Today will be a partial review; partial intro of new concepts

Crystallographic orientation representation

- Rotation matrices
- Euler
- Axis-angle
- Rodrigues
- Quaternions

} descriptors of orientation

- Descriptors are employed to represent different aspects of

macrotexture

microtexture

- All descriptors are defined in their appropriate space

- Crystallographic orientation — what we'll do
  - 3D when refered to crystals: 3 indep parameters
  - 2D crystal plane: 2 indep parameters

- crystal systems: grouping of xtals according to axial system used to describe lattice (cubic, hex, tetrag, rhom, tri, ortho, rhombohedral)

- Transformation between coordinate systems: through rotation matrices

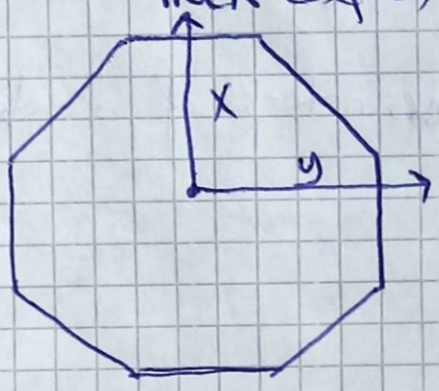
** To specify an orientation, it is necessary to set up terms of reference frames

- are relating to specimen
- are relating to crystals
- if you are doing characterization; are relating to lab coordinates

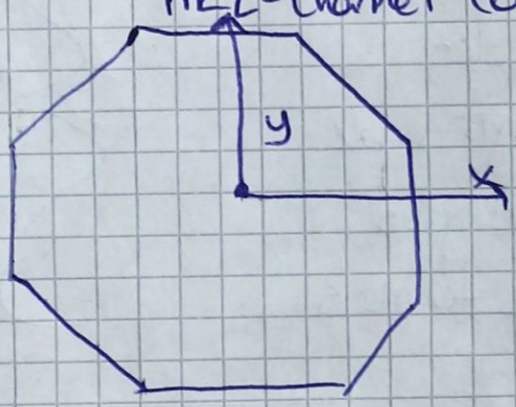
different sample coordinates for different softwares.

for hex coordinate system; let's look at RD(x) and TD(y) transverse definitions:

INCA (Oxford)

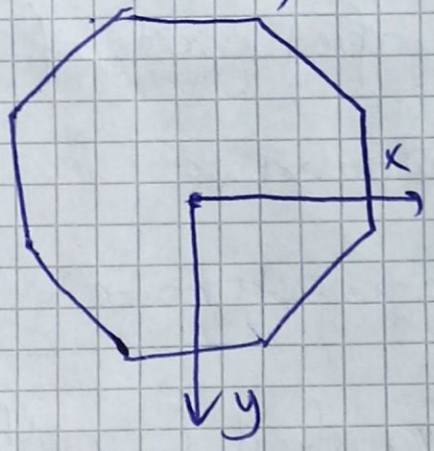


HKL-Channel (Oxford)

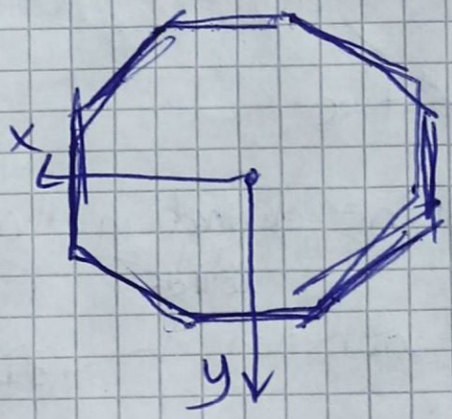


plus how to convert hex frame into orthonormal

OIM (TSL)

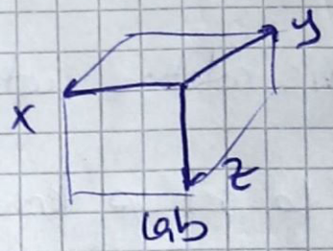


MTEX

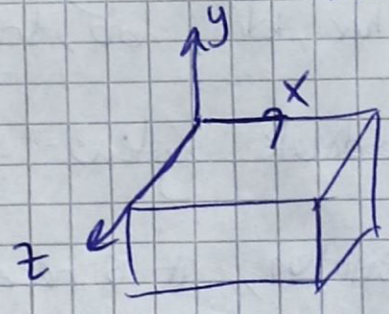


These are the crystal coordinate system differences. There is also lab frame differences (global)

TSL (OIM)



APS (HEDM)



2 choices to convert hex x-tal into orthonormal frame

$x=[10\bar{1}0]$, $y=[\bar{1}2\bar{1}0]$, $z=[0001]$

$y=[2\bar{1}\bar{1}0]$, $y=[01\bar{1}0]$, $z=[0001]$

from hex coordinate to orthonormal; transformation matrices

premultiply ← a zone axis referenced to xtal coordinate system, by rotation matrix

$$\begin{bmatrix} a & b\cos\gamma & c\cos\beta \\ 0 & b\sin\gamma & \dfrac{c(\cos\alpha - \cos\beta\cos\gamma)}{\sin\gamma} \\ 0 & 0 & \dfrac{c(1+2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma)^{1/2}}{\sin\gamma} \end{bmatrix}$$

α, β, γ = angles lattice
a, b, c = parameters lattice

for hex crystals; the transformation matrix becomes

$$L_{\text{hex-ort}} = \begin{pmatrix} a & -a/2 & 0 \\ 0 & a\sqrt{3}/2 & 0 \\ 0 & 0 & c \end{pmatrix}. \qquad L[\text{axis}]$$

from orth to hex

$$L^{-1}[\text{axis}]$$

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crystallographic orientation: is defined as: the position of xtal system wrt the specimen coordinate system.

misorientation = orientation of one crystal wrt another

now; here comes in the active vs. passive rotations.

Euler Bunge says: 3 rotations that will bring sample (S) into crystal (C)

passive = S into C (TSL-OIM) Active = C into S

Review of Euler and Rotation

Euler Angles and rotation matrices are the centrality in the field; but they cause confusion as they source ambiguity of definitions? Not really man!

A single rotation can be defined by a rotation axis; and angular offset about the axis

axis-angle pair, most basic.

Euler showed 3 sequential rotations about different axes can describe orientations.

Rotation can be described by 3×3 rotation matrices, R (or g).
↳ (single axis-angle) or 3 sequential (Euler)

R = bridge the relative state of vectors to coordinate systems before and after rotation.

(left-multiplying R acting on column vectors

$$R^{-1} = R^T$$
$$\det R = 1$$

$$v = R\,(v) \rightarrow \begin{bmatrix} - \\ - \\ - \end{bmatrix}$$

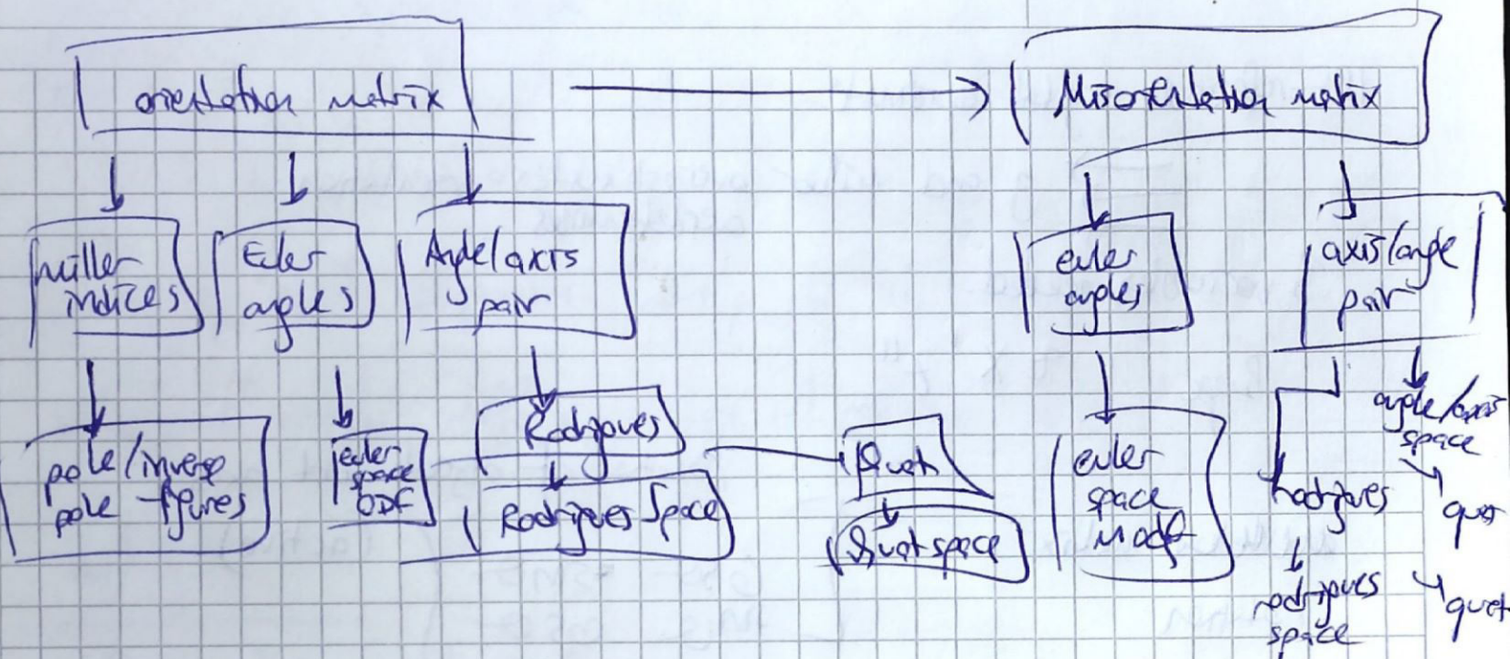
(3×1) (3×3) (3×1) column vector

Rotation matrix

$$C_c = g\,C_s$$

g → rows and columns are unit vectors.

cross product of 2 rows or columns gives the third.



Symetry

full solution premultiply

$O \times g$

24 = cubic
hex = 12
ort = 4

Miller Indices orientation

$$g = \begin{pmatrix} u/N_1 & q/N_2 & h/N_3 \\ v/N_1 & r/N_2 & k/N_3 \\ w/N_1 & s/N_2 & l/N_3 \end{pmatrix}$$

N = normalization

$\{qrs\}$ = specimen Y in xtal coor = $(hkl) \times [uvw]$

for cubic (because indices for plane & direction identical)

but; nearest family - can be away from (hkl) [uvw]

specimen symmetry also affects solution

(110) [001] → Goss cubic

PF = reference ⇒ specimen coordinate

unit quets = Euler-Rodrigues Parameters

IPF = reference crystal coordinate

⇒ g and miller overestimates orientation
overdetermines

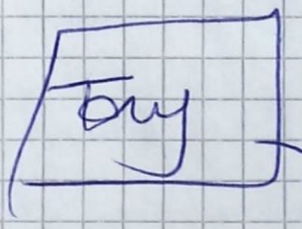
3 variables needed.

Bunge $z X' Z''$

rotation of object wrt axis

rotation matrix

$$\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$ (active)



$$\rightarrow \begin{bmatrix} \cos & \sin \\ -\sin & \cos \end{bmatrix}$$ passive (coordinate sys)

Euler space

most general triclinic xtal no sample sym

$0 < \theta_1, \theta_2 < 360$; $0 < \Phi < 180°$

max size

sample symmetry affects the size of θ_1
reduces

Rolling → normally introduce orthorhombic sample symmetry
2 mirror planes (1 RD 1 TD)

so $0 \leq \theta_1 \leq 90$

1 mirror → $0 \leq \theta_1 \leq 180$ monoclinic symmetry
shear deformation
torsion

Note page 38 from book.

misorientation through angle-axis

$M = g_1^{-1} g_2$

reference grain orientation

get g - M composer from page 41.

misor vs rotation difference = choice of reference axes

Rodrigues

Born from axis-angle

$\rho = \tan\left(\frac{\theta}{2}\right) r$

beauty = a vector that lies in a Cartesian coordinate system, that can be chosen to correspond to either xtl or specimen axes.

RF-space → population of vectors

smallest R from smallest θ.

lie closest to the origin of RF space.

here smallest θ is most convenient to select to represent R-space.

1988 → Frank - Rodrigues

Euler more continuous orientation distribution

Rodrigues → microtexture

FZ - R space → periodic

fibre → lie on a straight line in R-F space

lines represent rotations about fixed axis → geodesic lines