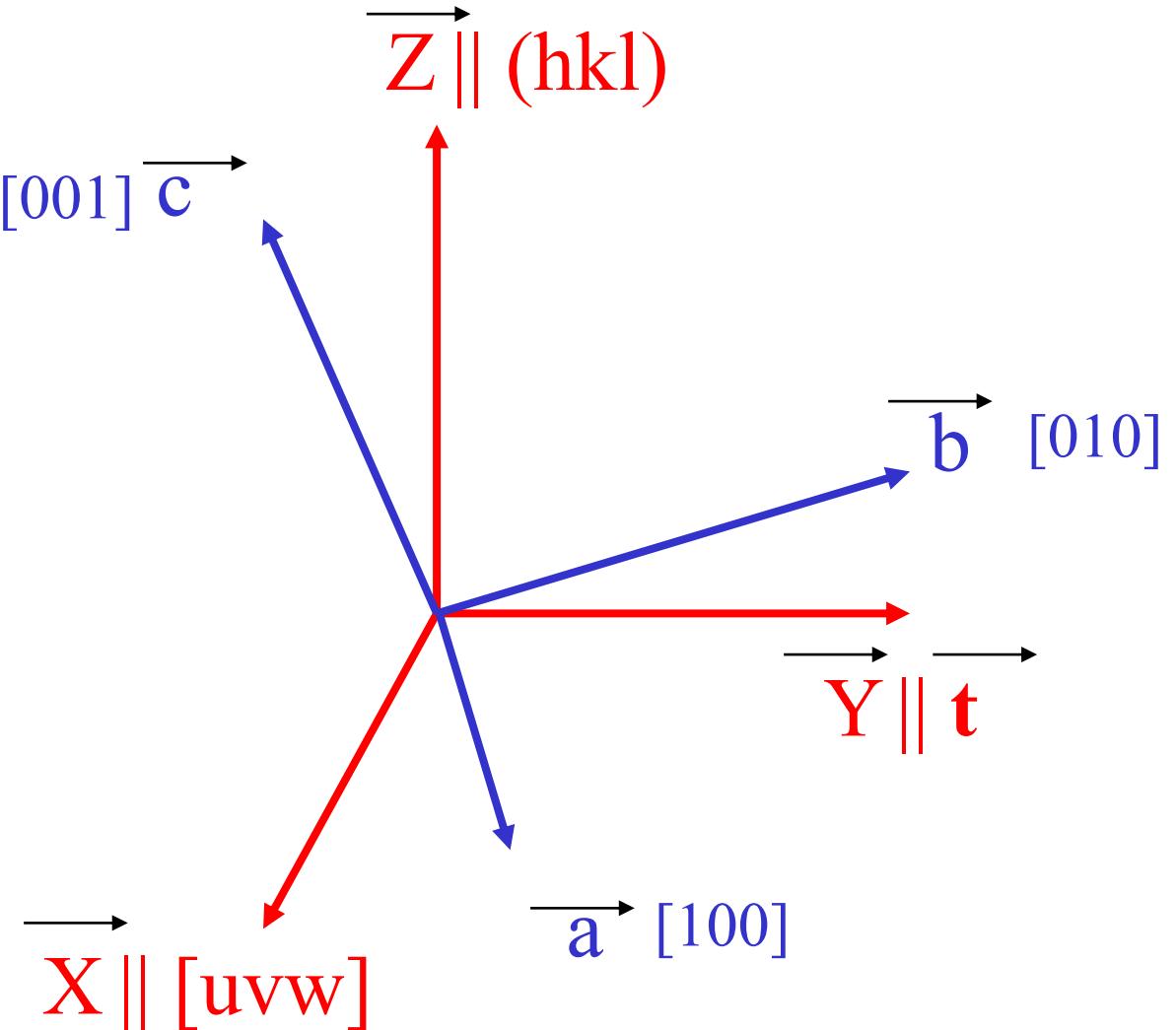
$$\vec{Z} = (2, 3, 15)$$

$$X \quad \vec{X} = (-10, -3, 2)$$

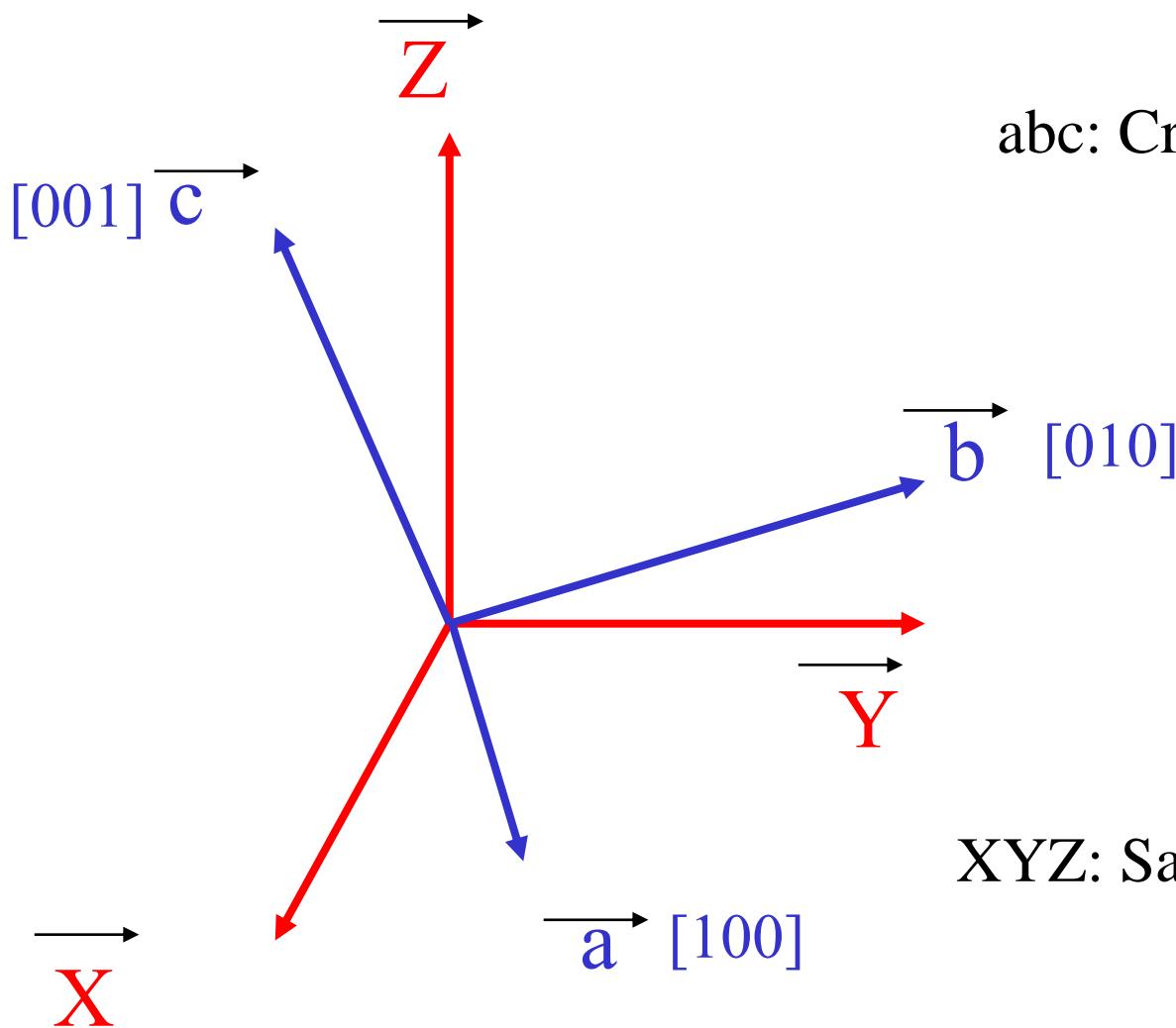
Orientation Description I: $\{hkl\} <uvw>$

Miller index
notation of
texture component
specifies direction
 \parallel to sample axes.

$$T = hkl \times uvw$$



Coordinate Description

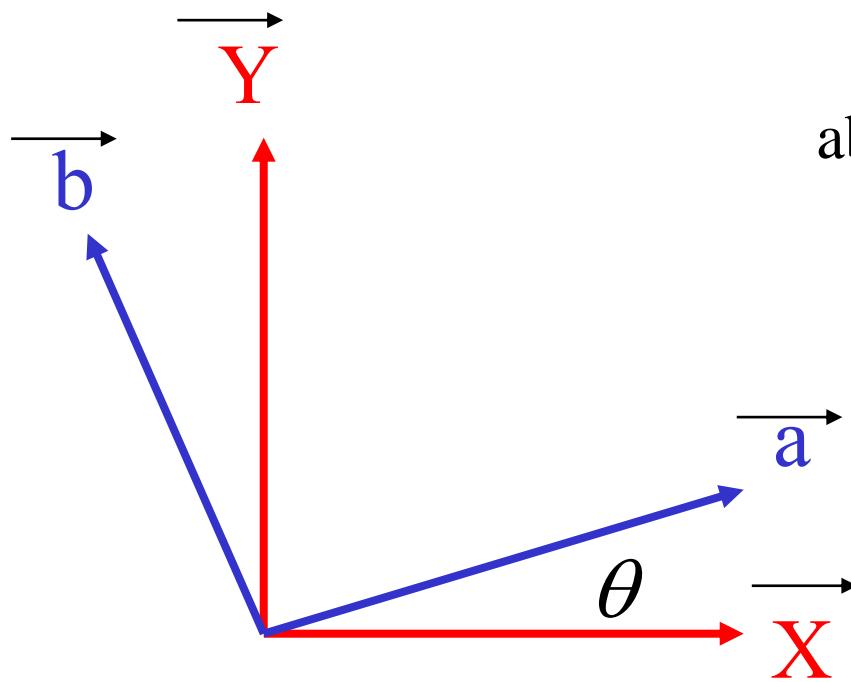


abc: Crystal coordinates

XYZ: Sample coordinates

How to determine the orientation using matrix?

Coordinate Transformation 2D



ab: Crystal coordinates

$$x_0 = l \cos \theta$$

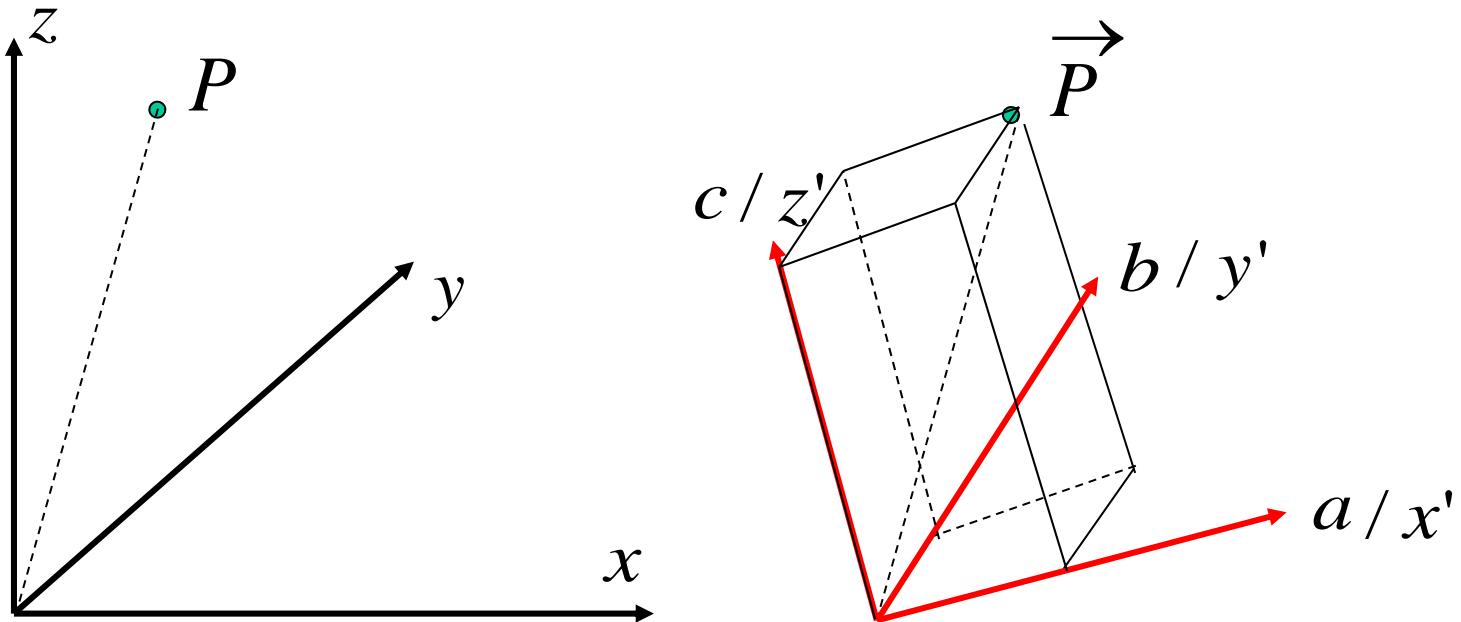
$$y_0 = l \sin \theta$$

$$\theta = \cos^{-1}(x_0 / l)$$

XY: Sample coordinates

What is the transformation matrix?

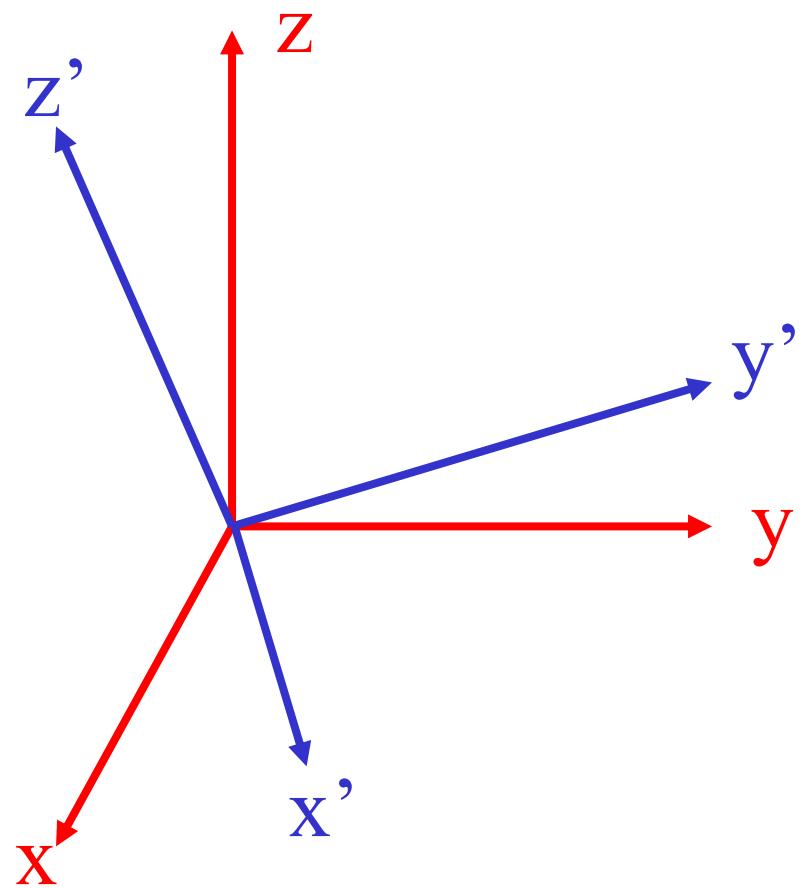
Description of Transformation Matrix



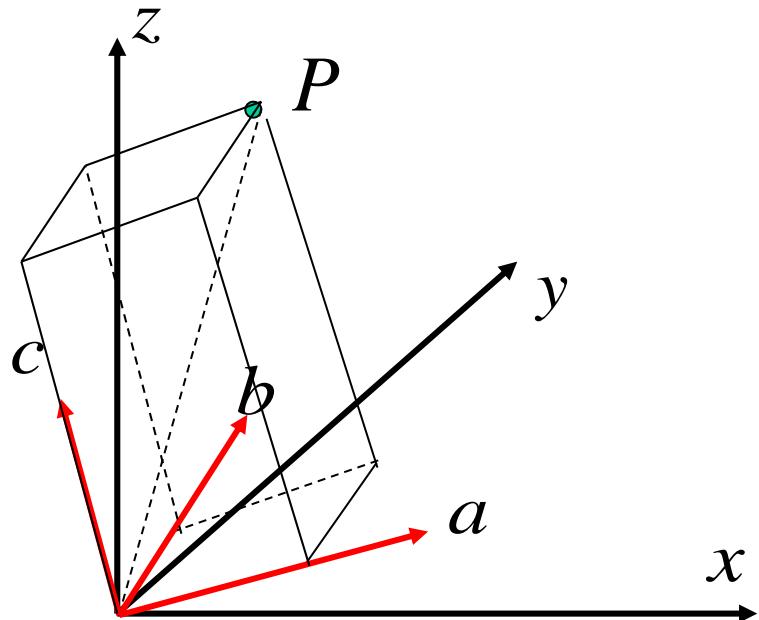
Transformation of Axis

Old coord. to new coord.

$$\begin{array}{ccc} & \text{old} & \\ x' & y' & z' \\ \text{x} & \left(\begin{array}{ccc} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{array} \right) \\ \text{y} \\ \text{z} \end{array}$$



Transformation Matrix



$$\vec{P}_{xyz} = p_x \mathbf{i}_x + p_y \mathbf{j}_y + p_z \mathbf{k}_z$$

$$\vec{P}_{abc} = p_a \mathbf{i}_a + p_b \mathbf{j}_b + p_c \mathbf{k}_c$$

$$P_{abc} = T P_{xyz}$$

$$P = p_x \mathbf{i}_x + p_y \mathbf{j}_y + p_z \mathbf{k}_z$$

$$p_a = \mathbf{i}_a \cdot P = \mathbf{i}_a \cdot \mathbf{i}_x p_x + \mathbf{i}_a \cdot \mathbf{j}_y p_y + \mathbf{i}_a \cdot \mathbf{k}_z p_z$$

$$p_b = \mathbf{j}_b \cdot P = \mathbf{j}_b \cdot \mathbf{i}_x p_x + \mathbf{j}_b \cdot \mathbf{j}_y p_y + \mathbf{j}_b \cdot \mathbf{k}_z p_z$$

$$p_c = \mathbf{k}_c \cdot P = \mathbf{k}_c \cdot \mathbf{i}_x p_x + \mathbf{k}_c \cdot \mathbf{j}_y p_y + \mathbf{k}_c \cdot \mathbf{k}_z p_z$$

Orientation Transformation: S to C

$$\begin{bmatrix} p_a \\ p_b \\ p_w \end{bmatrix} = \begin{bmatrix} \mathbf{i}_a \cdot \mathbf{i}_x & \mathbf{i}_a \cdot \mathbf{j}_y & \mathbf{i}_a \cdot \mathbf{k}_z \\ \mathbf{j}_b \cdot \mathbf{i}_x & \mathbf{j}_b \cdot \mathbf{j}_y & \mathbf{j}_b \cdot \mathbf{k}_z \\ \mathbf{k}_c \cdot \mathbf{i}_x & \mathbf{k}_c \cdot \mathbf{j}_y & \mathbf{k}_c \cdot \mathbf{k}_z \end{bmatrix} \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix}$$

Crystal coordinate

$$C_c = g_{cs} \cdot C_s$$

sample coordinate

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix} \cdot \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Orientation Transformation: C to S

$$p_x = \mathbf{i}_x \cdot P = \mathbf{i}_x \cdot \mathbf{i}_u p_u + \mathbf{i}_x \cdot \mathbf{j}_v p_v + \mathbf{i}_x \cdot \mathbf{k}_w p_w$$

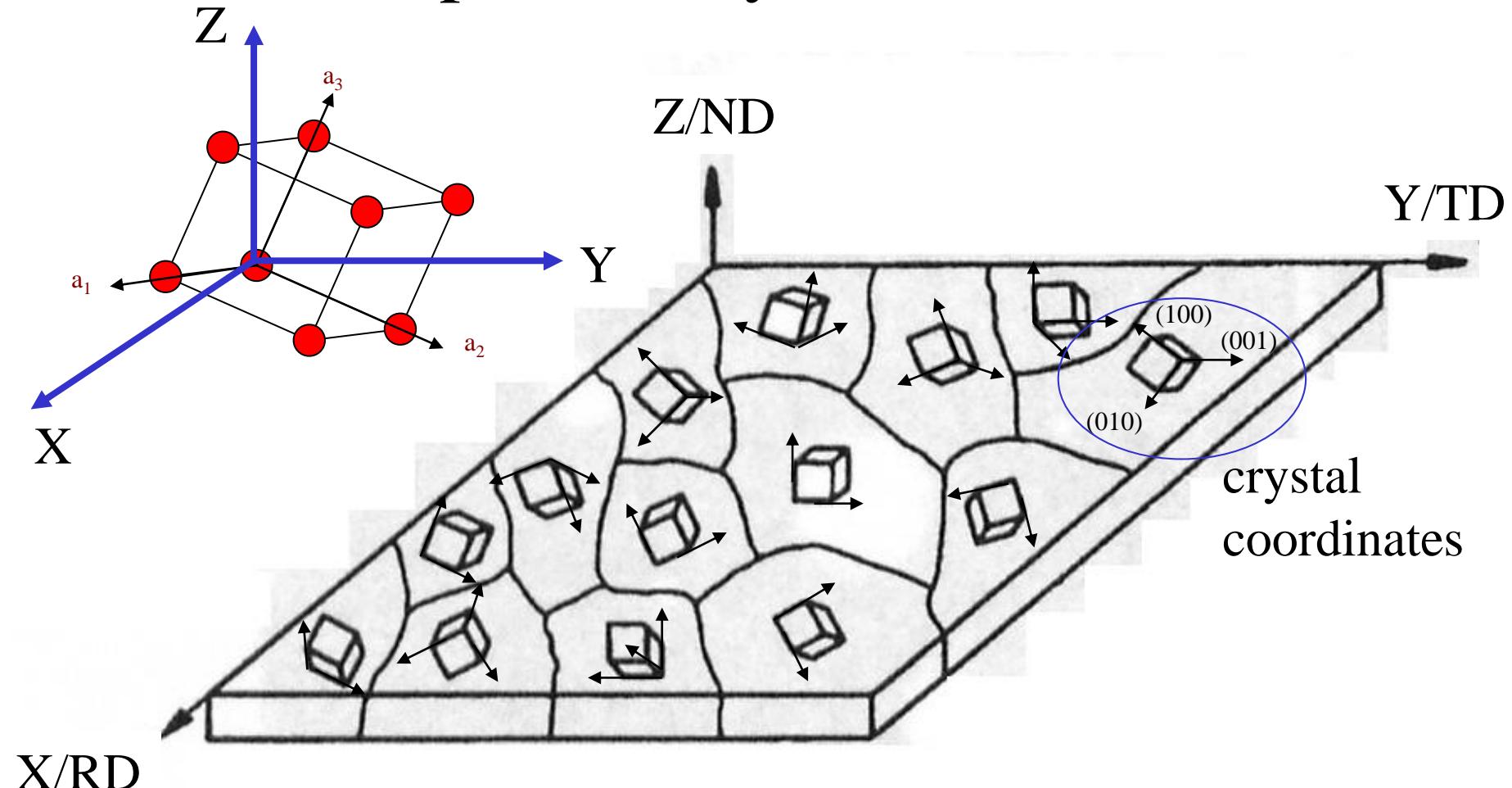
$$p_y = \mathbf{j}_y \cdot P = \mathbf{j}_y \cdot \mathbf{i}_u p_u + \mathbf{j}_y \cdot \mathbf{j}_v p_v + \mathbf{j}_y \cdot \mathbf{k}_w p_w$$

$$p_z = \mathbf{k}_z \cdot P = \mathbf{k}_z \cdot \mathbf{i}_u p_u + \mathbf{k}_z \cdot \mathbf{j}_v p_v + \mathbf{k}_z \cdot \mathbf{k}_w p_w$$

sample coordinate $C_s = g_{cs}^{-1} C_c = g_{cs}^T C_c$ Crystal coordinate

$$\begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} = \begin{bmatrix} \mathbf{i}_x \cdot \mathbf{i}_u & \mathbf{i}_x \cdot \mathbf{j}_v & \mathbf{i}_x \cdot \mathbf{k}_w \\ \mathbf{j}_y \cdot \mathbf{i}_u & \mathbf{j}_y \cdot \mathbf{j}_v & \mathbf{j}_y \cdot \mathbf{k}_w \\ \mathbf{k}_z \cdot \mathbf{i}_u & \mathbf{k}_z \cdot \mathbf{j}_v & \mathbf{k}_z \cdot \mathbf{k}_w \end{bmatrix} \begin{bmatrix} p_u \\ p_v \\ p_w \end{bmatrix}$$

Sample vs. Crystal Coordinates



Sample coordinates (X , Y , Z) are defined as reference coordinates.

<http://aluminium.matter.org.uk/content/html/eng>

Rotation (Orientation) matrix

An orientation is defined as “the position of the crystal coordinate system with respect to the specimen coordinate system”.

$$C_C = g \cdot C_S$$

$$g = \begin{pmatrix} \cos \alpha_1 & \cos \beta_1 & \cos \gamma_1 \\ \cos \alpha_2 & \cos \beta_2 & \cos \gamma_2 \\ \cos \alpha_3 & \cos \beta_3 & \cos \gamma_3 \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix}$$

angle between crystal axis [100] and X

angle between crystal axis [010] with Y

angle between crystal axis [001] with X

Definition of an Axis Transformation:

sample

$$\begin{array}{c}
 \text{crystal} \\
 100 = \begin{pmatrix} \text{RD} & \text{TD} & \text{ND} \\ g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix} \\
 010 = \begin{pmatrix} b_1 & t_1 & n_1 \\ b_2 & t_2 & n_2 \\ b_3 & t_3 & n_3 \end{pmatrix} \\
 001
 \end{array}$$

Sample to Crystal

The diagram illustrates the transformation between sample and crystal coordinate systems. It shows three sets of orthogonal axes: sample axes (red), crystal axes (blue), and intermediate axes (purple).

- Sample Axes:** Represented by red arrows. The vertical axis is labeled \overrightarrow{Z} , the horizontal axis is labeled \overrightarrow{Y} , and the diagonal axis is labeled \overrightarrow{X} .
- Crystal Axes:** Represented by blue arrows. The vertical axis is labeled \overrightarrow{c} and $[001]$. The diagonal axis is labeled \overrightarrow{b} and $[010]$. The horizontal axis is labeled \overrightarrow{a} and $[100]$.
- Intermediate Axes:** Represented by purple arrows. They connect the sample axes to the crystal axes, indicating the orientation of each axis.

The transformation matrix C_c is given by:

$$C_c = g_{cs} \cdot C_s$$

Determination of matrix from Miller Indices

$$\hat{\mathbf{n}} = \frac{(h, k, l)}{\sqrt{h^2 + k^2 + l^2}} \quad \hat{\mathbf{b}} = \frac{(u, v, w)}{\sqrt{u^2 + v^2 + w^2}}$$

$$\hat{\mathbf{t}} = \frac{\hat{\mathbf{n}} \times \hat{\mathbf{b}}}{|\hat{\mathbf{n}} \times \hat{\mathbf{b}}|}$$

Sample

$$g_{ij} = Crystal \begin{pmatrix} b_1 & t_1 & n_1 \\ b_2 & t_2 & n_2 \\ b_3 & t_3 & n_3 \end{pmatrix}$$

Miller Indices vs. Matrix

$$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$$

[100] direction →

[010] direction →

[001] direction →

Miller Indices vs. Matrix

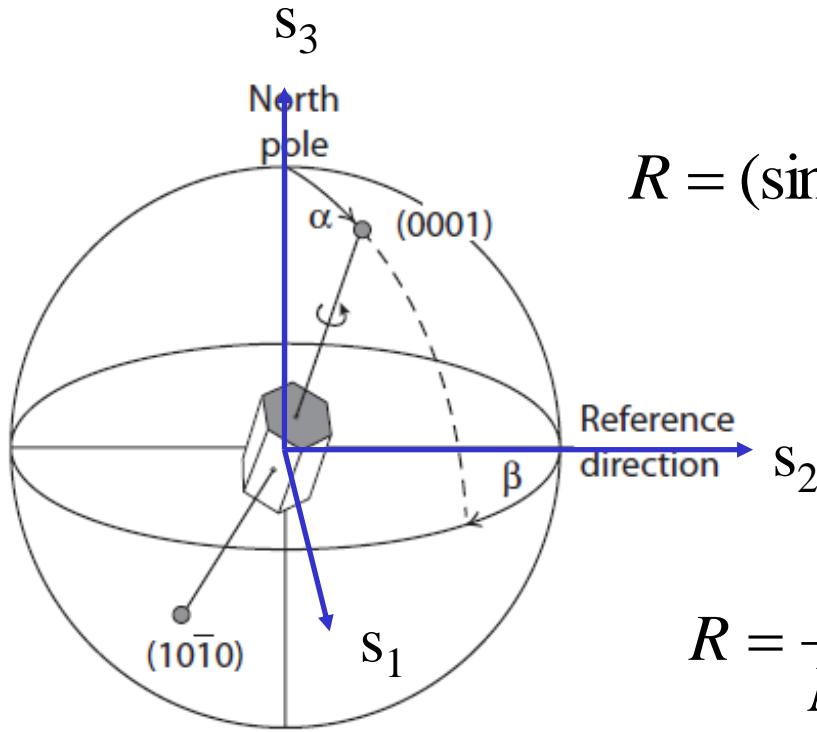
- The *columns* represent components of three other unit vectors:

$$[uvw] \equiv RD \quad TD \quad ND \equiv (hkl)$$

$$\begin{bmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{bmatrix}$$

- Where the Columns are the direction cosines (i.e. hkl or uvw) for the RD, TD and Normal directions in the *crystal coordinate system*.

Orientation of a plane



$$R = (\sin \alpha \cos \beta)s_1 + (\sin \alpha \sin \beta)s_2 + (\cos \alpha)s_3$$

sample coordinates

$$R = \frac{1}{N} (X_{c_1} + Y_{c_2} + Z_{c_3})$$

crystal coordinates

Orientation of the basal plane (0001) in a hexagonal crystal. The position of the (0001) pole on the unit sphere with regard to an external reference frame is described by the two angles α and β . However, since the crystal can still rotate about the (0001) pole, for an unequivocal definition of the orientation of the crystal more information, here the position of the $(10\bar{1}0)$ pole, is required.

Definition of orientation

$$\begin{matrix} \text{sample} \\ \left(\begin{array}{c} \sin \alpha \cos \beta \\ \sin \alpha \sin \beta \\ \cos \alpha \end{array} \right) \end{matrix} = \begin{pmatrix} g_{11} & g_{21} & g_{31} \\ g_{12} & g_{22} & g_{32} \\ g_{13} & g_{23} & g_{33} \end{pmatrix} \cdot \begin{matrix} \text{crystal} \\ \left(\begin{array}{c} X / N \\ Y / N \\ Z / N \end{array} \right) \end{matrix}$$

1. determine the pole figure angles α and β
2. index the pole
3. determine the orientation matrix g

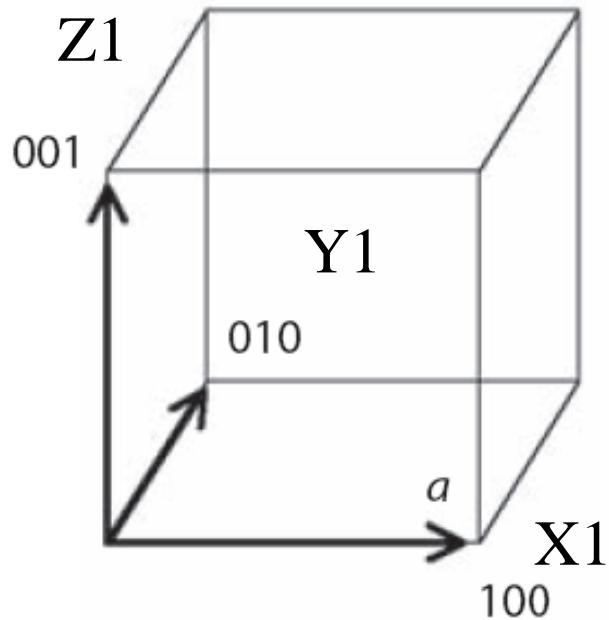
Inverse pole figure

$$s_i = (\sin \gamma_i \cos \delta_i) c_1 + (\sin \gamma_i \sin \delta_i) c_2 + (\cos \gamma_i) c_3$$

$$\begin{matrix} \text{sample} \\ \left(\begin{array}{c} \sin \gamma \cos \delta \\ \sin \gamma \sin \delta \\ \cos \delta \end{array} \right) \end{matrix} = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix} \cdot \begin{matrix} \text{crystal} \\ \left(\begin{array}{c} X_s \\ Y_s \\ Z_s \end{array} \right) \end{matrix}$$

Non-cubic Crystal Coordinate systems

Cubic



$$\vec{b}' = \begin{pmatrix} 0 \\ a \\ 0 \end{pmatrix} = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\vec{b}$$

$$\vec{a}' = \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$\vec{a}$$

$$\vec{c}' = \begin{pmatrix} 0 \\ 0 \\ a \end{pmatrix} = \begin{pmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$\vec{c}$$

orthorhombic

Transformation matrix

$$\nu_C = L \nu_T$$

$$\vec{a}' = \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \vec{a}$$

$$\vec{b}' = \begin{pmatrix} 0 \\ b \\ 0 \end{pmatrix} = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \vec{b}$$

$$\vec{c}' = \begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix} = \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \vec{c}$$

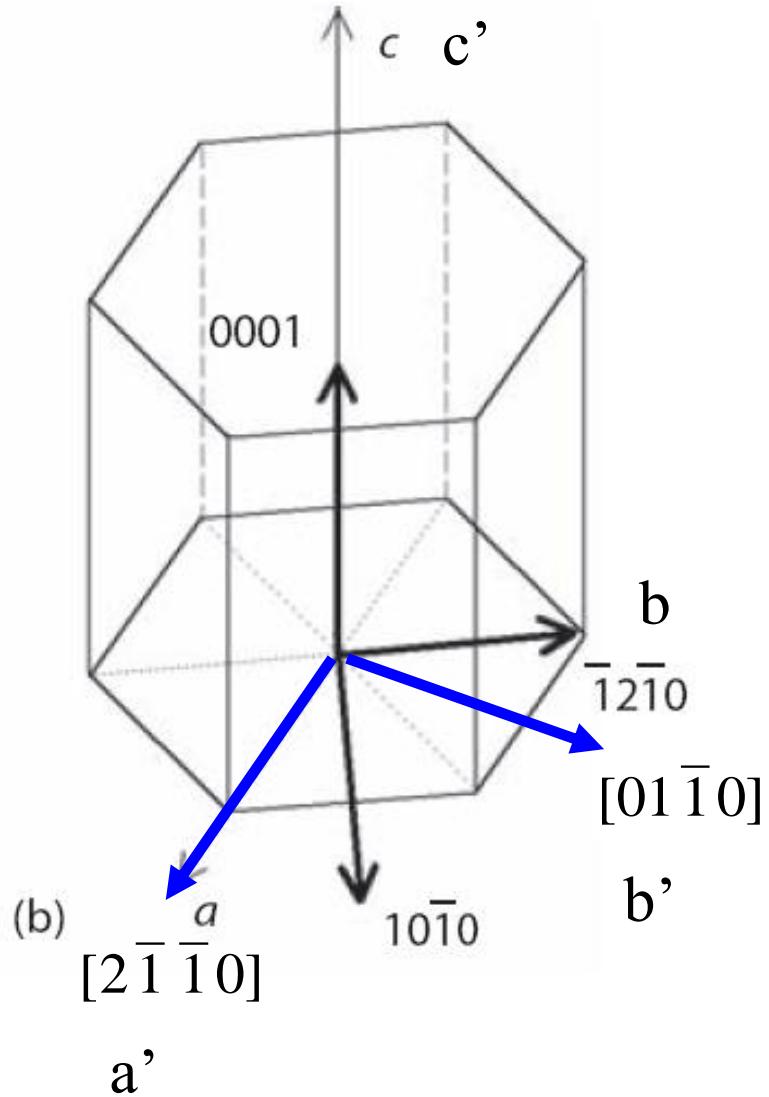
Non-cubic Crystal Coordinate systems

hexagonal

$$\begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} a & -a/2 & 0 \\ 0 & a\sqrt{3}/2 & 0 \\ 0 & 0 & c \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

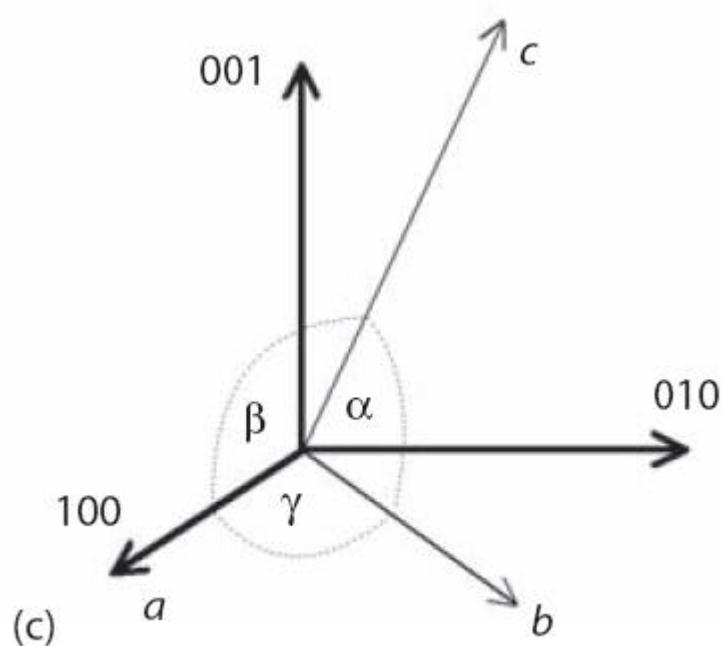
$$\begin{pmatrix} -a/2 \\ a\sqrt{3}/2 \\ 0 \end{pmatrix} = \begin{pmatrix} a & -a/2 & 0 \\ 0 & a\sqrt{3}/2 & 0 \\ 0 & 0 & c \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 0 \\ 0 \\ c \end{pmatrix} = \begin{pmatrix} a & -a/2 & 0 \\ 0 & a\sqrt{3}/2 & 0 \\ 0 & 0 & c \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$



triclinic

Transformation of an zone axis



$$l_{11} = a$$

$$l_{12} = b \cos \gamma$$

$$l_{13} = c \cos \beta$$

$$l_{21} = 0$$

$$l_{22} = b \sin \gamma$$

$$l_{23} = c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma$$

$$l_{31} = 0$$

$$l_{32} = 0$$

$$l_{33} = \left[c(1 + 2 \cos \alpha \cos \beta \cos \gamma - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma)^{1/2} \right] / \sin \gamma$$

$$L = \begin{pmatrix} a & b \cos \gamma & c \cos \beta \\ 0 & b \sin \gamma & c(\cos \alpha - \cos \beta \cos \gamma) / \sin \gamma \\ 0 & 0 & \left[c(1 + 2 \cos \alpha \cos \beta \cos \gamma - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma)^{1/2} \right] / \sin \gamma \end{pmatrix}$$

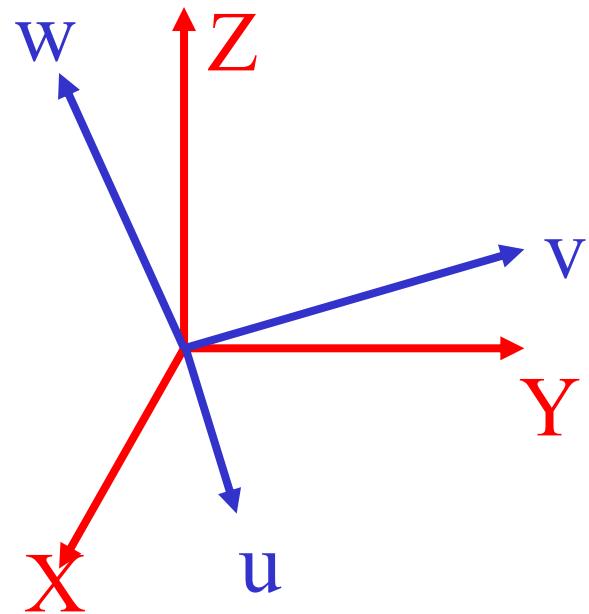
$$\nu_C = L \nu_T$$

Orientation Description II: Bunge Euler angles

Rotation 1 (ϕ_1): rotate axes (anticlockwise) about the (sample) 3 [ND] axis; \mathbf{Z}_1 .

Rotation 2 (Φ): rotate axes (anticlockwise) about the (rotated) 1 axis [100] axis; \mathbf{X} .

Rotation 3 (ϕ_2): rotate axes (anticlockwise) about the (crystal) 3 [001] axis; \mathbf{Z}_2 .



Orientation Description II: Bunge Euler angles

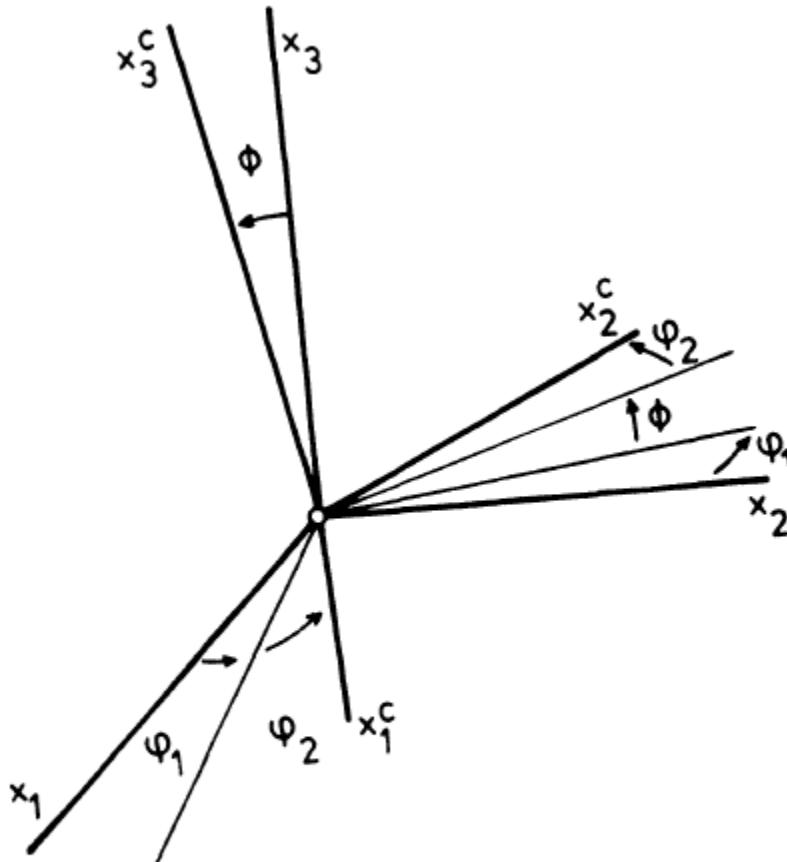
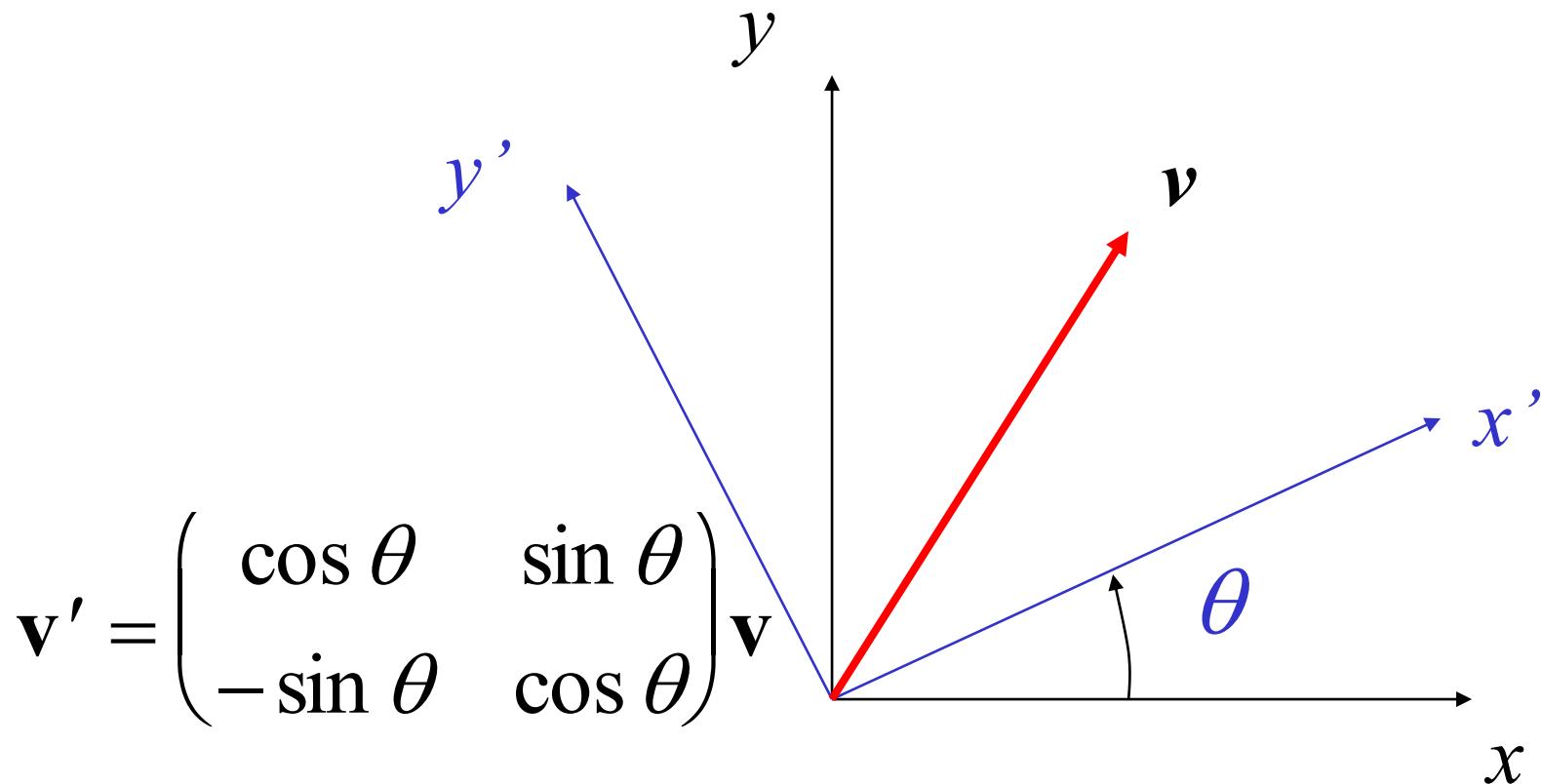


Figure 1 Euler angles used for the description of a crystal orientation. $\langle x_i \rangle$ are the sample axes; for example: x_1 = rolling direction, x_3 = normal direction. $\langle x_i^c \rangle$ are the coordinate axes of the crystal system, e.g. the $\langle 1\ 0\ 0 \rangle$ axes in case of cubic crystal symmetry.

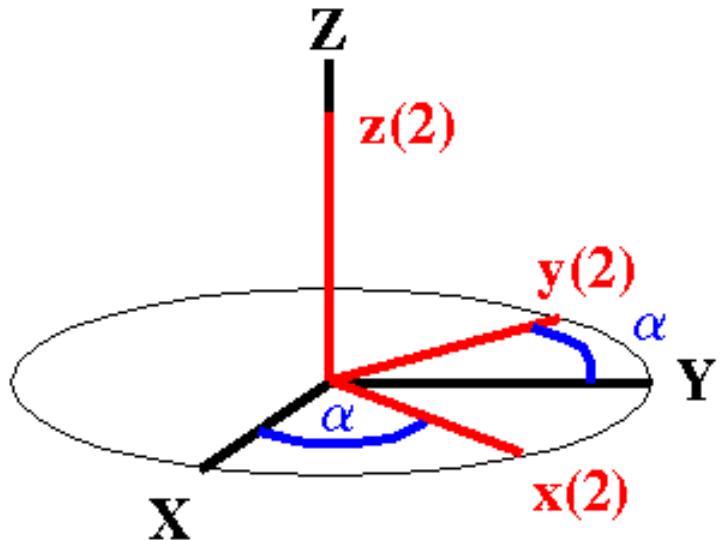
Rotation Matrix in a 2D plane:



N.B. *Passive Rotation/ Transformation of Axes*

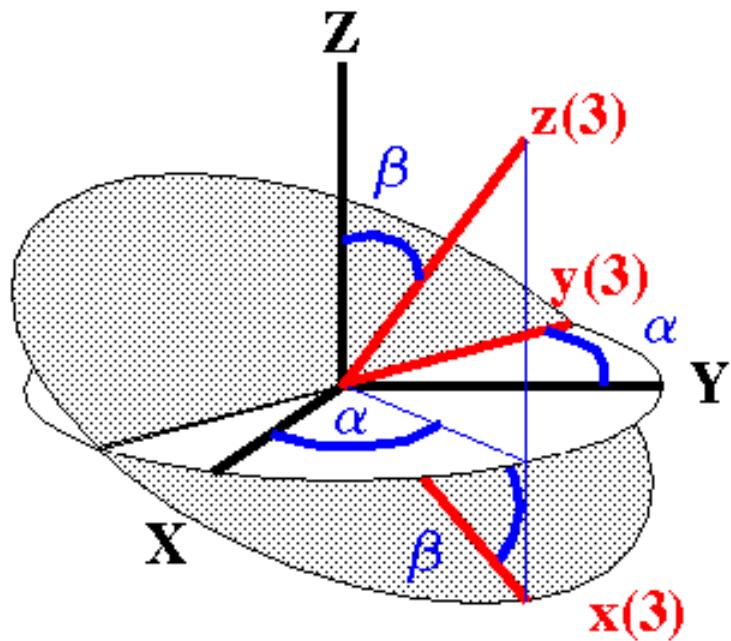
x, y = old axes; x', y' = new axes

Bunge Euler angles to Matrix, 1st Rotation



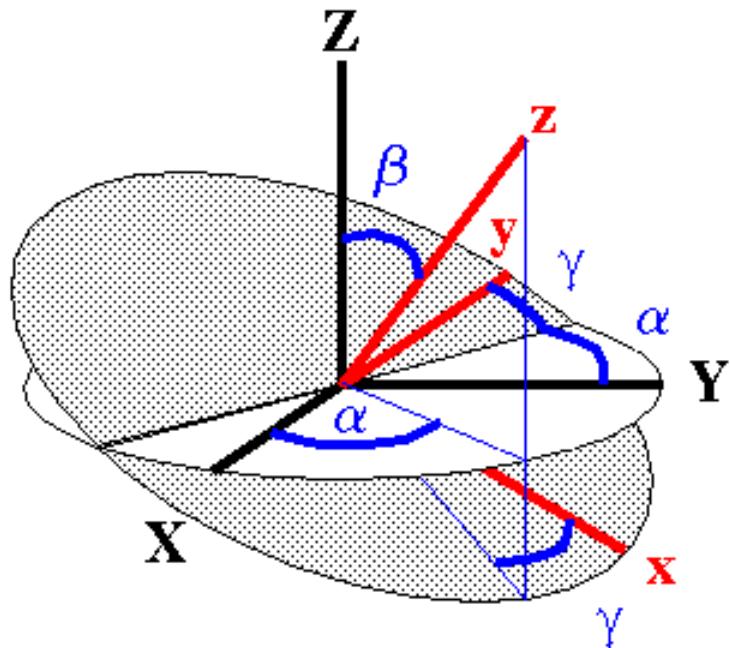
$$g_{\phi_1} = \begin{pmatrix} \cos \phi_1 & \sin \phi_1 & 0 \\ -\sin \phi_1 & \cos \phi_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Bunge Euler angles to Matrix, 2st Rotation



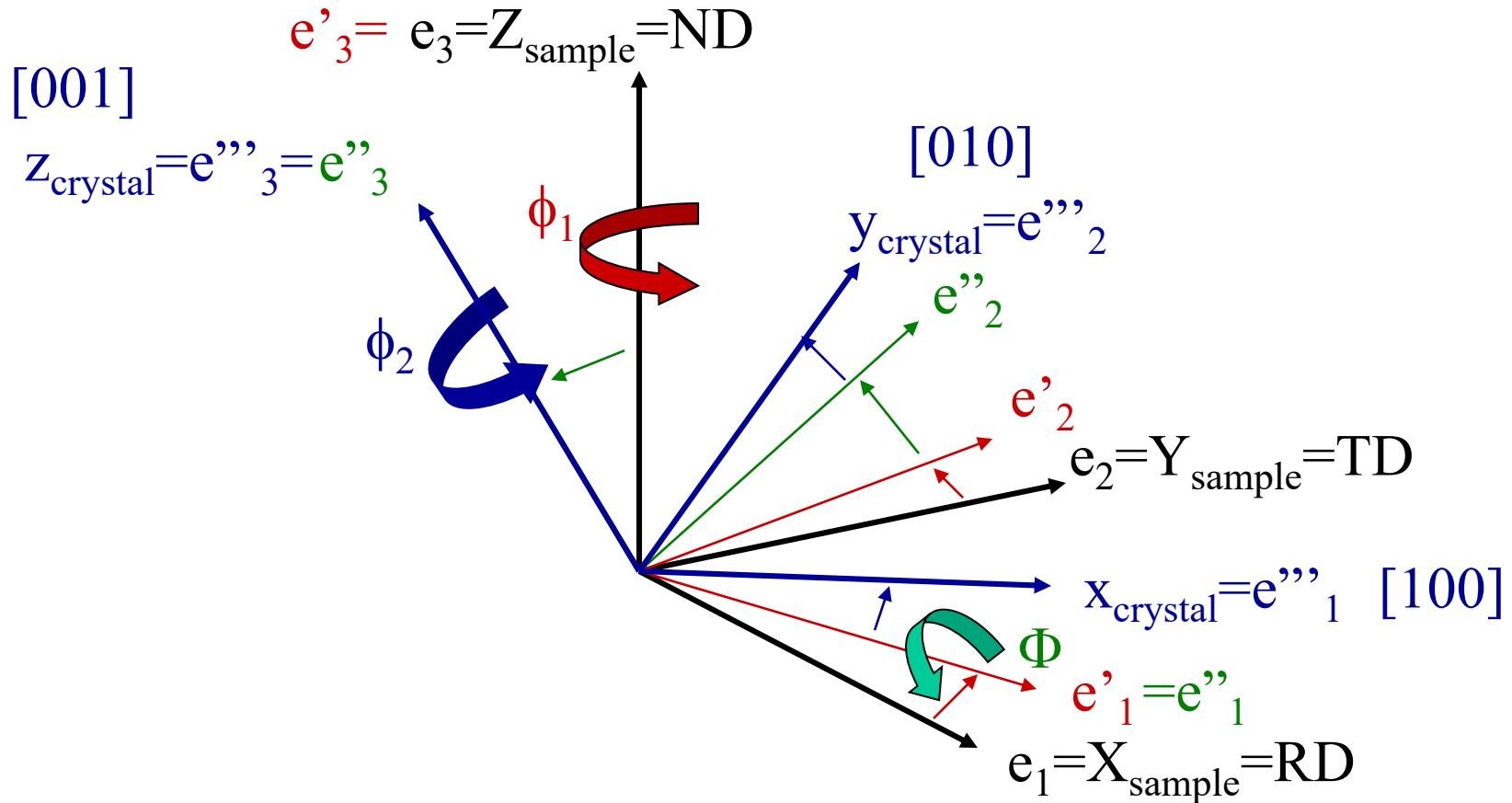
$$g_\Phi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \Phi & \sin \Phi \\ 0 & -\sin \Phi & \cos \Phi \end{pmatrix}$$

Bunge Euler angles to Matrix, 3st Rotation



$$g_{\phi_2} = \begin{pmatrix} \cos \phi_2 & \sin \phi_2 & 0 \\ -\sin \phi_2 & \cos \phi_2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Principle of Bunge Euler Angles



<http://www.youtube.com/watch?v=ImPBVQJRSwY&feature=related>

Bunge Angles vs. Matrix

$$g = g_{\varphi_2} \cdot g_{\Phi} \cdot g_{\varphi_1}$$

[uvw]

$$\cos \varphi_1 \cos \varphi_2$$

$$-\sin \varphi_1 \sin \varphi_2 \cos \Phi$$

$$-\cos \varphi_1 \sin \varphi_2$$

$$-\sin \varphi_1 \cos \varphi_2 \cos \Phi$$

$$\sin \varphi_1 \sin \Phi$$

$$\sin \varphi_1 \cos \varphi_2$$

$$+\cos \varphi_1 \sin \varphi_2 \cos \Phi$$

$$-\sin \varphi_1 \sin \varphi_2$$

$$+\cos \varphi_1 \cos \varphi_2 \cos \Phi$$

$$-\cos \varphi_1 \sin \Phi$$

(hkl)

$$\sin \varphi_2 \sin \Phi$$

$$\cos \varphi_2 \sin \Phi$$

$$\cos \Phi$$

Summary of Orientation Descriptions

$$a_{ij} = \text{Crystal} \begin{pmatrix} b_1 & t_1 & n_1 \\ b_2 & t_2 & n_2 \\ b_3 & t_3 & n_3 \end{pmatrix} = \begin{pmatrix} \cos \varphi_1 \cos \varphi_2 & \sin \varphi_1 \cos \varphi_2 \\ -\sin \varphi_1 \sin \varphi_2 \cos \Phi & +\cos \varphi_1 \sin \varphi_2 \cos \Phi \\ -\cos \varphi_1 \sin \varphi_2 & -\sin \varphi_1 \sin \varphi_2 \\ -\sin \varphi_1 \cos \varphi_2 \cos \Phi & +\cos \varphi_1 \cos \varphi_2 \cos \Phi \\ \sin \varphi_1 \sin \Phi & -\cos \varphi_1 \sin \Phi \end{pmatrix} \begin{pmatrix} \sin \varphi_2 \sin \Phi \\ \cos \varphi_2 \sin \Phi \\ \cos \varphi_2 \end{pmatrix}$$

Sample

Miller indices from Euler angle matrix

Compare the
indices matrix
with the Euler
angle matrix.

$$h = n \sin \Phi \sin \varphi_2$$

$$k = n \sin \Phi \cos \varphi_2$$

$$l = n \cos \Phi$$

$$u = n' (\cos \varphi_1 \cos \varphi_2 - \sin \varphi_1 \sin \varphi_2 \cos \Phi)$$

$$v = n' (-\cos \varphi_1 \sin \varphi_2 - \sin \varphi_1 \cos \varphi_2 \cos \Phi)$$

$$w = n' \sin \Phi \sin \varphi_1$$

n, n' = factors to make integers

Euler angles from Miller indices

Inversion of
the previous
relations:

$$\cos \Phi = \frac{l}{\sqrt{h^2 + k^2 + l^2}}$$

$$\cos \varphi_2 = \frac{k}{\sqrt{h^2 + k^2}}$$

$$\sin \varphi_1 = \frac{w}{\sqrt{u^2 + v^2 + w^2}} \frac{\sqrt{h^2 + k^2 + l^2}}{\sqrt{h^2 + k^2}}$$

Caution: it is more reliable to go from Miller indices to an orientation matrix, and *then* calculate the Euler angles. Extra credit: show that the following surmise is correct. If a plane, hkl , is chosen in the lower hemisphere, $l < 0$, show that the Euler angles are *incorrect*.

Other Euler angle definitions

- A confusing aspect of texture analysis is that there are multiple definitions of the Euler angles.
- Definitions according to *Bunge*, *Roe* and *Kocks* are in common use.
- Components have *different values of Euler angles* depending on which definition is used.
- The *Bunge* definition is the most common.
- The differences between the definitions are based on differences in the sense of rotation, and the choice of rotation axis for the second angle.

3D Euler space

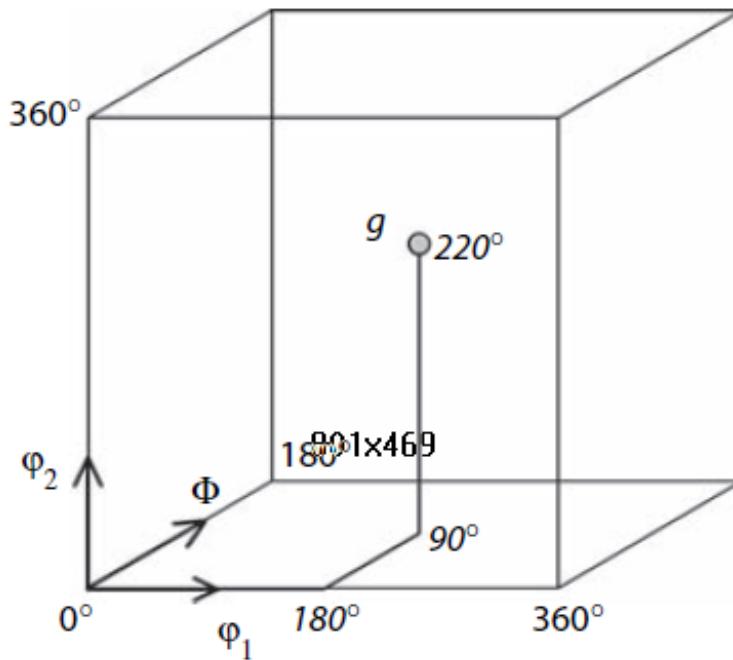


FIGURE 2.11

Representation of orientations in a three-dimensional orientation space defined by the Euler angles. Each orientation g corresponds to a point in the Euler space whose coordinates are given by the three Euler angles $\varphi_1, \Phi, \varphi_2$ describing the orientation (Bunge's convention).

3D Euler space

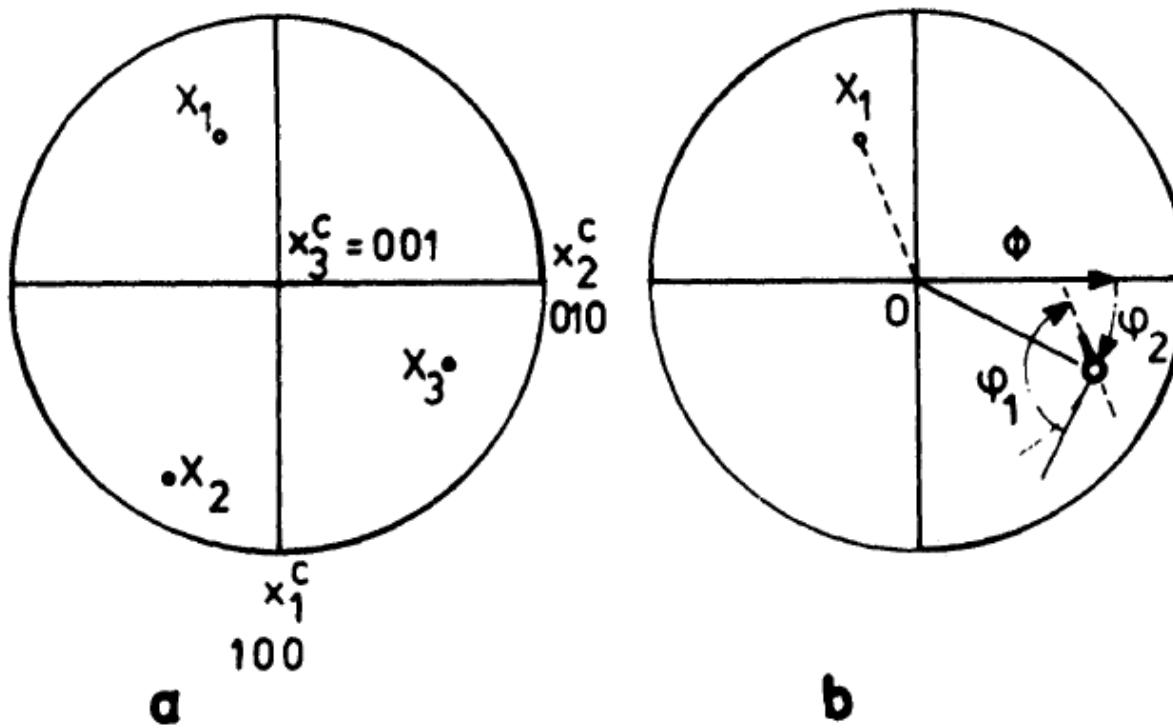


Figure 3 Inverse pole figure representation of a crystal orientation (example for cubic metals). (a) The three specimen axes are plotted in a (001) standard projection. (b) The representation of the axis x_3 depends only on the Euler angles Φ and ϕ_2 , used as polar coordinates. This is also true for non-cubic lattice symmetries.

Sample and crystal symmetries

Size of the Euler Space Necessary to Represent Unequivocally Orientations for Different Sample and Crystal Symmetries

Crystal System	Laue Class	Crystal Symmetry	Sample Symmetry		
			Φ	φ_2	Orthonormal φ_1
Triclinic	$\bar{1}$	180°	360°		
Monoclinic	$2/m$	180°	180°		
Orthorhombic	mmm	90°	180°		
Trigonal	$\bar{3}$	180°	120°		
	$\bar{3}m$	90°	120°	90°	180°
Tetragonal	$4/m$	180°	90°		
	$4/mmm$	90°	90°		
Hexagonal	$6/m$	180°	60°		
	$6/mmm$	90°	60°		
Cubic	$m\bar{3}$	90° ^a	180°		
	$m\bar{3}m$	90° ^a	90°		

^aThreefold symmetry due to $120^\circ\langle 111 \rangle$ symmetry.

Symmetry element

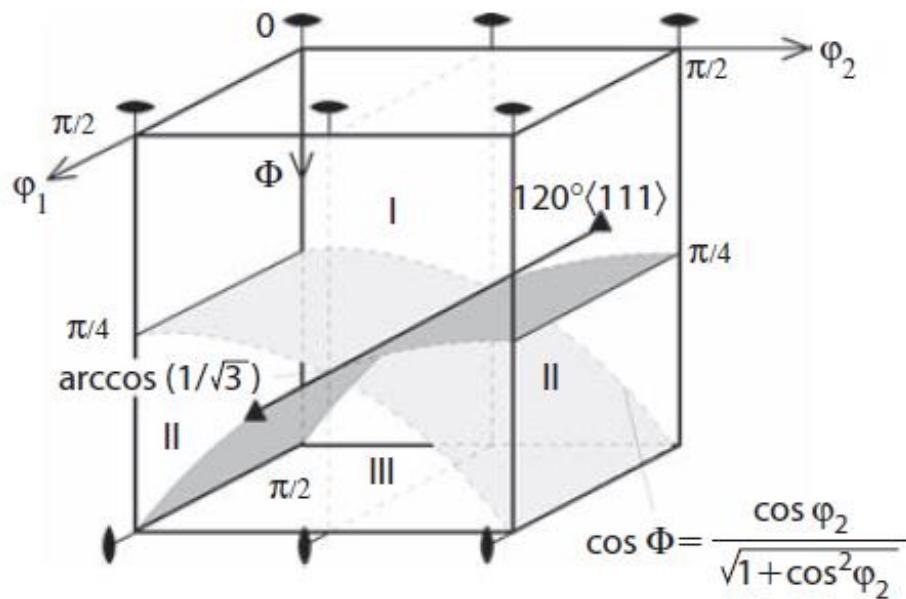
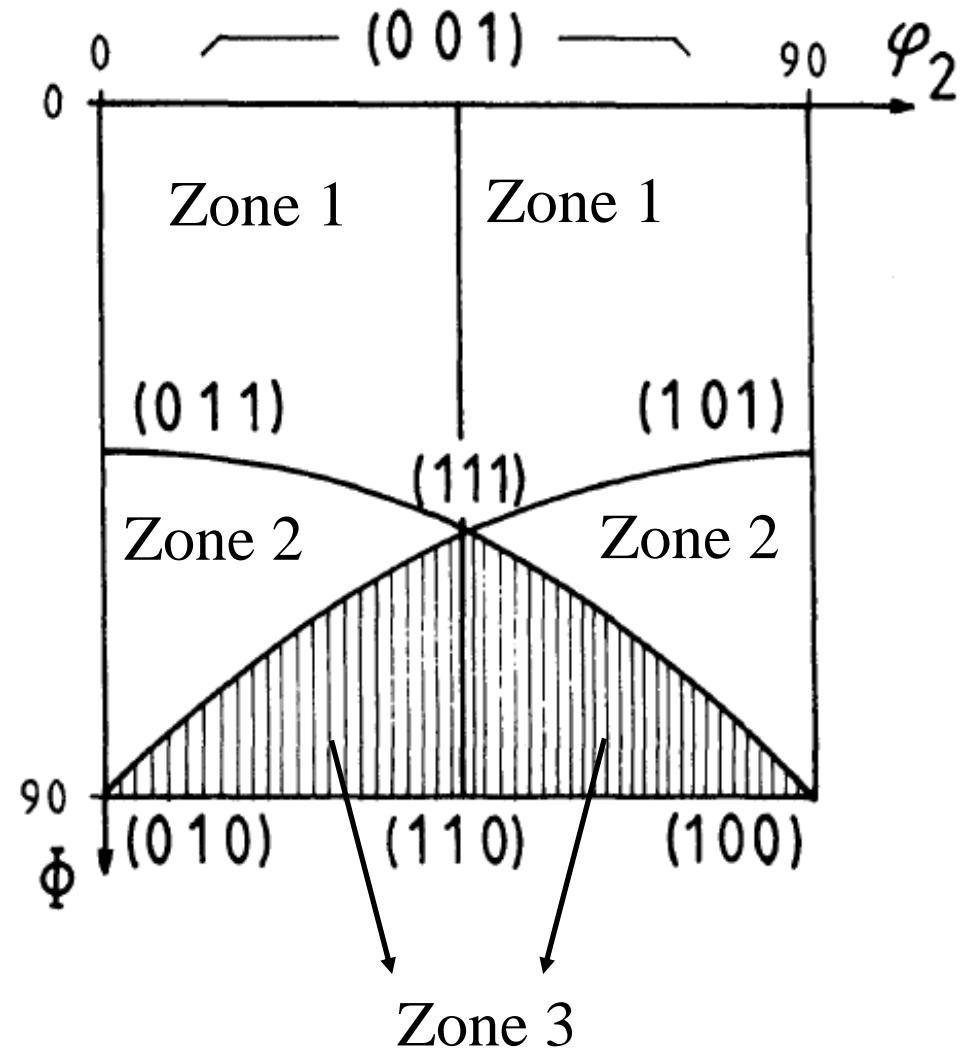
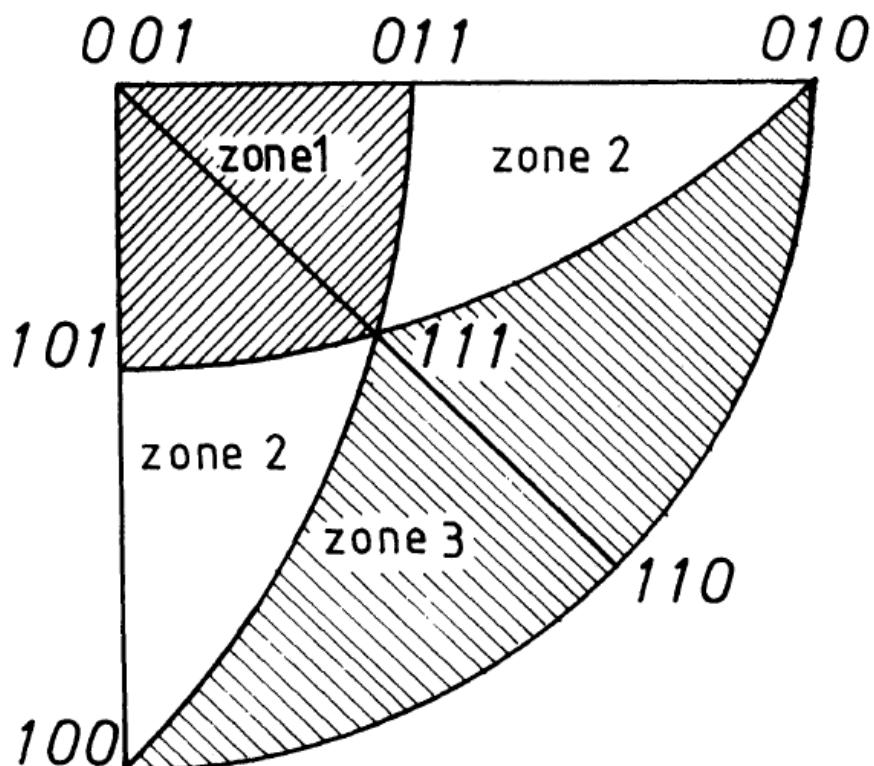


FIGURE 2.12

Symmetry elements in the Euler space for cubic crystal symmetry and orthonormal sample symmetry.

Symmetry element



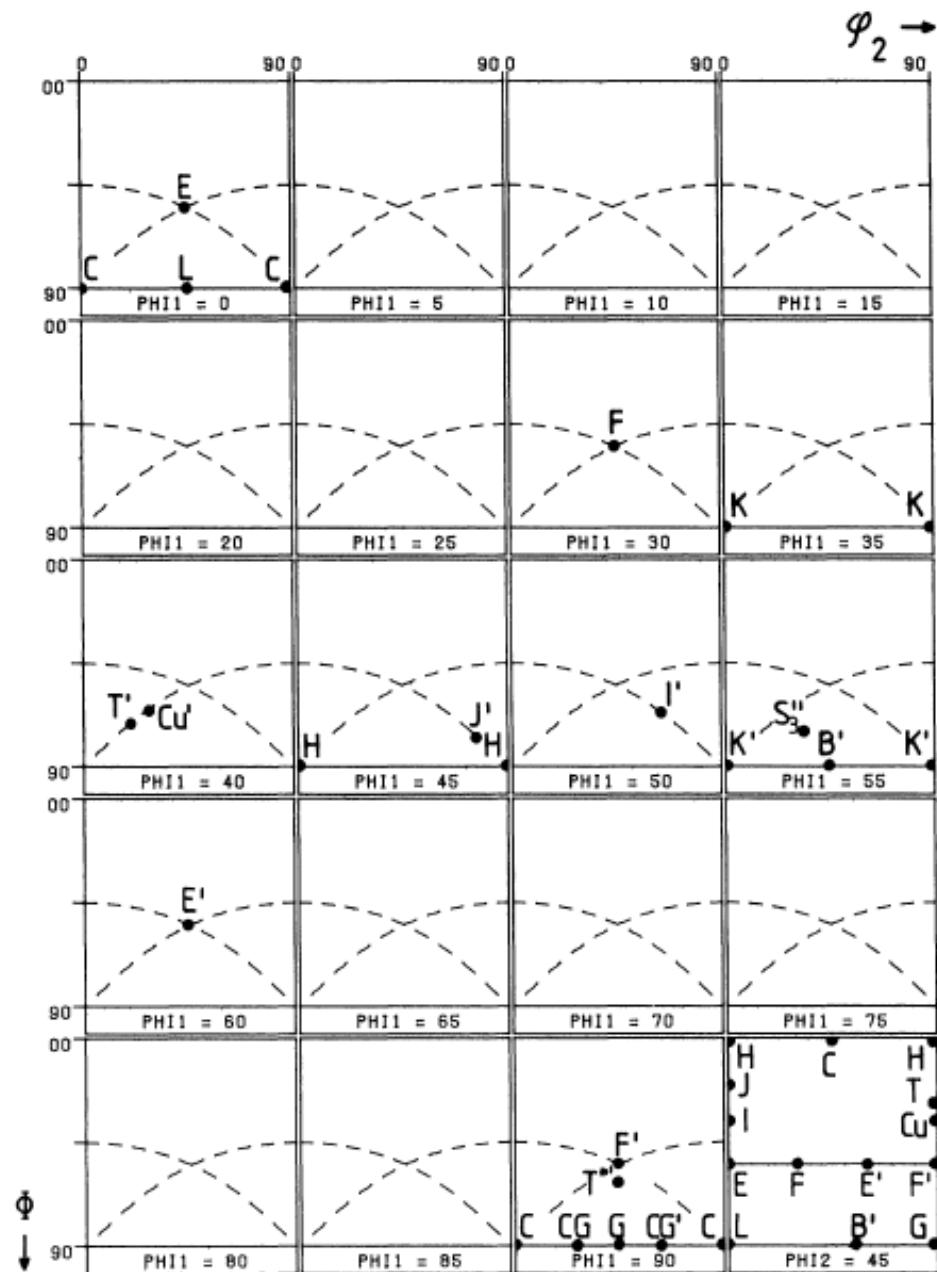


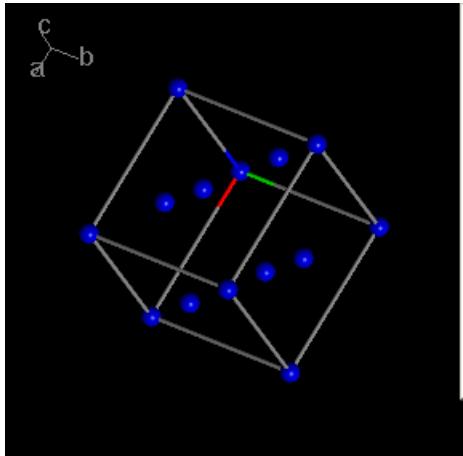
Figure 6 Euler diagram consisting of 19 $\phi_1 = \text{constant}$ sections and a $\phi_2 = 45^\circ$ section. The zone 3 representation of various frequently used crystal orientations are shown (case of cubic crystal symmetry), except in the $\phi_2 = 45^\circ$ section, where zone 1 and zone 2 representations are also shown.

Code	(A)	(B)	Euler angles		
			ϕ_1	Φ	ϕ_2
C	$(0\ 0\ 1)[1\ 0\ 0]$	$(0\ 0\ 1)[\bar{1}\ 0\ 0]$	180	90	0
		$(0\ 0\ 1)[0\ 1\ 0]$	180	90	90
		$(0\ 0\ \bar{1})[1\ 0\ 0]$	0	90	0
		$(0\ 0\ \bar{1})[0\ \bar{1}\ 0]$	0	90	90
		$(0\ \bar{1}\ 0)[0\ 0\ 1]$	90	90	90
		$(1\ 0\ 0)[0\ 0\ 1]$	90	90	0
CG'	$(0\ 2\ 1)[1\ 0\ 0]$	$(1\ \bar{2}\ 0)[0\ 0\ 1]$	90	90	63.43
CG	$(0\ 2\ 1)[\bar{1}\ 0\ 0]$	$(2\ \bar{1}\ 0)[0\ 0\ 1]$	90	90	26.56
G	$(0\ 1\ 1)[1\ 0\ 0]$	$(1\ \bar{1}\ 0)[0\ 0\ 1]$	90	90	45
B	$(0\ 1\ 1)[2\ \bar{1}\ 1]$	$(0\ \bar{1}\ 1)[\bar{2}\ 1\ 1]$	150	54.74	45
		$(1\ 0\ \bar{1})[1\ \bar{2}\ 1]$	30	54.74	45
B'	$(0\ \bar{1}\ \bar{1})[2\ \bar{1}\ 1]$	$(1\ \bar{1}\ 0)[\bar{1}\ \bar{1}\ 2]$	90	54.74	45
S ₃	$(\bar{1}\ \bar{2}\ \bar{3})[6\ 3\ \bar{4}]$	$(1\ \bar{2}\ 3)[\bar{6}\ 3\ 4]$	147.4	72.06	37.69
S' ₃	$(\bar{1}\ \bar{2}\ \bar{3})[\bar{6}\ \bar{3}\ 4]$	$(2\ \bar{1}\ \bar{3})[3\ \bar{6}\ 4]$	32.57	72.06	52.31
T'	$(4\ 4\ 11)[11\ 11\ \bar{8}]$	$(4\ \bar{4}\ \bar{11})[11\ \bar{11}\ 8]$	27.21	90	45
T	$(4\ 4\ 11)[\bar{11}\ \bar{11}\ 8]$	$(4\ \bar{4}\ 11)[\bar{11}\ 11\ 8]$	152.78	90	45
Cu'	$(1\ 1\ 2)[1\ 1\ \bar{1}]$	$(1\ \bar{1}\ \bar{2})[1\ \bar{1}\ 1]$	35.26	90	45
Cu	$(1\ 1\ 2)[\bar{1}\ \bar{1}\ 1]$	$(1\ \bar{1}\ 2)[\bar{1}\ 1\ 1]$	144.74	90	45
H	$(0\ 0\ 1)[1\ 1\ 0]$	$(0\ 0\ 1)[\bar{1}\ 1\ 0]$	180	90	45
		$(0\ 0\ \bar{1})[1\ \bar{1}\ 0]$	0	90	45

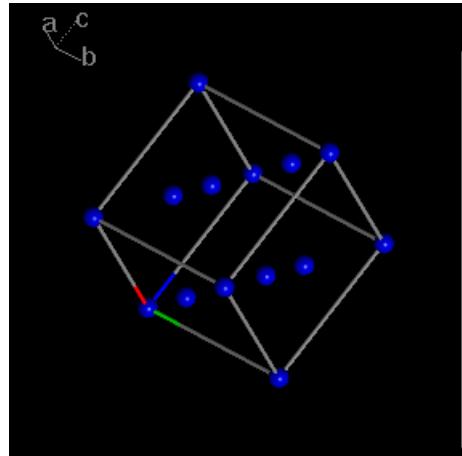
Table 2 (contd.)

Code	(A)	(B)	Euler angles		
			ϕ_1	Φ	ϕ_2
K'	$(0\ 0\ 1)[3\ 2\ 0]$	$(0\ 0\ 1)[\bar{2}\ \bar{3}\ 0]$	180	90	56.31
		$(0\ 0\ 1)[3\ \bar{2}\ 0]$	0	90	33.69
K	$(0\ 0\ \bar{1})[3\ 2\ 0]$	$(0\ 0\ \bar{1})[\bar{2}\ \bar{3}\ 0]$	0	90	56.31
		$(0\ 0\ 1)[\bar{3}\ 2\ 0]$	180	90	33.69
I'	$(1\ 1\ 2)[\bar{1}\ 1\ 0]$	$(1\ \bar{1}\ \bar{2})[\bar{1}\ \bar{1}\ 0]$	0	54.74	45
		$(1\ \bar{2}\ 1)[\bar{1}\ 0\ 1]$	120	54.74	45
I	$(1\ 1\ 2)[1\ \bar{1}\ 0]$	$(\bar{1}\ \bar{1}\ 2)[\bar{1}\ 1\ 0]$	180	54.74	45
		$(2\ \bar{1}\ 1)[0\ \bar{1}\ 1]$	60	54.74	45
J'	$(1\ 1\ 4)[\bar{1}\ 1\ 0]$	$(1\ 1\ \bar{4})[1\ \bar{1}\ 0]$	0	70.53	45
J	$(1\ 1\ 4)[1\ \bar{1}\ 0]$	$(\bar{1}\ \bar{1}\ 4)[\bar{1}\ 1\ 0]$	180	70.53	45
T*	$(11\ 8\ 11)[4\ \bar{1}\bar{1}\ 4]$	$(11\ \bar{1}\bar{1}\ \bar{8})[4\ \bar{4}\ 11]$	62.78	90	45
T**	$(11\ 8\ 11)[\bar{4}\ 11\ \bar{4}]$	$(11\ \bar{1}\bar{1}\ 8)[\bar{4}\ 4\ 11]$	117.21	90	45
E'	$(1\ 1\ 1)[\bar{1}\ 1\ 0]$	$(1\ \bar{1}\ 1)[\bar{1}\ 0\ 1]$	129.2	65.90	26.56
E	$(1\ 1\ 1)[1\ \bar{1}\ 0]$	$(1\ \bar{1}\ \bar{1})[0\ \bar{1}\ 1]$	50.77	65.90	63.43
F	$(1\ 1\ 1)[\bar{2}\ 1\ 1]$	$(1\ \bar{1}\ \bar{1})[1\ \bar{1}\ 2]$	54.74	90	45
F'	$(1\ 1\ 1)[2\ \bar{1}\ \bar{1}]$	$(1\ \bar{1}\ 1)[\bar{1}\ 1\ 2]$	125.26	90	45
L	$(0\ 1\ 1)[0\ \bar{1}\ 1]$	$(1\ 0\ 1)[\bar{1}\ 0\ 1]$	135	90	0
		$(0\ \bar{1}\ 1)[0\ 1\ 1]$	135	90	90
		$(0\ \bar{1}\ \bar{1})[0\ \bar{1}\ 1]$	45	90	90
		$(1\ 0\ \bar{1})[1\ 0\ 1]$	45	90	0

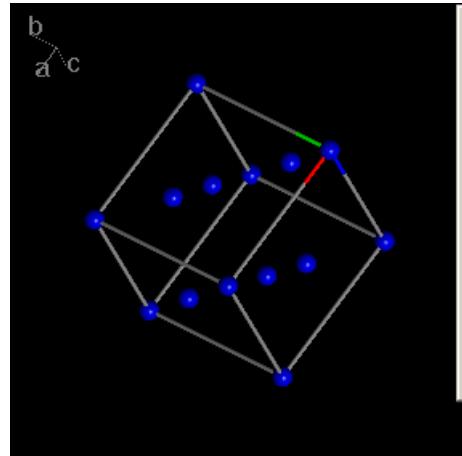
(307, 36, 26)



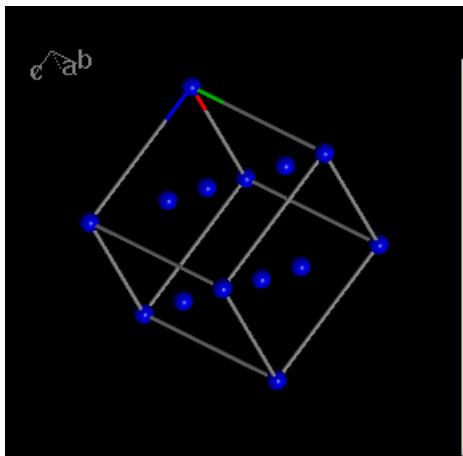
(233, 105, 56)



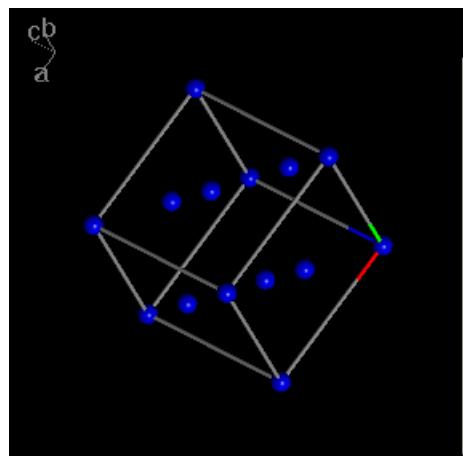
(121, 143, 333)



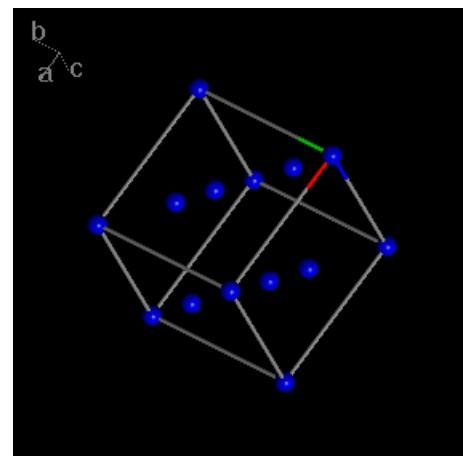
(53, 74, 304)



(333, 122, 18)



(121, 143, 153)



Crystal Symmetry

$$g_i = g_i^C \cdot g$$

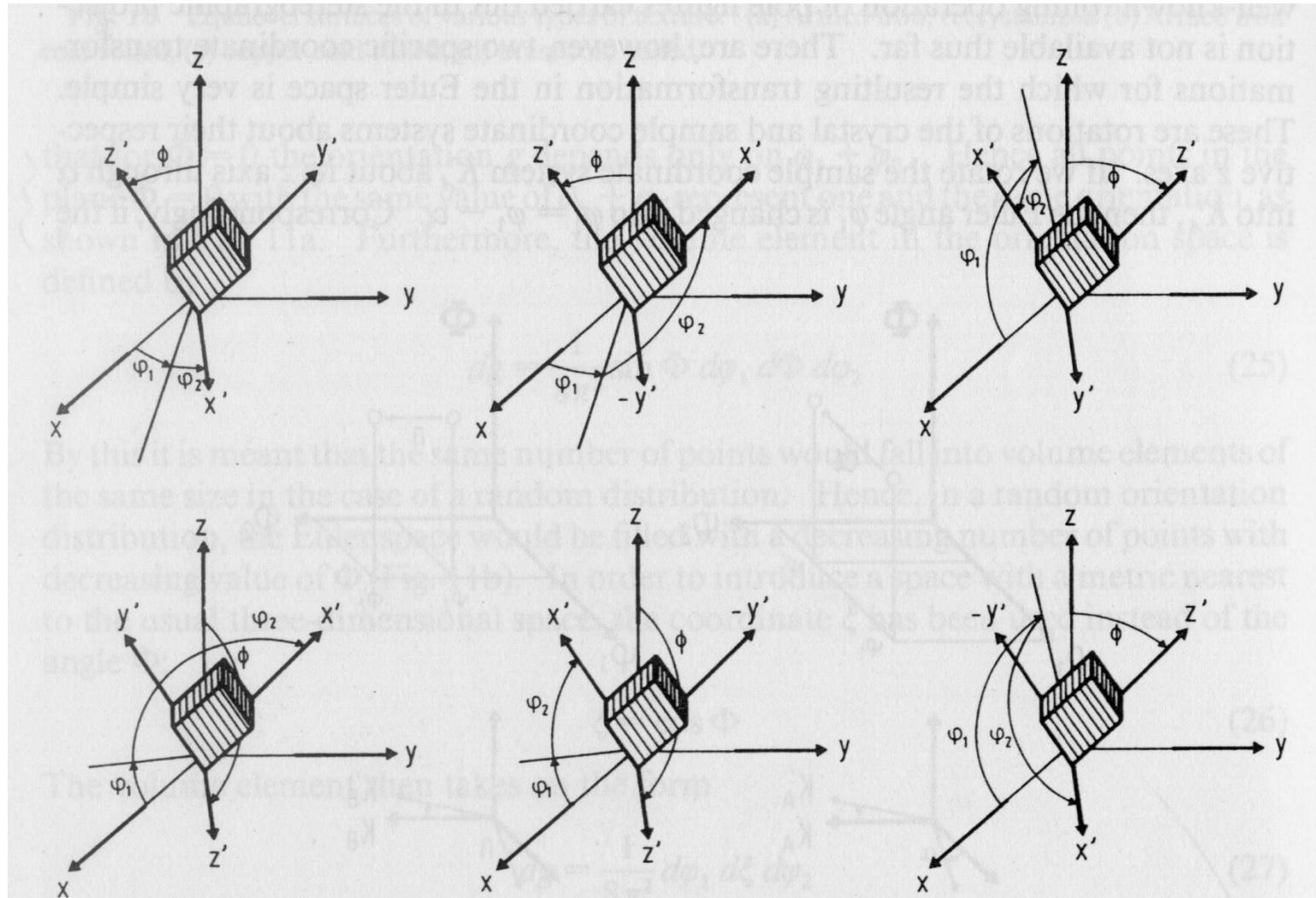


Fig. 13 Different choices of the crystal coordinate system K_B according to crystal symmetry.

Crystal Symmetry

Table II. Symmetry operators of rotation groups

tetragonal branch	hexagonal branch	cubic branch																																																																																																																																																																																																																																																																																																																																																																																																
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The dashed boxes
in this column
make up group 4.

The dashed boxes
in this column
make up group 32.

The dashed box
in this column
comprises the 3-fold axes only.

Matrix representation of the rotation point groups for 432

Matrix number 1

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Matrix number 5

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

Matrix number 9

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

Matrix number 13

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

Matrix number 19

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

Matrix number 2

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

Matrix number 6

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

Matrix number 10

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

Matrix number 14

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

Matrix number 20

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

Matrix number 3

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

Matrix number 7

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

Matrix number 11

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

Matrix number 16

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

Matrix number 22

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

Matrix number 4

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

Matrix number 8

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

Matrix number 12

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

Matrix number 17

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

Matrix number 23

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

Matrix number 18

$$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Matrix number 24

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

Taken from subroutine by D. Raabe

24 symmetry matrix for cubic (123)[63-4]

TABLE 2.2

Twenty-Four Equivalent Descriptions for (123)[63 $\bar{4}$]

Ideal Orientation	Orientation Matrix	Angle/Axis Pair ($\theta/u \ v \ w$)	Rodrigues Vector ($R_1 \ R_2 \ R_3$)	Euler Angles ($\varphi_1 \ \Phi \ \varphi_2$)	Ideal Orientation	Orientation Matrix	Angle/Axis Pair ($\theta/u \ v \ w$)	Rodrigues Vector ($R_1 \ R_2 \ R_3$)	Euler Angles ($\varphi_1 \ \Phi \ \varphi_2$)
(123)[63 $\bar{4}$]	0.768 -0.582 0.267 0.384 0.753 0.535 -0.512 -0.308 0.802	48.6°/0.562 -0.520 -0.644	0.254 -0.235 -0.291	307.0° 36.7° 26.6°	($\bar{3}\bar{1}\bar{2}$)[46 $\bar{3}$]	0.512 0.308 -0.802 0.768 -0.582 0.267 -0.384 -0.753 -0.535	143.3°/0.854 0.350 -0.385 -1.163	2.577 1.055	333.0° 122.3° 288.4°
(32 $\bar{1}$)[$\bar{4}\bar{3}\bar{6}$]	-0.512 -0.308 0.802 0.384 0.753 0.535 -0.768 0.582 -0.267	120.9°/-0.028 -0.915 -0.403	-0.048 -1.613 -0.711	232.9° 105.5° 56.3°	($\bar{2}\bar{3}\bar{1}$)[346]	0.384 0.753 0.535 0.512 0.308 -0.802 -0.768 0.582 -0.267	106.7°/-0.722 -0.680 0.126 0.169	-0.971 -0.914	232.9° 105.5° 146.3°
($\bar{1}\bar{2}\bar{3}$)[$\bar{6}3\bar{4}$]	-0.768 0.582 -0.267 0.384 0.753 0.535 0.512 0.308 -0.802	155.3°/0.271 0.933 0.237	1.239 4.263 1.081	121.0° 143.3° 333.4°	($\bar{2}\bar{3}\bar{1}$)[$\bar{3}46$]	-0.384 -0.753 -0.535 0.512 0.308 -0.802 0.768 -0.582 0.267	113.9°/-0.120 0.712 -0.692 -1.062	-0.185 1.094	52.9° 74.5° 213.7°
($\bar{3}\bar{2}\bar{1}$)[436]	0.512 0.308 -0.802 0.384 0.753 0.535 0.768 -0.582 0.267	74.6°/0.579 0.814 -0.039	0.441 0.620 -0.030	52.9° 74.5° 303.7°	($\bar{3}\bar{1}\bar{2}$)[$\bar{4}\bar{6}3$]	-0.512 -0.308 0.802 -0.768 0.582 -0.267 -0.384 -0.753 -0.535	137.1°/0.357 -0.871 0.338 -0.384 -0.753 -0.535	0.907	333.0° 122.3° 108.4°
(13 $\bar{2}$)[64 $\bar{3}$]	0.768 -0.582 0.267 -0.512 -0.308 0.802 -0.384 -0.753 -0.535	122.5°/0.922 -0.386 -0.041	1.679 -0.704 -0.075	333.0° 122.3° 18.4°	(21 $\bar{3}$)[364]	0.384 0.753 0.535 0.768 -0.582 0.267 0.512 0.308 -0.802	178.6°/-0.832 -0.457 -0.315 -0.257 1.10	-67.983	121.0° 143.3° 63.4°
(1 $\bar{2}\bar{3}$)[63 $\bar{4}$]	0.768 -0.582 0.267 -0.384 -0.753 -0.535 0.512 0.308 -0.802	153.3°/-0.937 0.272 -0.220	-3.944 1.146 -0.925	121.0° 143.3° 153.4°	(13 $\bar{2}$)[$\bar{6}43$]	-0.768 0.582 -0.267 -0.512 -0.308 0.802 0.384 0.753 0.535	140.4°/0.038 0.511 0.859 0.384 0.753 0.535	0.107 1.421	153.0° 57.7° 341.6°
(1 $\bar{3}\bar{2}$)[643]	0.768 -0.582 0.267 0.512 0.308 -0.802 0.384 0.753 0.535	72.2°/-0.816 0.061 -0.574	-0.595 0.045 -0.419	153.0° 57.7° 161.6°	($\bar{3}\bar{2}\bar{1}$)[$\bar{4}\bar{3}\bar{6}$]	-0.512 -0.308 0.802 -0.384 -0.753 -0.535 0.768 -0.582 0.267	177.3°/0.493 -0.351 0.796 -0.768 0.582 0.267	20.621 -14.661	52.9° 74.5° 123.7°
(2 $\bar{1}\bar{3}$)[364]	0.384 0.753 0.535 -0.768 0.582 -0.267 -0.512 -0.308 0.802	67.4°/0.022 -0.567 0.824	0.015 -0.378 0.550	301.0° 36.7° 116.6°	($\bar{2}\bar{1}\bar{3}$)[$\bar{3}\bar{6}4$]	-0.384 -0.753 -0.535 -0.768 0.582 -0.267 0.512 0.308 -0.802	143.3°/-0.482 0.876 0.013 0.512 0.308 -0.802	-1.453 2.644	121.0° 143.3° 243.4°
($\bar{1}\bar{2}\bar{3}$)[$\bar{6}3\bar{4}$]	-0.768 0.582 -0.267 -0.384 -0.753 -0.535 -0.512 -0.308 0.802	149.3°/-0.222 -0.240 0.945	-0.807 -0.872 3.440	301.0° 36.7° 206.6°	(13 $\bar{2}$)[$\bar{6}43$]	-0.768 0.582 -0.267 0.512 0.308 -0.802 -0.384 -0.753 -0.535	175.9°/-0.339 -0.808 0.481 -0.384 -0.753 -0.535	-9.362 -22.343	333.0° 122.3° 198.4°
($\bar{2}\bar{1}\bar{3}$)[$\bar{3}\bar{6}4$]	-0.384 -0.753 -0.535 0.768 -0.582 0.267 -0.512 -0.308 0.802	125.6°/0.354 0.014 -0.935	0.688 0.027 -1.820	301.0° 36.7° 296.6°	($\bar{3}\bar{2}\bar{1}$)[436]	0.512 0.308 -0.802 -0.384 -0.753 -0.535 0.768 -0.582 -0.267	138.9°/-0.850 0.026 0.527 -0.768 0.582 -0.267	-2.269 0.068	232.9° 105.5° 236.3°
(231)[346]	0.384 0.753 0.535 -0.512 -0.308 0.802 0.768 -0.582 0.267	109.2°/0.732 0.124 0.670	1.030 0.174	52.9° 74.5° 33.7°					
(312)[$\bar{4}\bar{6}3$]	-0.512 -0.308 0.802 0.768 -0.582 0.267 0.384 0.753 0.535	141.2°/-0.388 -0.334 -0.859	-1.102 -0.948 -2.442	153.0° 57.7° 71.6°					
($\bar{2}\bar{3}\bar{1}$)[$\bar{3}\bar{4}\bar{6}$]	-0.384 -0.753 -0.535 -0.512 -0.308 0.802 -0.768 0.582 -0.267	168.4°/0.548 -0.582 -0.600	5.413 -5.748 -5.920	239.2° 105.5° 326.3°					
($\bar{3}\bar{1}\bar{2}$)[463]	0.512 0.308 -0.802 -0.768 0.582 -0.267 0.384 0.757 0.535	71.7°/-0.537 0.625 0.567	-0.388 0.451	153.0° 57.7° 251.6°					

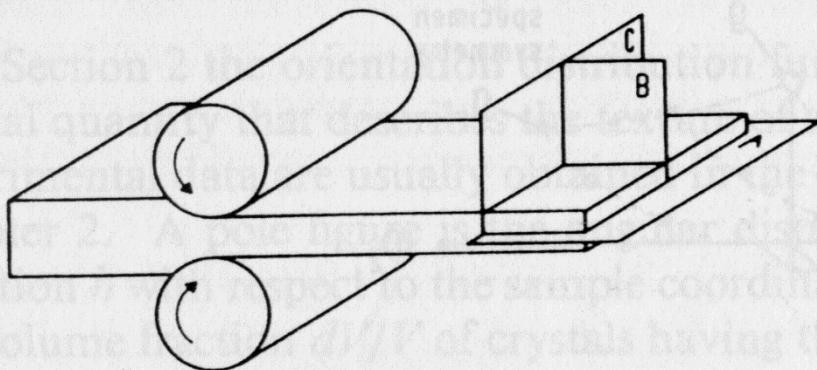
How to use a symmetry operator?

Goss: $\{110\}<001>$:
$$\begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \end{pmatrix}$$

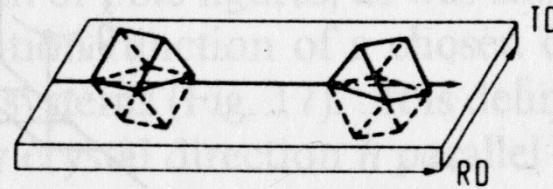
Pre-multiply by z-diad:
$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} 0 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 1 & 0 & 0 \end{pmatrix} \quad \text{which is } \{-1-10\}<001>$$

Sample Symmetry



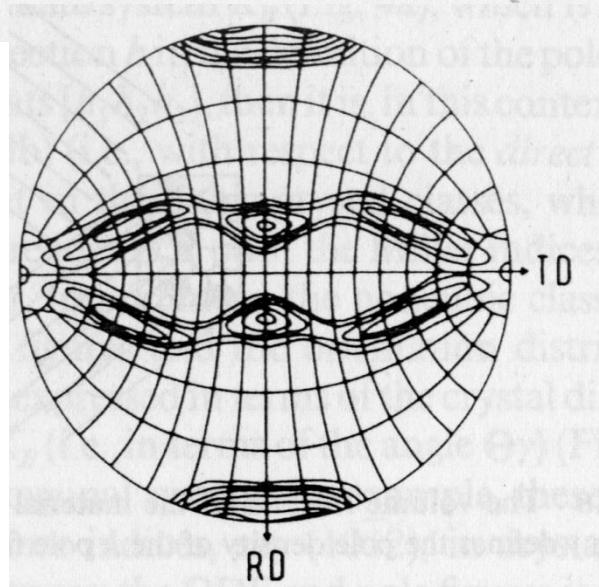
(a)



(b)

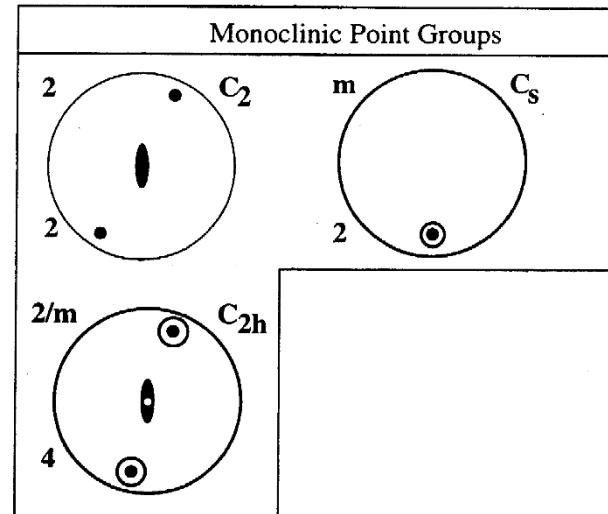
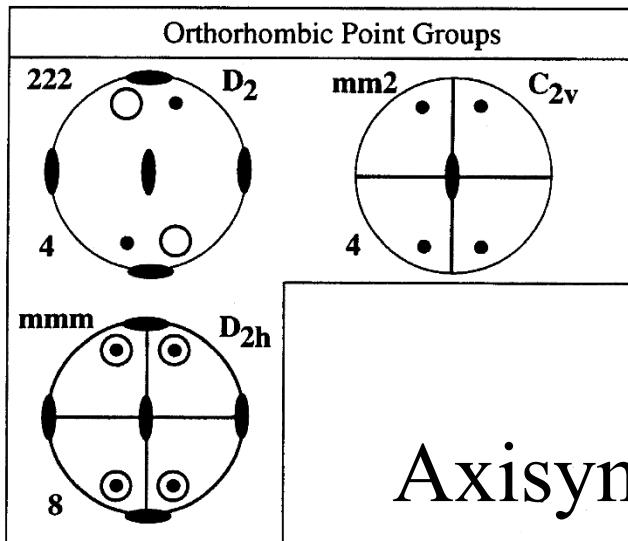
Fig. 15 (a) Possible sample symmetry in a rolled sheet. A, B, C are mirror planes. (b) Twofold axis of the sample symmetry.

$$g_j = g \cdot g_j^S$$



Sample Symmetry

Torsion, shear:
Monoclinic, 2.



Axisymmetric: C_∞

Rolling, plane strain
compression, mmm .

Otherwise,
triclinic.

Symmetry Relationships

- Note that the result of applying any available operator is equivalent to (physically indistinguishable in the case of crystal symmetry) from the starting configuration (not mathematically equal to!).
- Also, if you apply a sample symmetry operator, the result is generally physically different from the starting position. Why?! Because the sample symmetry is only a *statistical symmetry*, not an exact, physical symmetry.

$$g_{ij} = g_i^C \cdot g \cdot g_j^S$$

NB: if one writes an orientation as an *active rotation* (as in continuum mechanics), then the order of application of symmetry operators is reversed: premultiply by sample, and postmultiply by crystal!

Section Sizes: Crystal - Sample

- *Cubic-Orthorhombic:*
 $0 \leq \phi_1 \leq 90^\circ, 0 \leq \Phi \leq 90^\circ, 0 \leq \phi_2 \leq 90^\circ$
- *Cubic-Monoclinic:*
 $0 \leq \phi_1 \leq 180^\circ, 0 \leq \Phi \leq 90^\circ, 0 \leq \phi_2 \leq 90^\circ$
- *Cubic-Triclinic:*
 $0 \leq \phi_1 \leq 360^\circ, 0 \leq \Phi \leq 90^\circ, 0 \leq \phi_2 \leq 90^\circ$
- *But, these limits do not delineate a fundamental zone.*

Orientation description III: Angle/axis

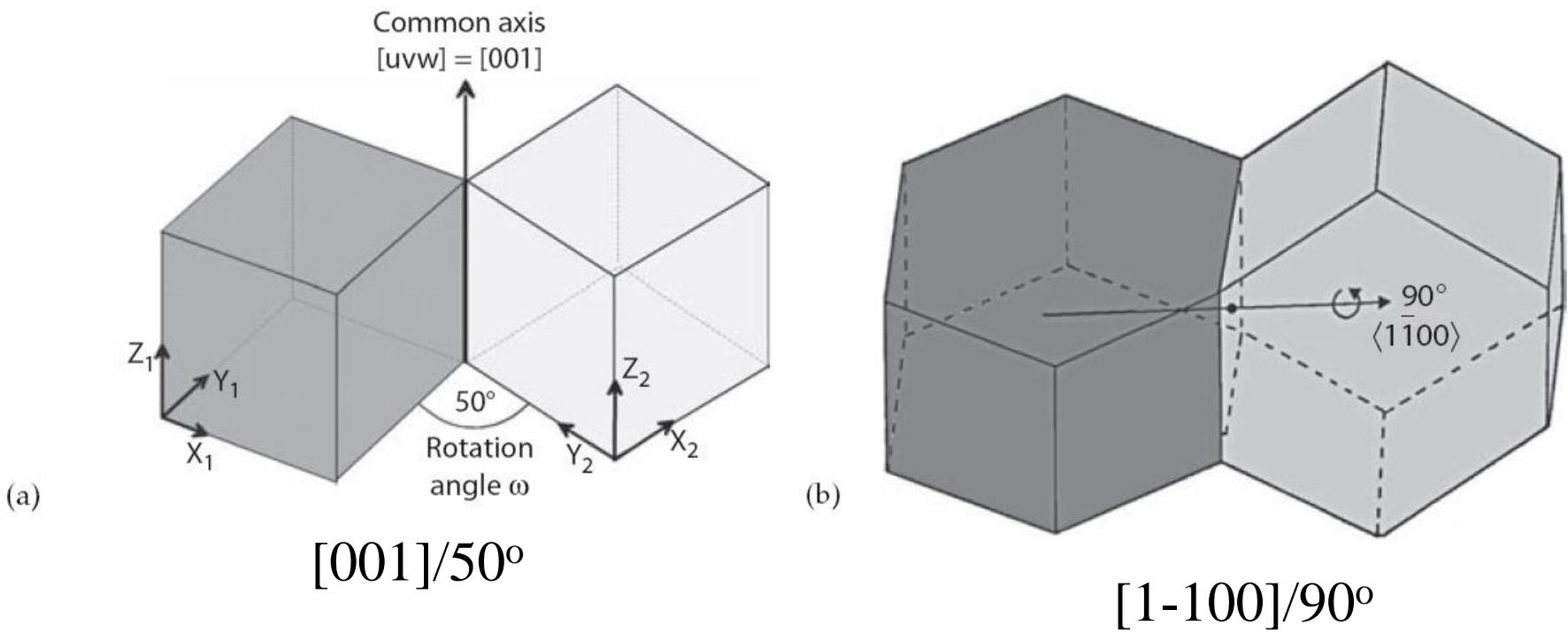
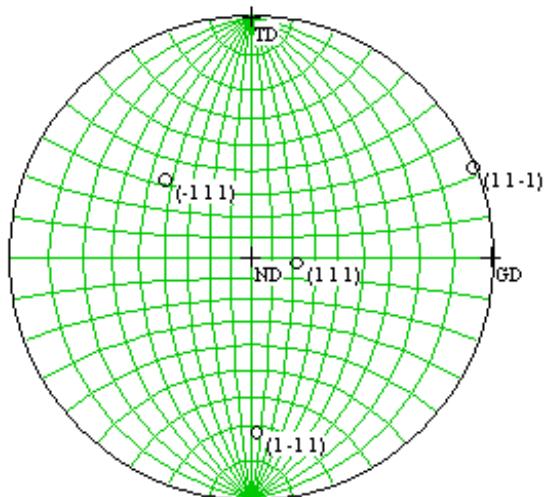


FIGURE 2.13

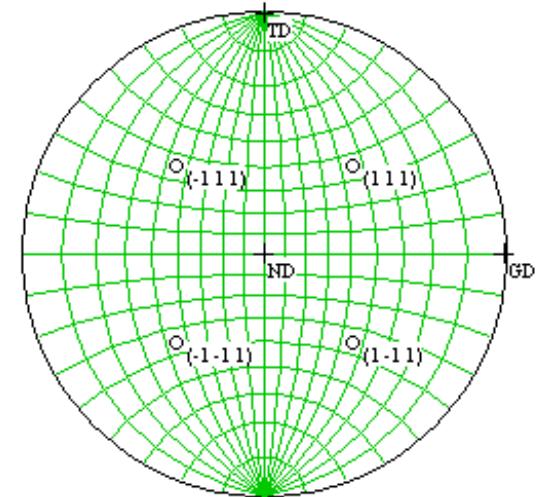
Diagram showing the angle/axis of rotation between (a) two cubes and (b) two hexagons.

Example of Orientation

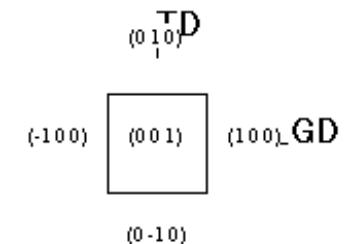
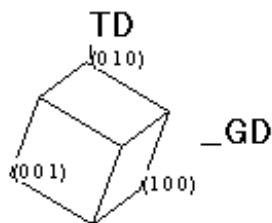
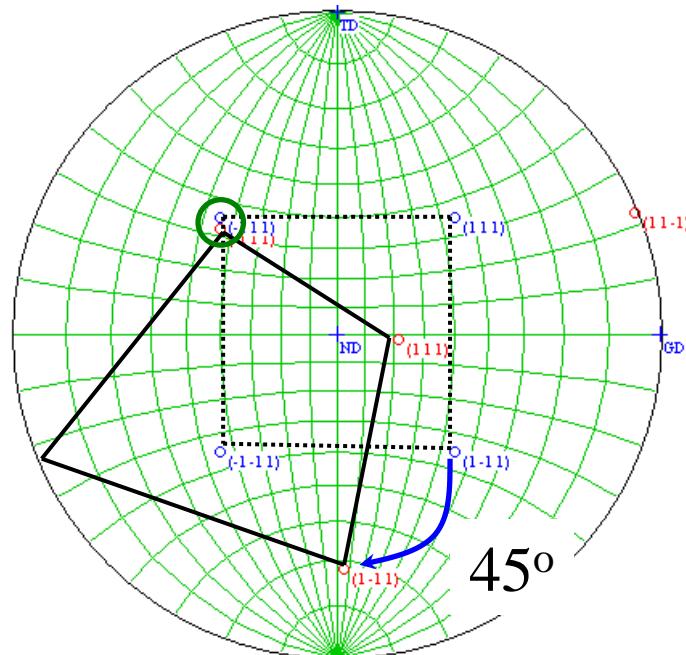
$(307^\circ, 37^\circ, 27^\circ)$



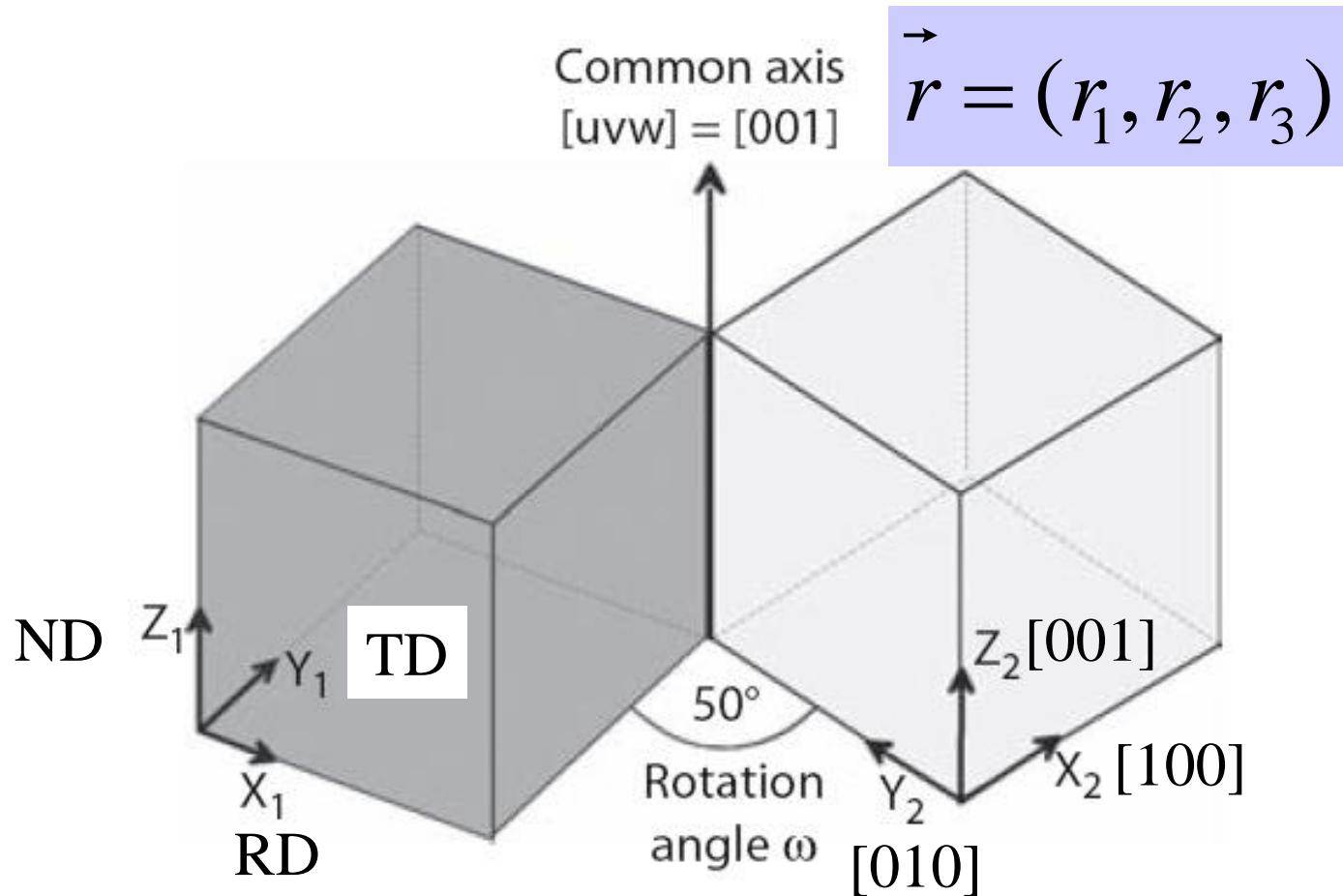
$(0^\circ, 0^\circ, 0^\circ)$



$[18, -15, -16]$ 45°



Orientation by angle/axis rotation



sample coordinates

$$\mathbf{C}_c = g_{cs} \cdot \mathbf{C}_s$$

crystal coordinates

Angle/axis of rotation

$$g = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix}$$

$$g_{11} = r_1^2(1 - \cos \theta) + \cos \theta$$

$$g_{12} = r_1 r_2 (1 - \cos \theta) - r_3 \sin \theta$$

$$g_{13} = r_1 r_3 (1 - \cos \theta) + r_2 \sin \theta$$

$$g_{21} = r_2 r_1 (1 - \cos \theta) + r_3 \sin \theta$$

$$g_{22} = r_2^2 (1 - \cos \theta) + \cos \theta$$

$$g_{23} = r_2 r_3 (1 - \cos \theta) - r_1 \sin \theta$$

$$g_{31} = r_3 r_1 (1 - \cos \theta) - r_2 \sin \theta$$

$$g_{32} = r_3 r_2 (1 - \cos \theta) + r_1 \sin \theta$$

$$g_{33} = r_3^2 (1 - \cos \theta) + \cos \theta$$

\vec{r} / θ

Angle/axis of rotation

\vec{r} / θ

$$\cos \theta = \frac{\text{Tr}(g) - 1}{2} = \frac{g_{11} + g_{22} + g_{33} - 1}{2}$$

$$r_1 = \frac{g_{23} - g_{32}}{2 \sin \theta}$$

$$r_2 = \frac{g_{31} - g_{13}}{2 \sin \theta}$$

$$r_3 = \frac{g_{12} - g_{21}}{2 \sin \theta}$$

The rotation is described as a right-handed screw operation and θ is always positive.

A negative angle is equivalent to changing the sign of r.

$\text{Tr}(g)$: the trace of matrix g

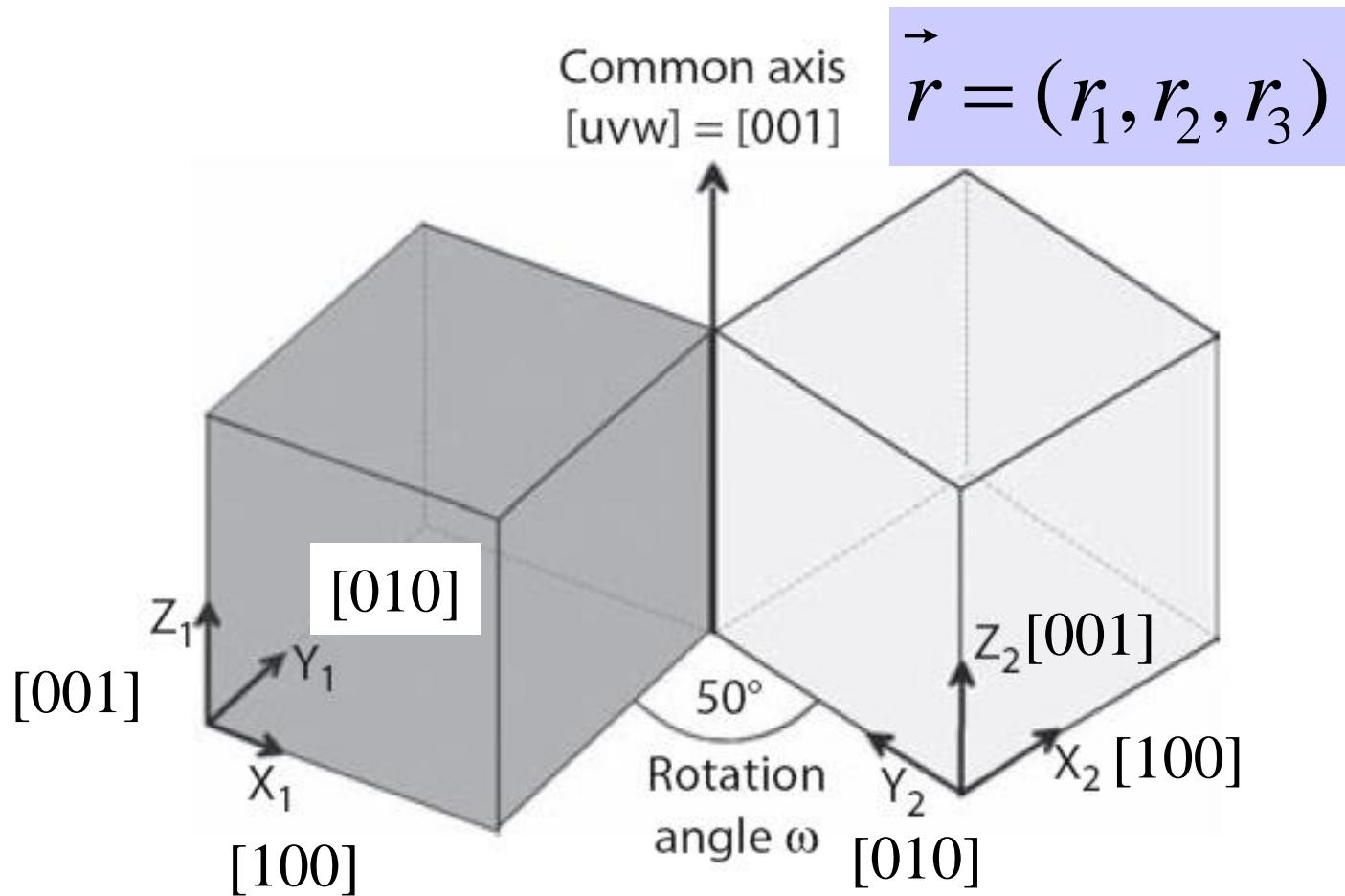
g_{ij} ($i, j = 1, 2, 3$): the elements of g

Angle/axis of misorientation

A misorientation is calculated from the orientations of grain 1 and grain 2 by

$$g_2 = M_{12} \cdot g_1$$

Misorientation by angle/axis rotation



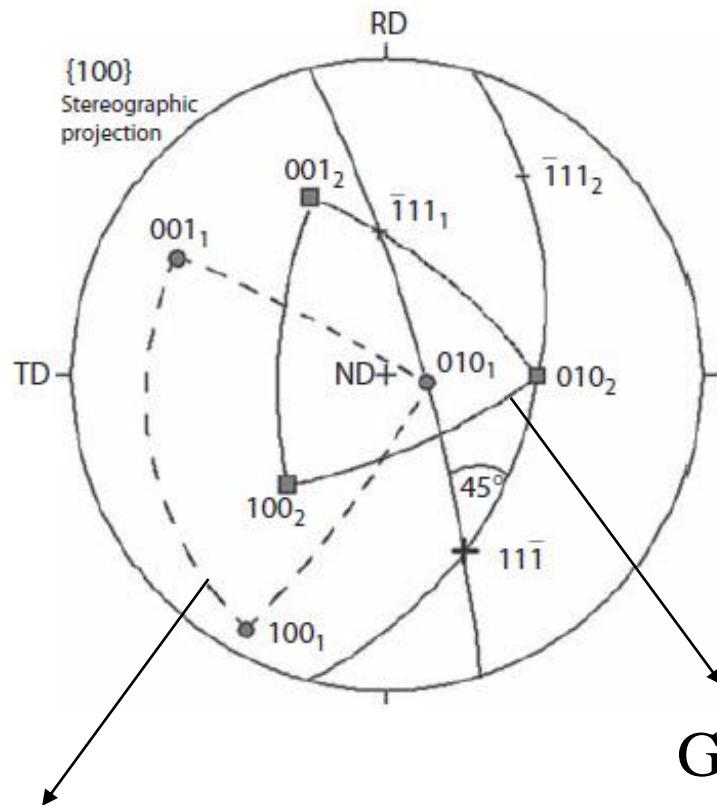
crystal coordinates of
grain 2

$$g_2 = M_{12} \cdot g_1$$

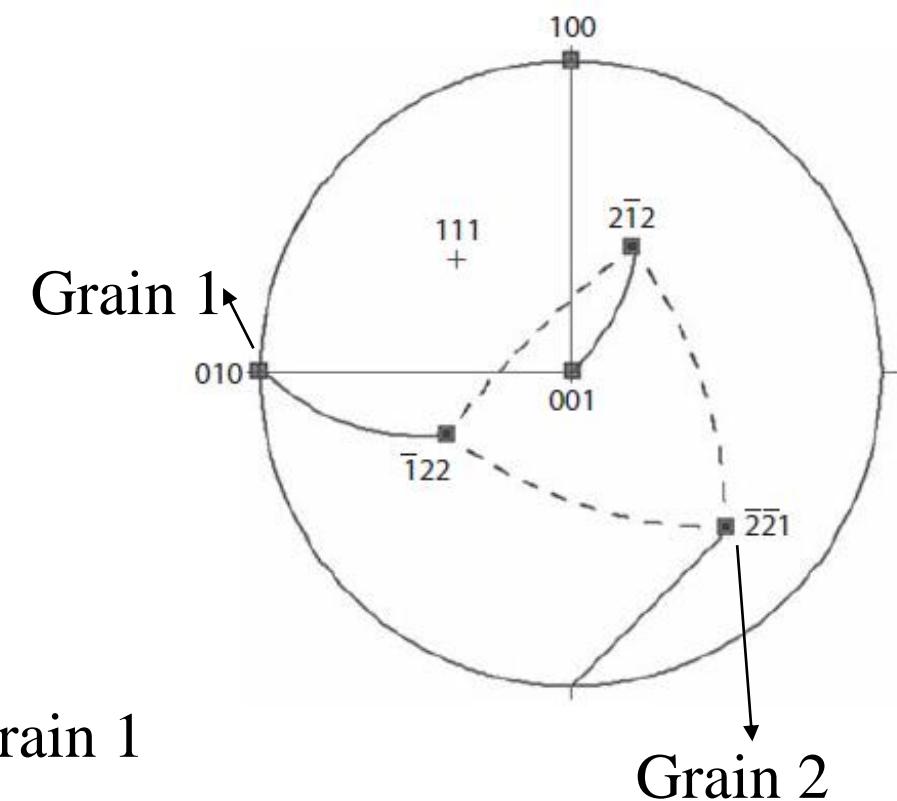
crystal coordinates
of grain 1

Orientation & misorientation

Orientation:
Reference (sample axes)



Misorientation:
Reference (grain 1)



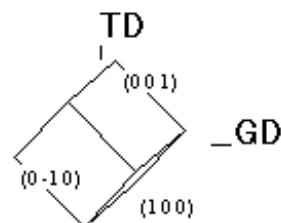
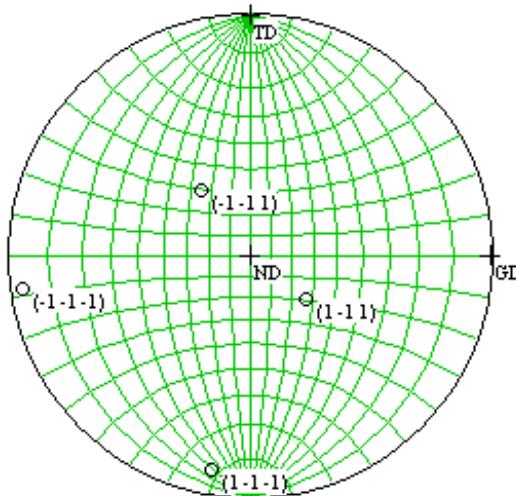
Grain 2

Grain 1

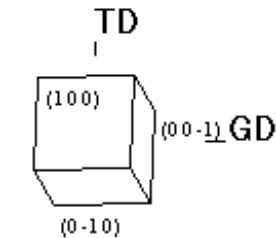
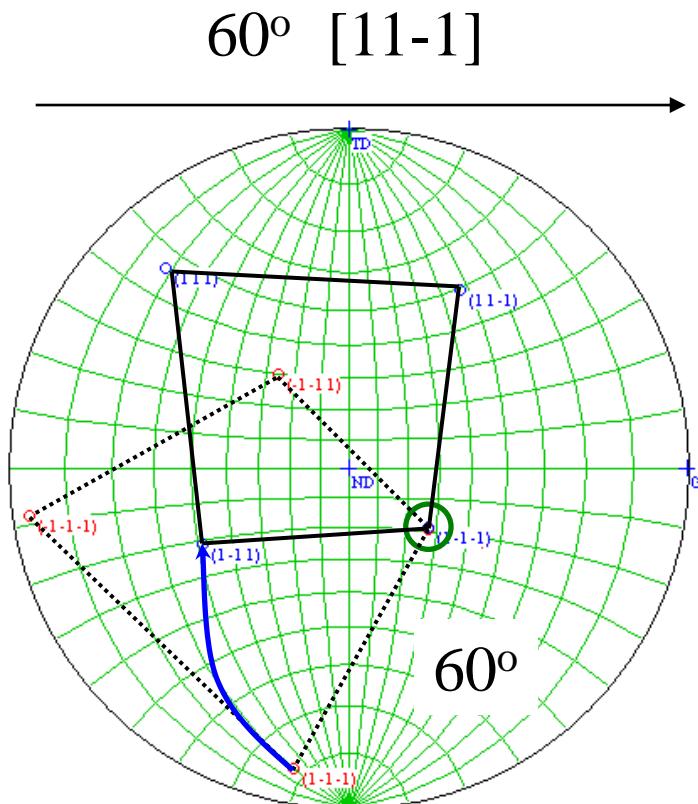
Grain 2

Example of Misorientation

$(136.4^\circ, 50.4^\circ, 176.4^\circ)$



$(271.9^\circ, 101.4^\circ, 110.6^\circ)$



Representation of Orientation

$$r_x = \cos \psi \sin \vartheta$$

$$r_y = \sin \psi \sin \vartheta$$

$$r_z = \cos \theta$$

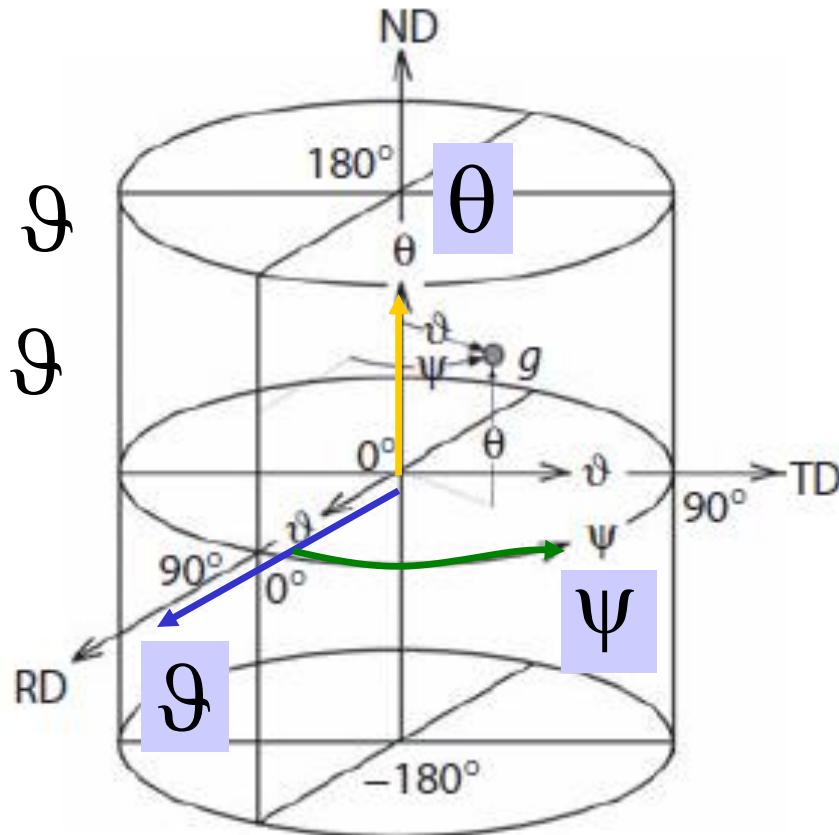


FIGURE 2.15

Representation of an orientation g given by the angle/axis description parameters r and θ in a cylindrical orientation space defined by the rotational parameters ϑ , ψ , and θ .

Rodrigues vector

The Rodrigues vector R combines the angle and axis of rotation into a mathematical entity.

$$\vec{R} = \vec{r} \cdot \tan\left(\frac{\theta}{2}\right)$$

$$R_1 = r_1 \cdot \tan\left(\frac{\theta}{2}\right)$$

$$R_2 = r_2 \cdot \tan\left(\frac{\theta}{2}\right)$$

$$R_3 = r_3 \cdot \tan\left(\frac{\theta}{2}\right)$$

Fundamental zone

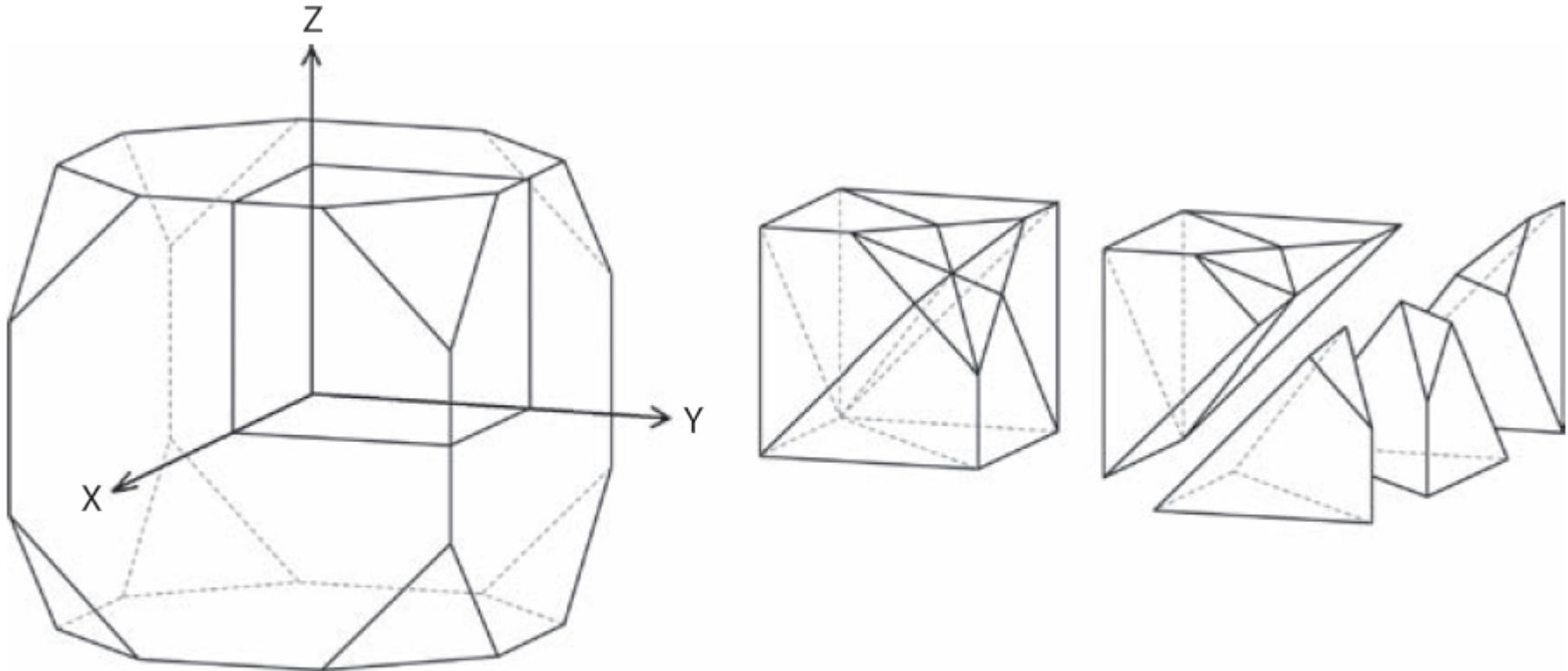


FIGURE 2.16

The fundamental zone of Rodrigues space for cubic symmetry, showing also the decomposition of the space into 48 subvolumes. (Adapted from Day, A., PhD Thesis, University of Bristol, U.K., 1994.)

Parameters of Rodrigues space

TABLE 2.4

Parameters of Rodrigues Space According to Crystal System

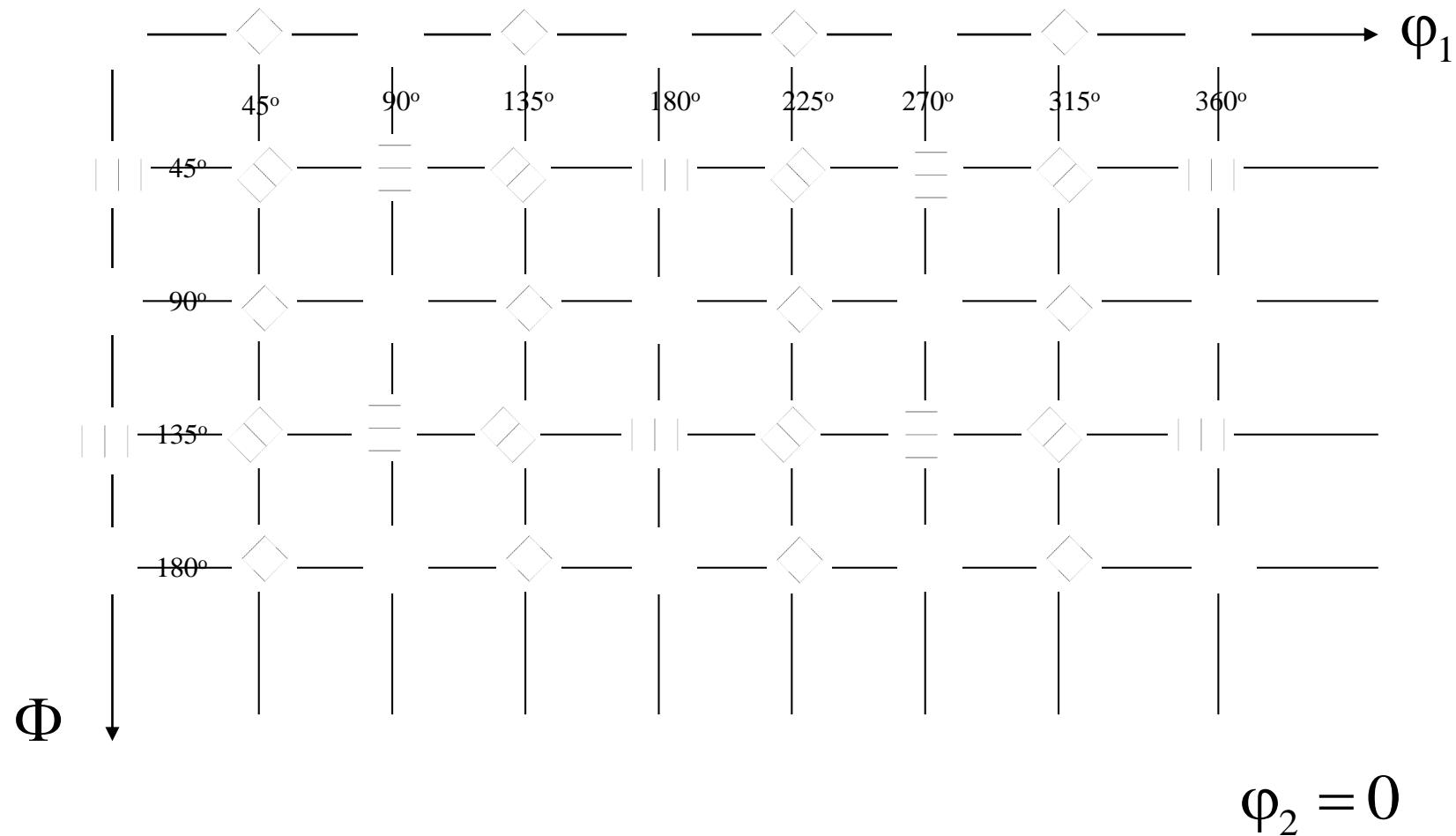
Crystal System	Distance of the Main Face from the Origin	Description	Subvolume Fraction
Cubic	$\tan \pi/8$	Six octagonal faces normal to the fourfold axes; eight triangular faces normal to the threefold axes	1/48
Hexagonal	$\tan \pi/4$	Two dodecagonal faces normal to the sixfold axis; 12 square faces normal to the diad axes	1/12
Trigonal	$\tan \pi/4$	Two hexagonal faces normal to the threefold axis; six square faces normal to the diad axes	1/6
Tetragonal	$\tan \pi/6$	Eight triangular faces perpendicular to the threefold axes (i.e., a regular octahedron)	1/24
Orthorhombic	$\tan \pi/4$	Six faces normal to the diads (i.e., a square)	1/8
Icosahedral	$\tan \pi/10$	Twelve pentagonal faces normal to the fivefold symmetry axes (i.e., a regular dodecahedron)	1/120

Source: Data from Morawiec, A. and Field, D.P., *Philos. Mag.*, 73A, 1113, 1996.

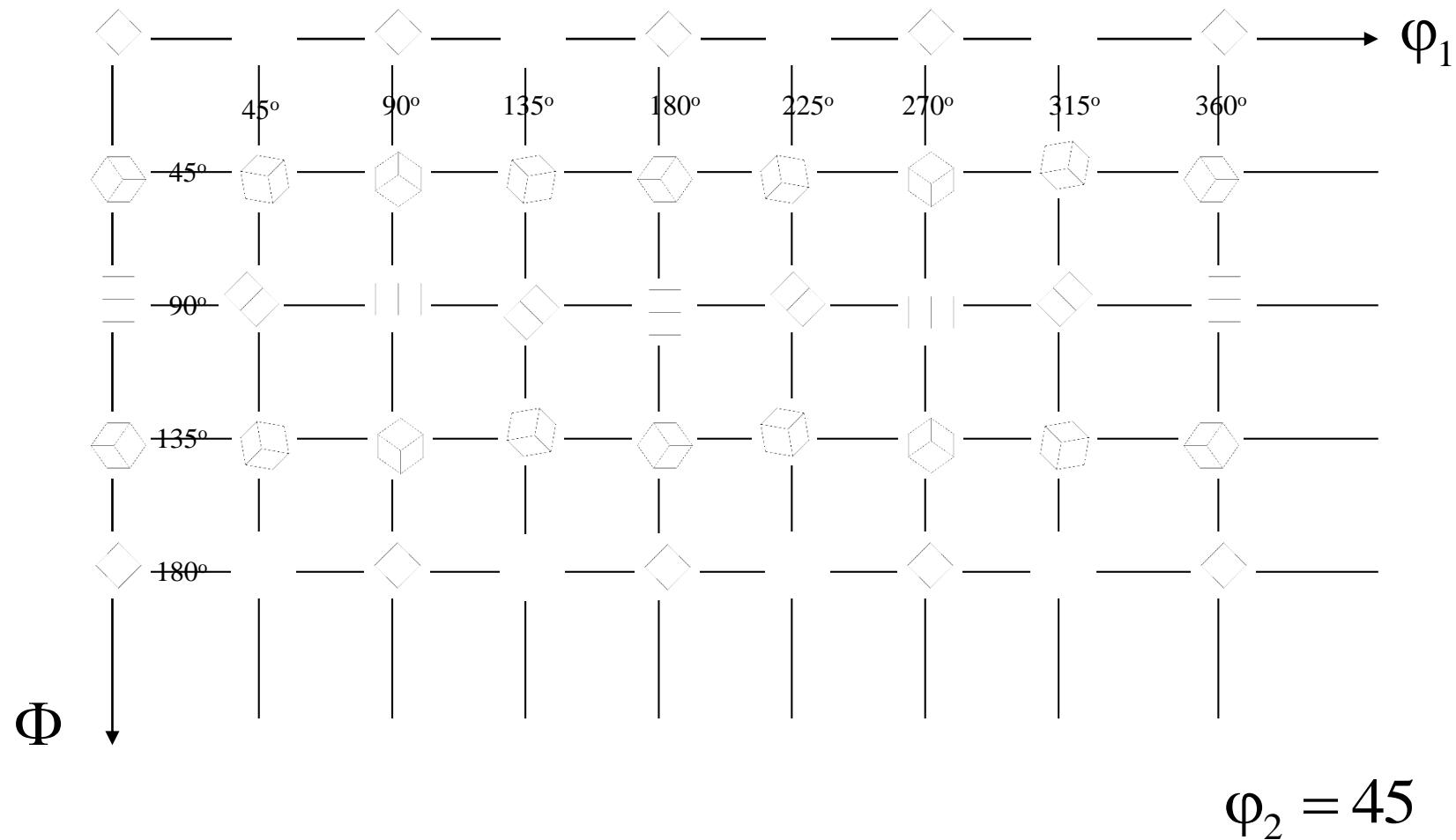
Properties of Rodrigues space

- The axis of rotation gives the direction of the R vector. Rotations about the same axis of rotation lie on a straight line that passes through the origin.
- The angle of rotation gives the length of the R vector. Small-angle boundaries cluster close to the origin.
- A fiber texture lies on a straight line that in general doesn't pass through the origin.
- The edges of zones in Rodrigues space are straight lines, and the faces of zones are planar.

Append: Symmetry in φ_1 for cubic



Append: Symmetry in φ_1 for cubic



Append: Symmetry in φ_1 for hexagonal

