Imperfections – deformation and microstructures in polycrystals

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2- Grain orientation

Objectives

How to represent a grain orientation?

- Coordinate systems
- Euler angles
  - Presentation
  - Bunge Euler angle
- Matrix representation
  - Definition
  - Properties
- Graphical representation :
  - Introduction to pole figures
  - Examples and applications.

2- Grain orientation
a- Coordinate systems

Representation of orientations

Need to define several coordinate systems (or *reference frames*)

- A reference frame for each crystallite
- A reference frame for the polycrystal, the sample

In texture analysis, we use Cartesian coordinate systems

Grain orientation

- Operation *sample reference frame → grain reference frame*

In 3D, the transformation between 2 Cartesian coordinate systems can be seen as

- Rotation matrices (in 3D)
- 3 subsequent rotations, defining Euler angles

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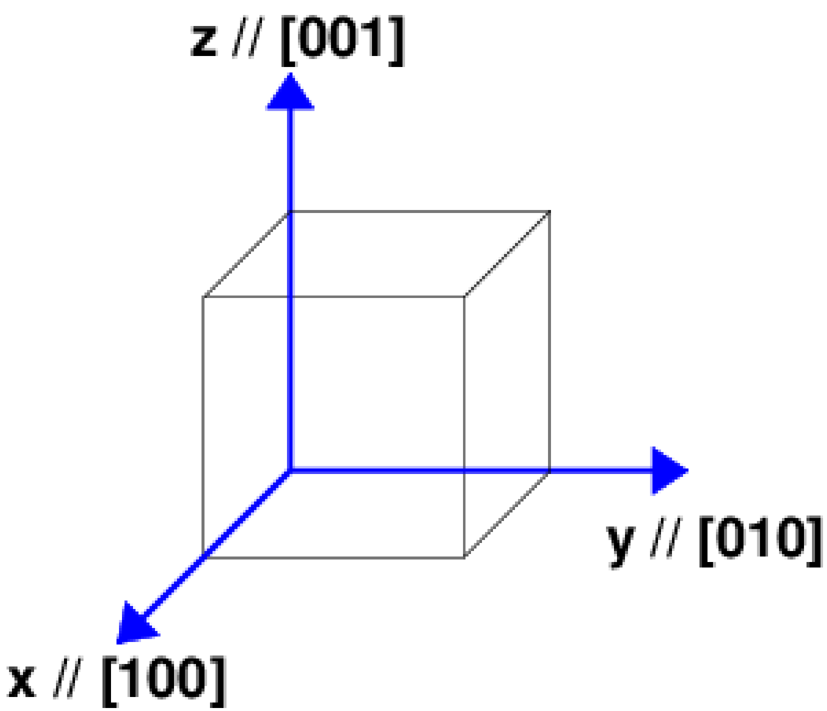
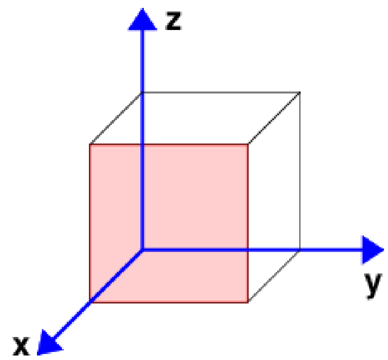
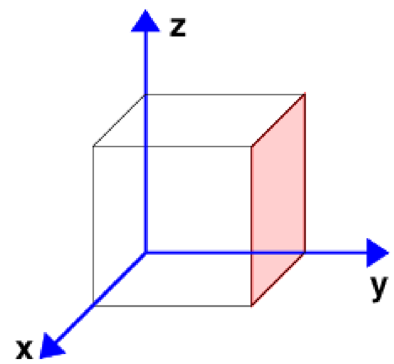
Crystal reference frame
Cubic symmetry

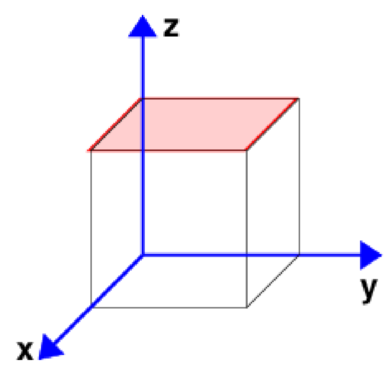




Plane : (100)
Normal to plane : [100]



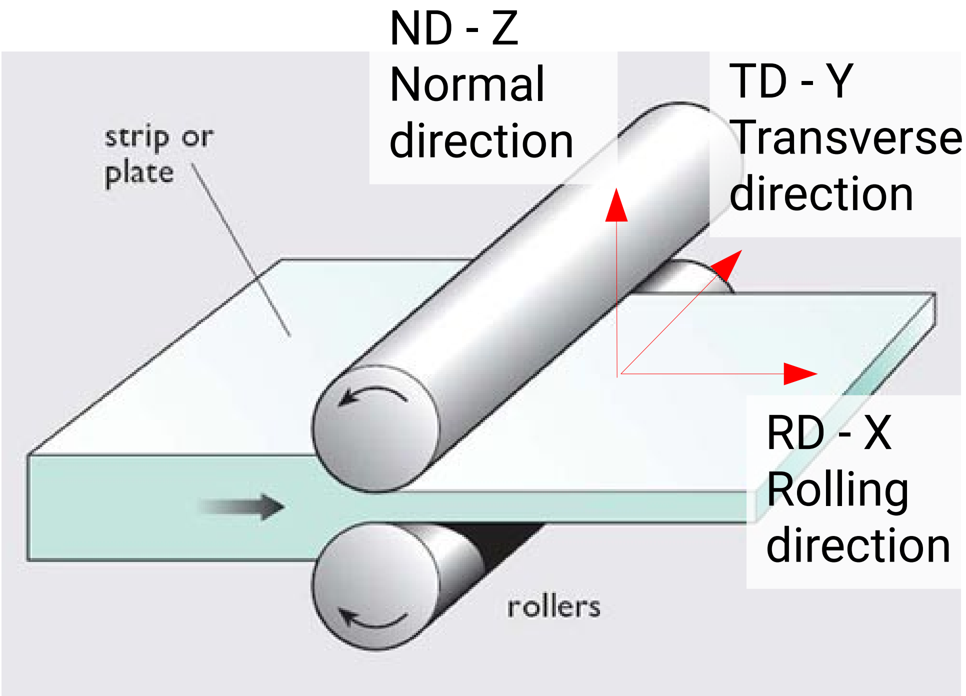
Plane : (010)
Normal to plane : [010]



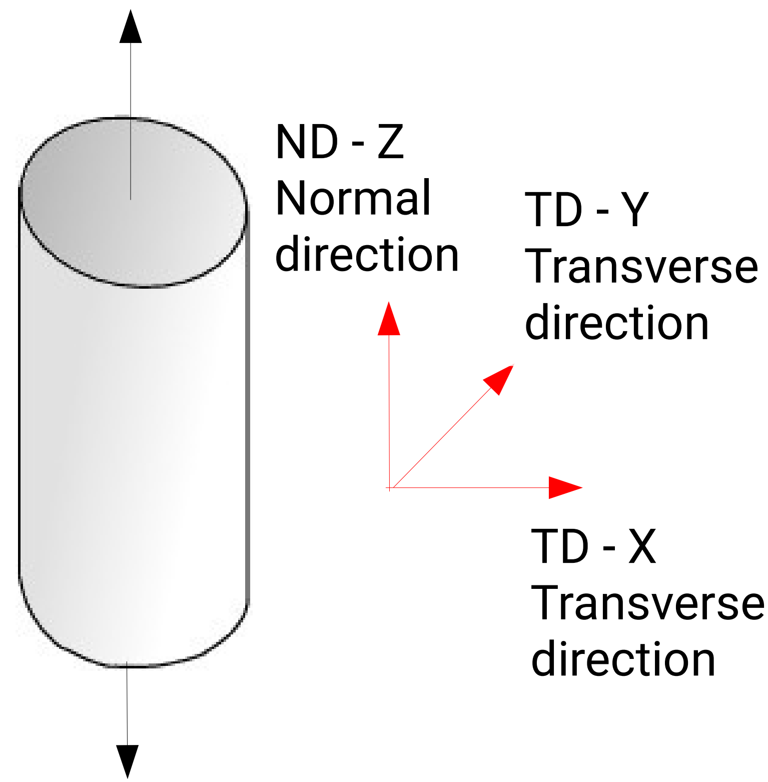
Plane : (001)
Normal to plane : [001]

Sample reference frame

Depends on process applied to the sample

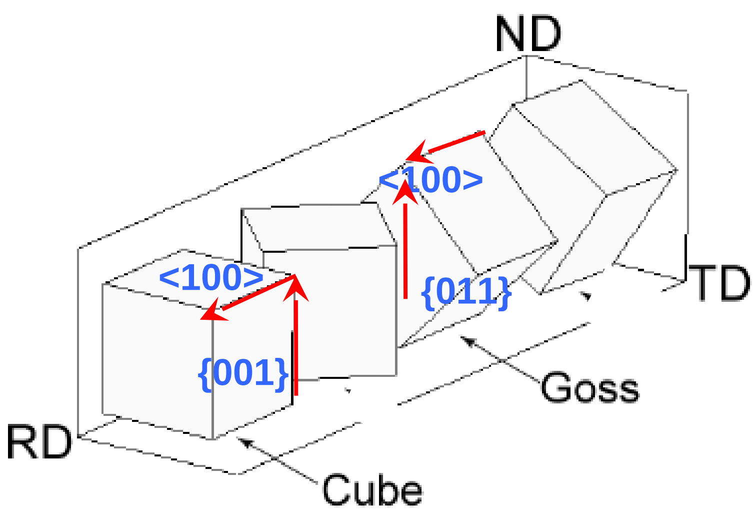


Rolling (laminage)



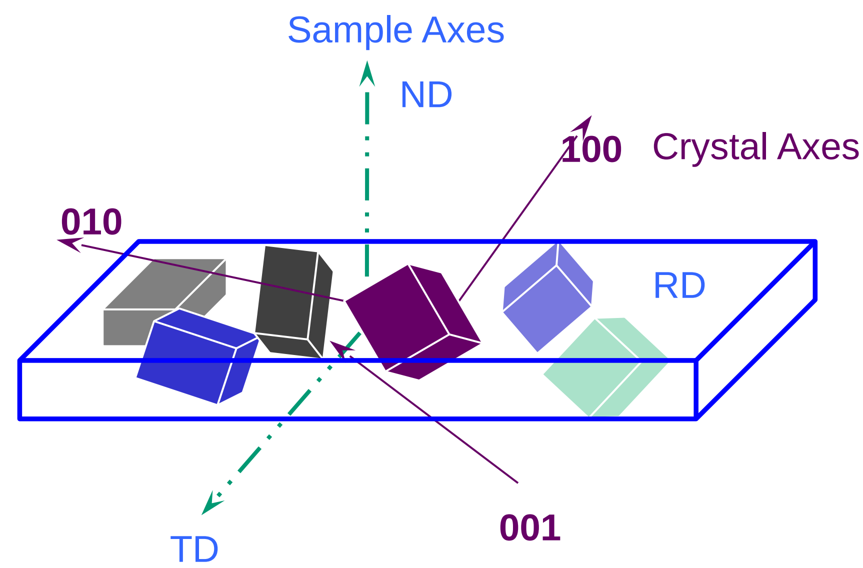
Tension

Crystal orientation



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

Defined with “standard” component or Euler angles to rotate from one coordinate system to the other



Rotation 1 (φ1): rotate sample axes about ND

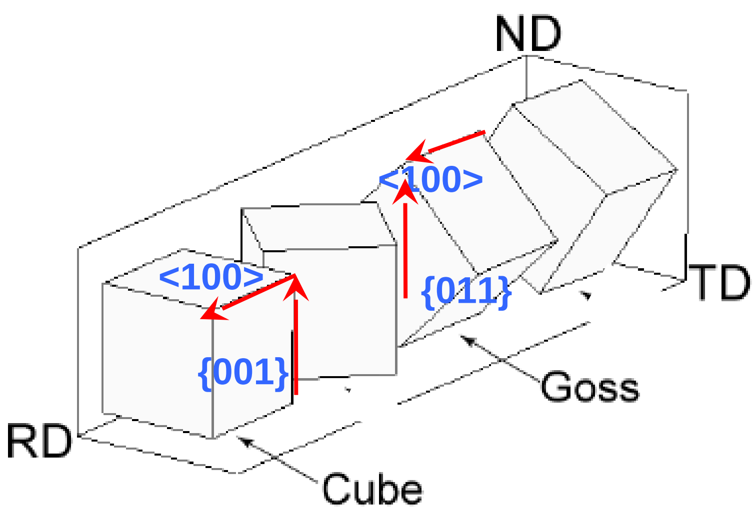
Rotation 2 (Φ): rotate sample axes about rotated RD

Rotation 3 (φ2): rotate sample axes about rotated ND

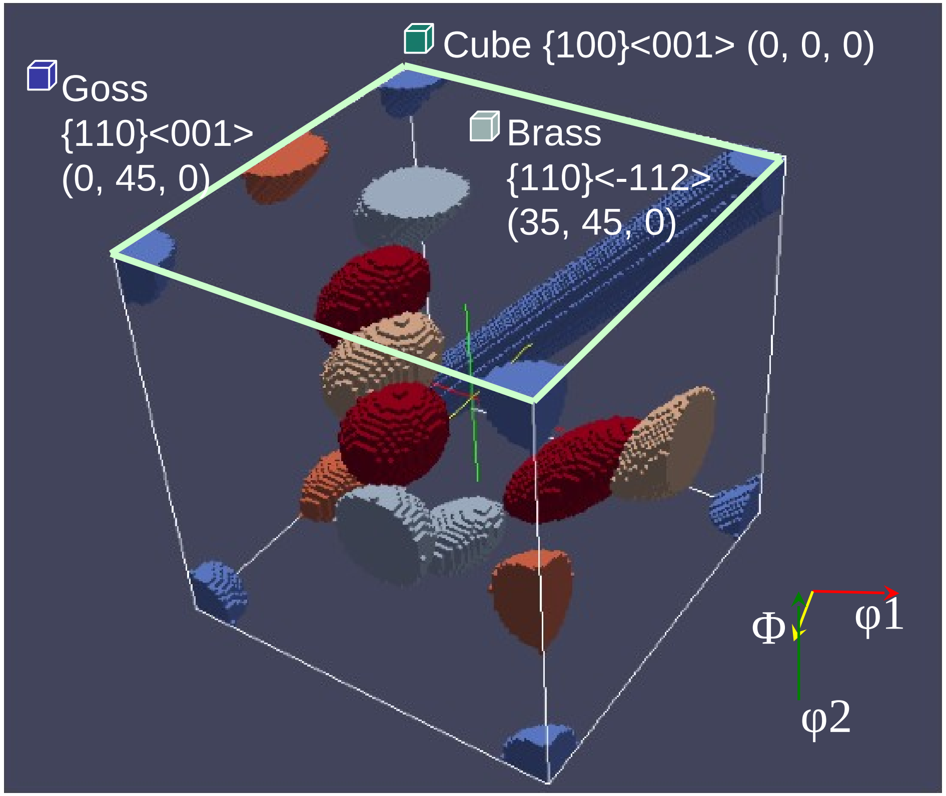
C. N. Tomé and R. A. Lebensohn, Crystal Plasticity, presentation at Pohang University of Science and Technology, Korea, 2009

Orientation space

Defined with “standard” component or Euler angles to rotate from one coordinate system to the other



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



2- Grain orientation
b- Euler angles

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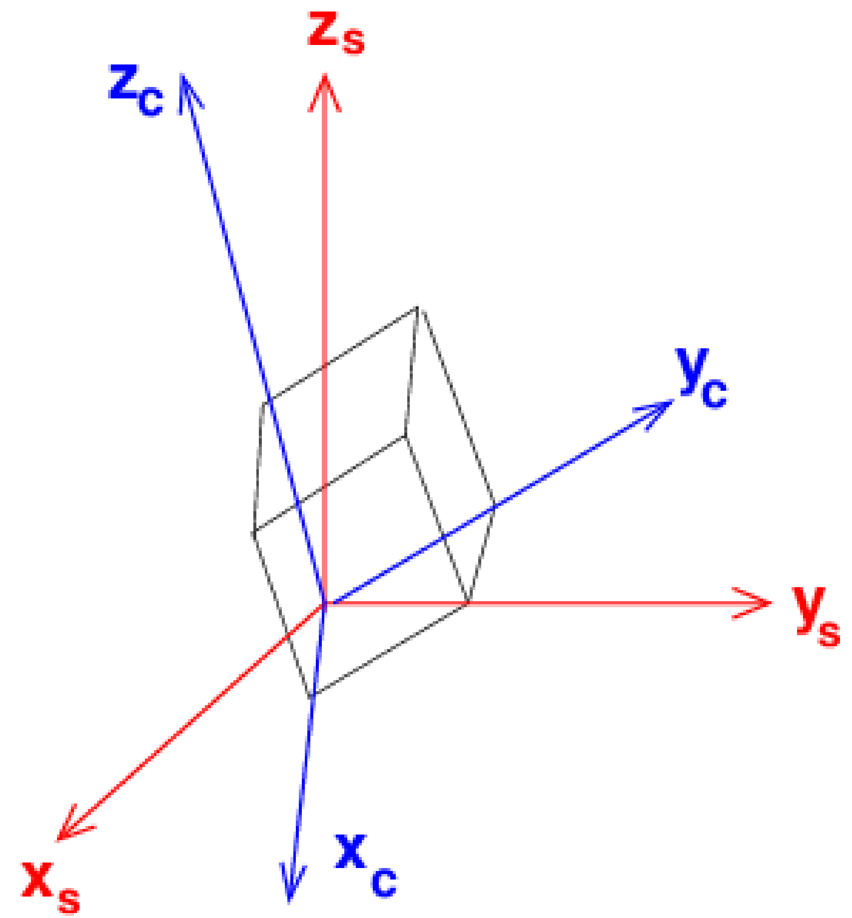
Reference frame transformation Bunge convention

Transformation from the sample reference frame to the crystal reference frame



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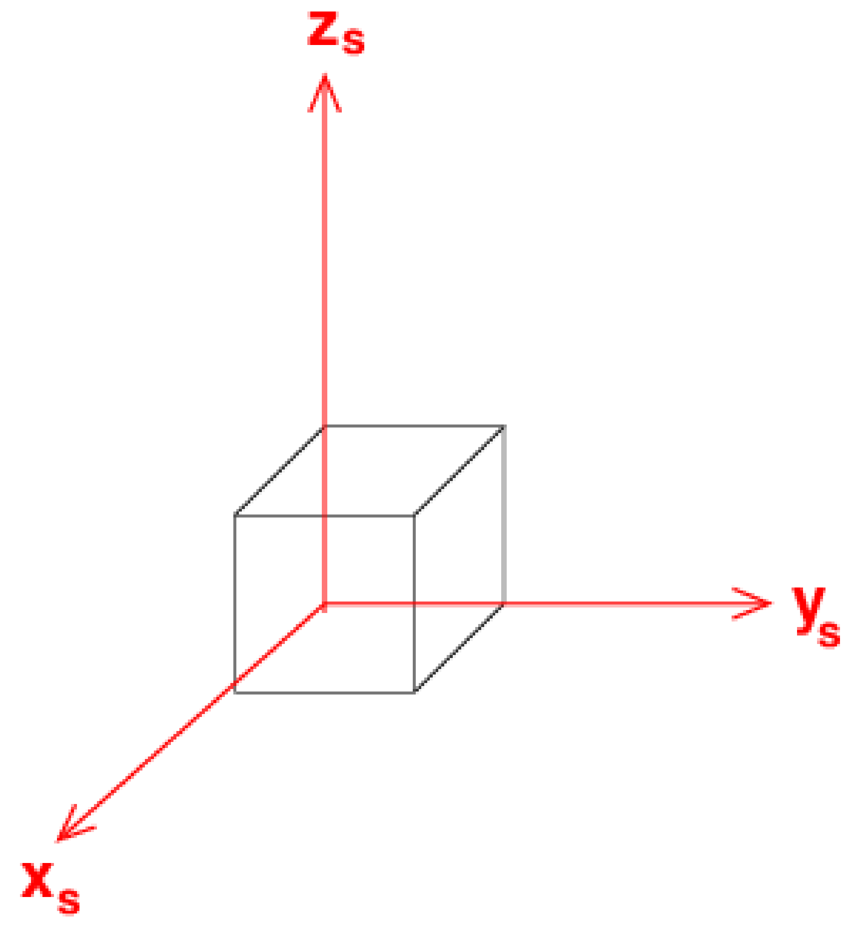
Reference frame transformation
Bunge convention

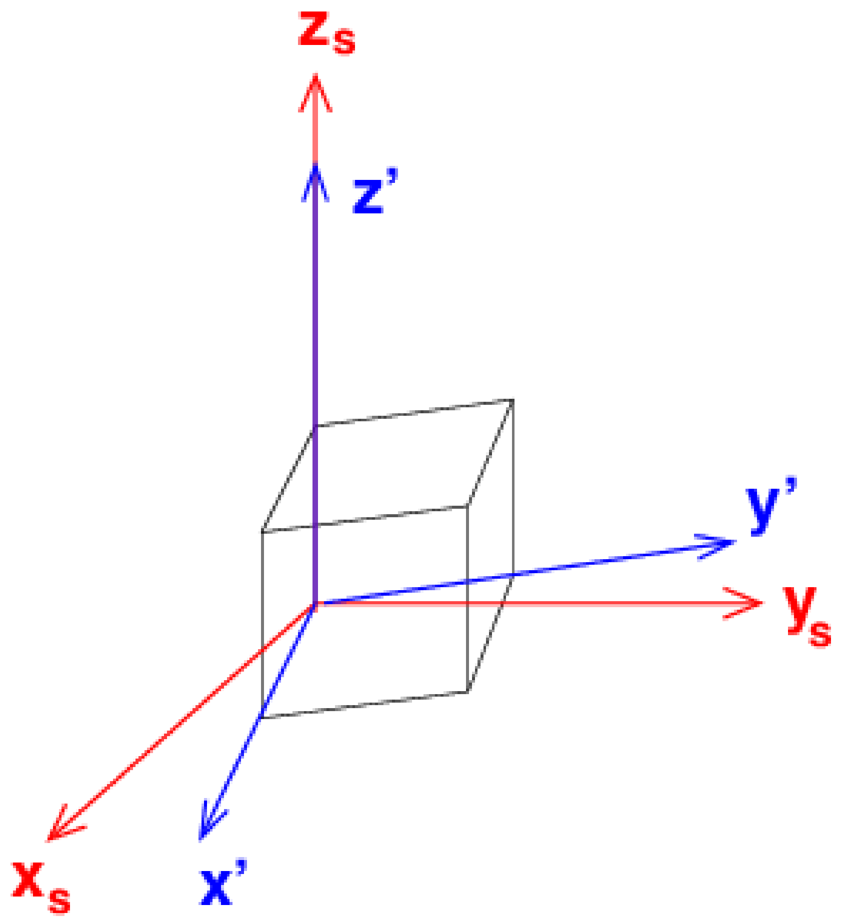
Transformation from the sample reference frame to the crystal reference frame



Reference frame transformation Bunge convention

Transformation from the sample reference frame to the crystal reference frame

- first rotation

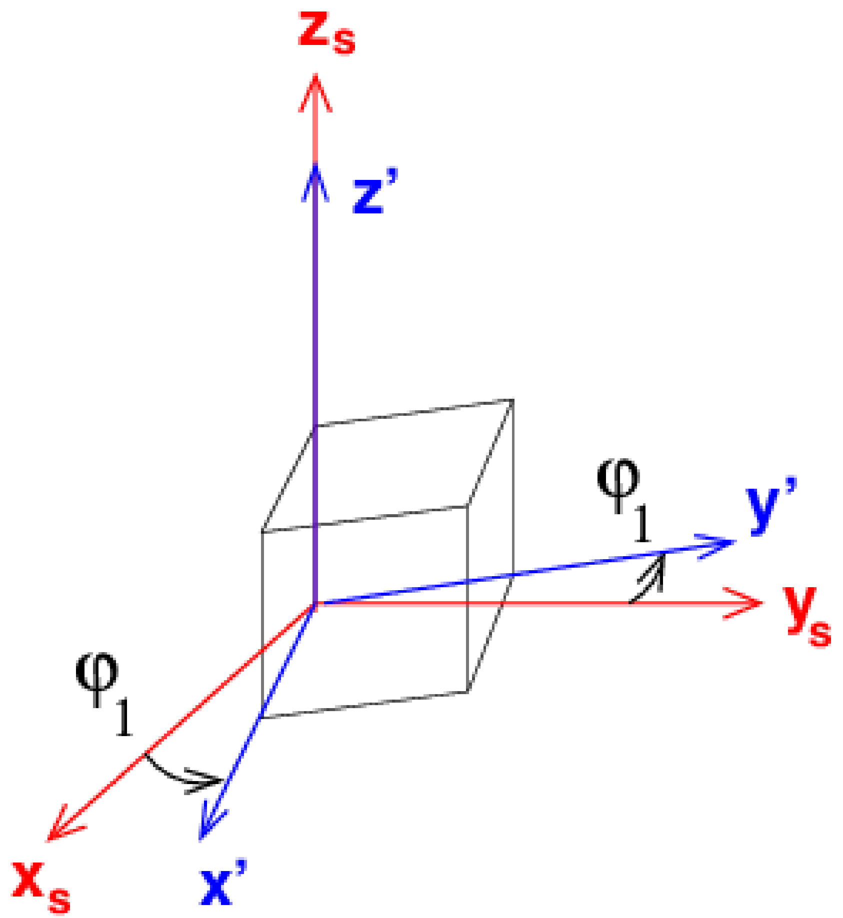


Reference frame transformation
Bunge convention

Transformation from the sample reference frame to the crystal reference frame

- first rotation

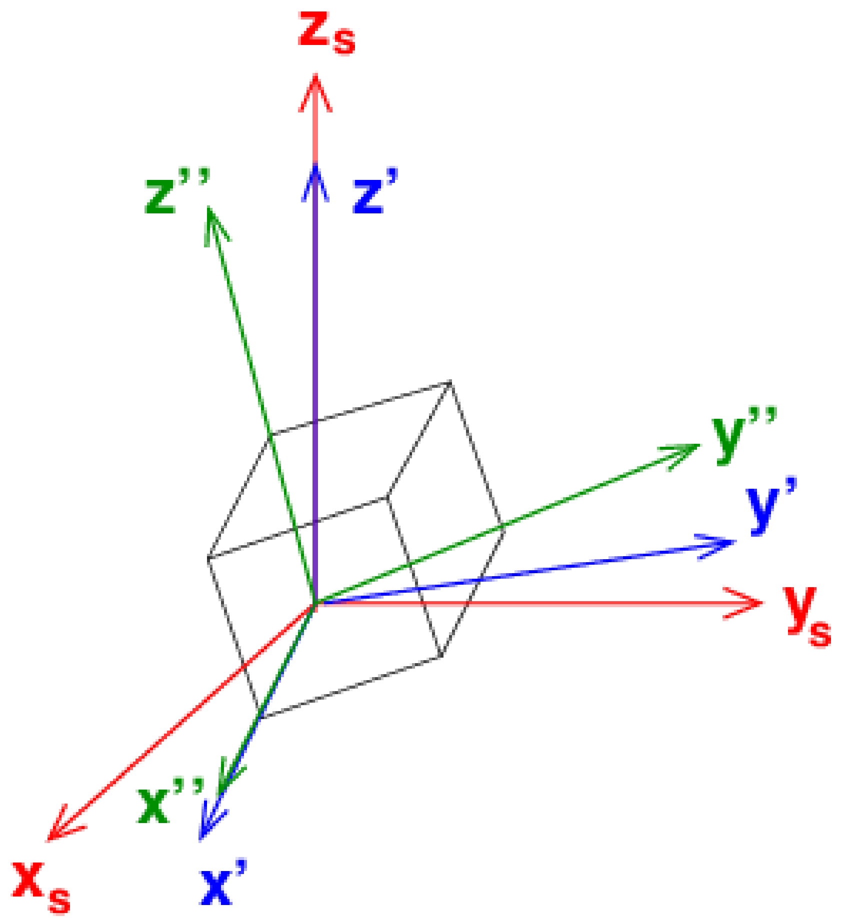
  φ_1 – rotation around z_s



Reference frame transformation
Bunge convention

Transformation from the sample reference frame to the crystal reference frame

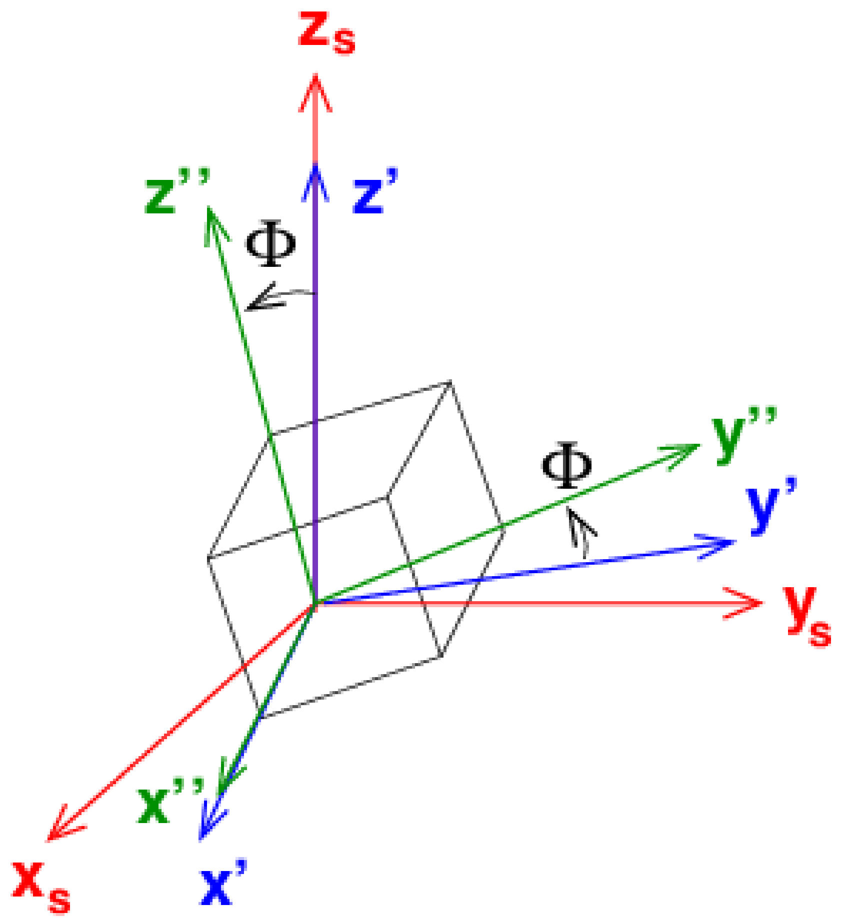
- first rotation
  - φ_1 – rotation around z_s
- second rotation



Reference frame transformation
Bunge convention

Transformation from the sample reference frame to the crystal reference frame

- first rotation
  - φ_1 – rotation around z_s
- second rotation
  - Φ – rotation around x'



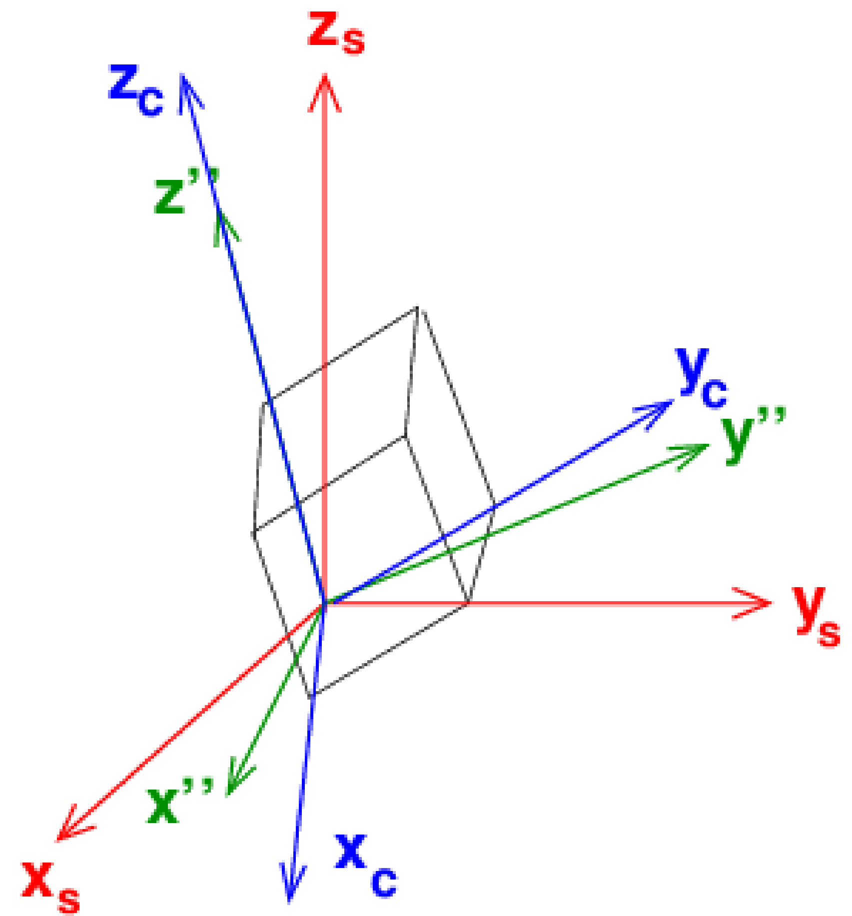
Reference frame transformation
Bunge convention

Transformation from the sample reference frame to the crystal reference frame

- first rotation

  φ_1 – rotation around z_s
- second rotation

  Φ – rotation around x'
- third rotation



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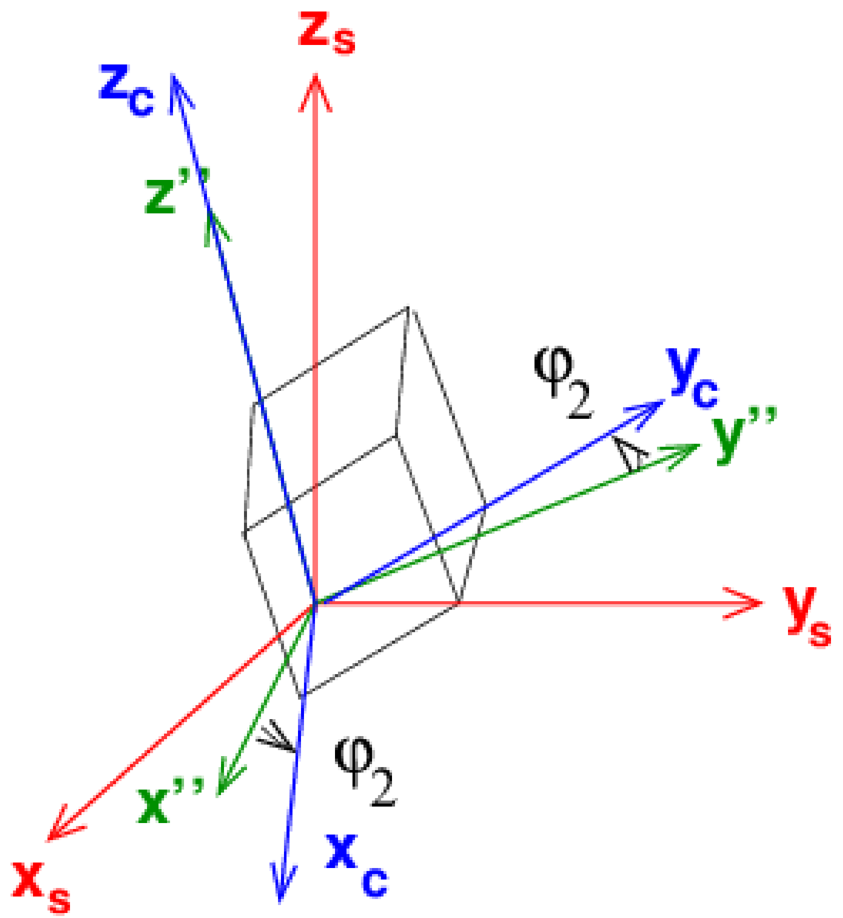
Reference frame transformation
Bunge convention

Transformation from the sample reference frame to the crystal reference frame

- first rotation
  - φ_1 – rotation around z_s
- second rotation
  - Φ – rotation around x'
- third rotation
  - φ_2 – rotation around z''



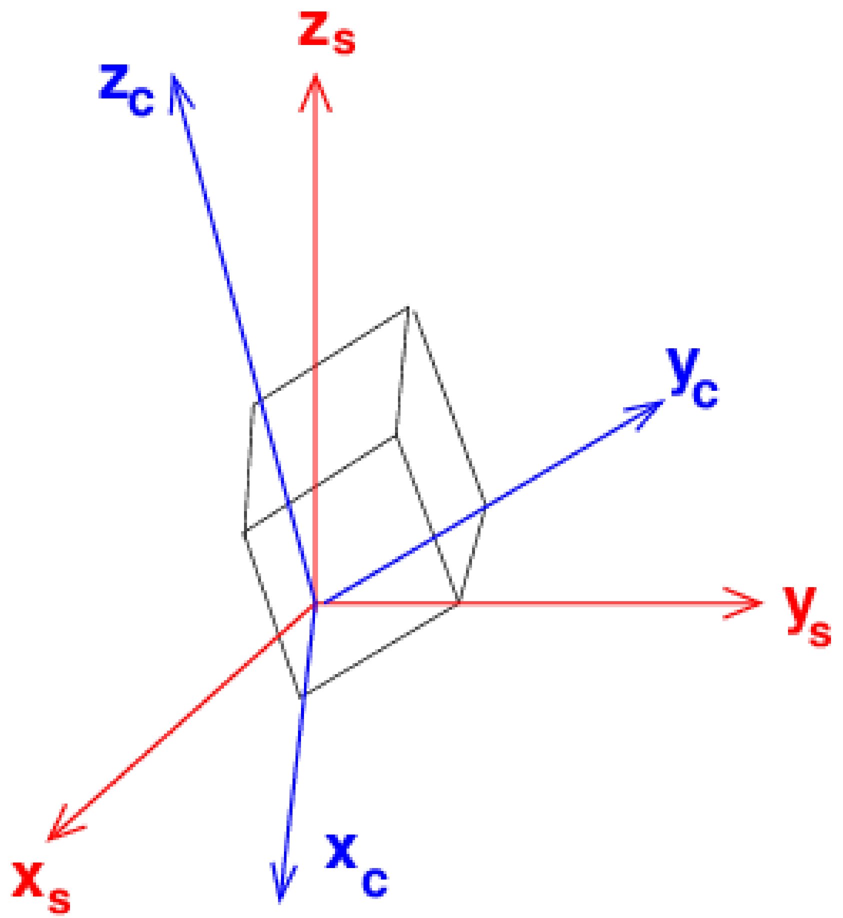
Reference frame transformation
Bunge convention

Transformation from the sample reference frame to the crystal reference frame

- first rotation
  - φ_1 – rotation around z_s
- second rotation
  - Φ – rotation around x'
- third rotation
  - φ_2 – rotation around z''

Crystal orientation defined by 3 Euler angles φ_1, Φ, et φ_2.

Bunge convention (there are others, Matthies, Roe, etc)



Why 3 angles?

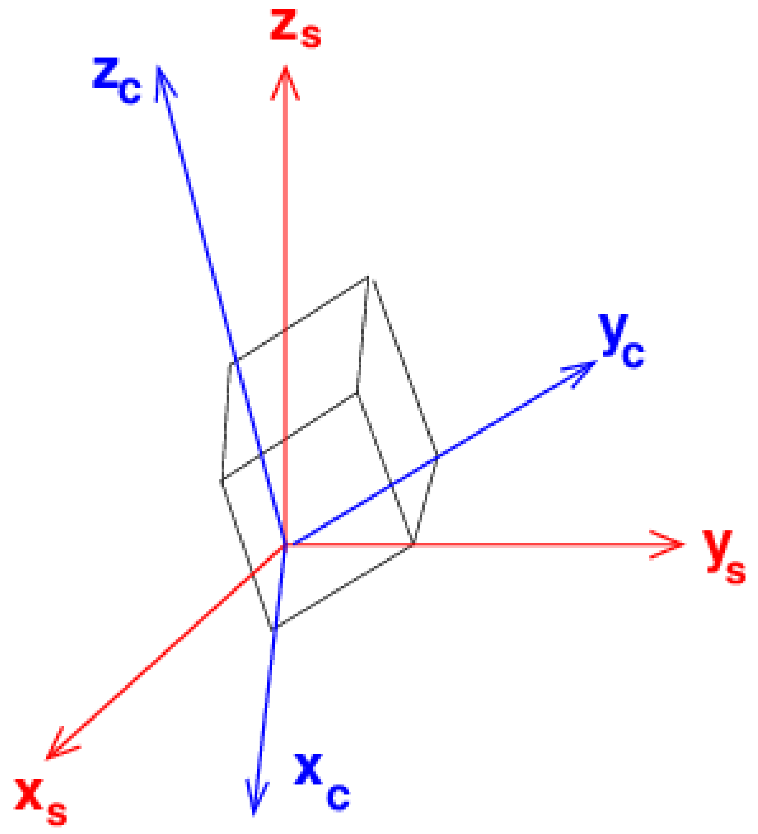
φ_1 – rotation around z_s

Φ – rotation around x'

φ_2 – rotation around z''

Angles φ_1 and Φ are used to locate [001] (z_c) in relation to the sample reference frame

Angle φ_2 adds a supplementary rotation to locate x_c and y_c



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2- Grain orientation
b- Marix representation

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Matrix representation

Rotations can be expressed as matrices

$$R_{\mathbf{x}}(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}, \quad R_{\mathbf{y}}(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}, \quad R_{\mathbf{z}}(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Direct θ rotation around X

Direct θ rotation around Y

Direct θ rotation around Z

To combine rotations: multiplication of corresponding matrices.

For instance, a rotation of α around **z**, followed by a rotation β around **x**, and then a rotation γ around ***z*** will be:

$$g(\alpha,\beta,\gamma) = g_z(\gamma) * g_x(\beta) * g_z(\alpha)$$

Pay attention to the order! The first rotation is on the right side of the equation!

Properties of rotation matrices

The inverse of a rotation matrix is its transpose

$$g^{-1} = {}^{t}g$$

The product of 2 rotations is a rotation

$$g_3 = g_2 * g_1$$

In dimension >2, order matters when multiplying rotation matrices

$$g_1 * g_2 \neq g_2 * g_1$$

They are orthogonal (they do not change vector length)

$$\det(g) = 1$$

$$\sqrt{(g_{11}^2 + g_{12}^2 + g_{13}^2)} = 1$$

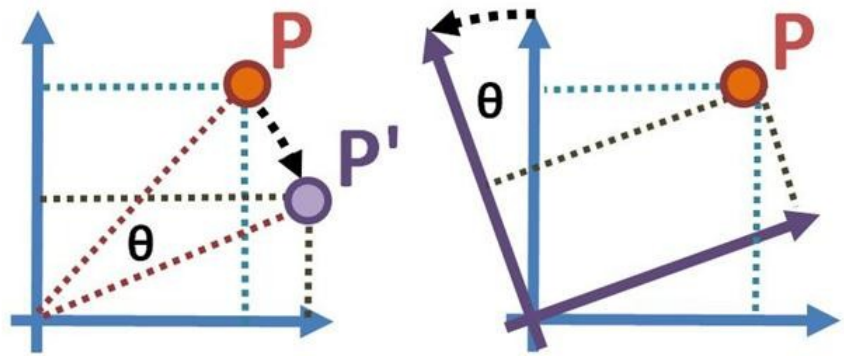
$$\sqrt{(g_{i1}^2 + g_{i2}^2 + g_{i3}^2)} = 1$$

$$\sqrt{(g_{1i}^2 + g_{2i}^2 + g_{3i}^2)} = 1$$

Passive rotation – active rotation

Active rotation:
The point moves in a fixed reference frame

$\theta < 0$



$\theta > 0$

Passive rotation:
Le point is fixed and the reference frame moves

In materials science, we express physical properties (stress, elasticity, etc) in different reference frames

- The sample reference frame
- The crystal reference frame
- Etc

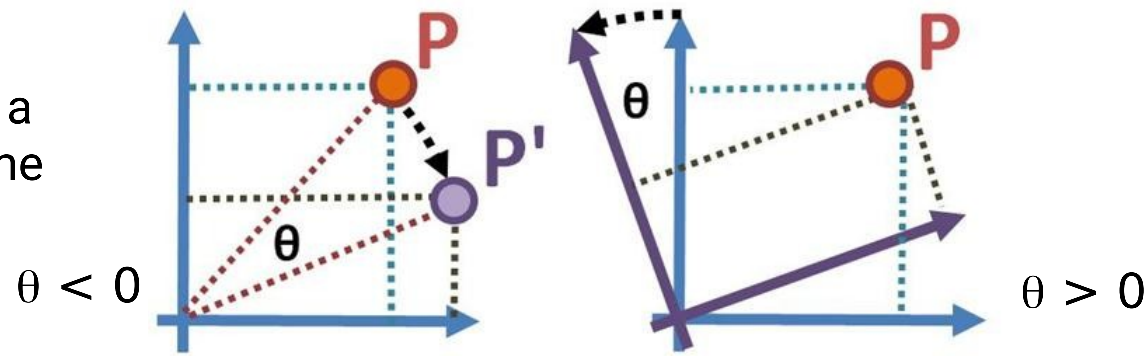
The sample, itself, does not move.

In mechanics, we study movements. The sample moves. Mechanics uses active rotations.

In texture analysis, we are moving reference frames, not the sample : texture analysis uses *passive rotations*.

Passive rotation – active rotation

Active rotation:
The point moves in a fixed reference frame



Passive rotation:
Le point is fixed and the reference frame moves

$$\begin{cases} x' = x\cos\theta - y\sin\theta \\ y' = x\sin\theta + y\cos\theta \end{cases}$$

$$g = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

$$\begin{cases} x' = x\cos\theta + y\sin\theta \\ y' = -x\sin\theta + y\cos\theta \end{cases}$$

$$g = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

Bunge angles – Rotation matrices

Rotation 1 (φ_1): rotates and axis 3 (*z*) of the sample reference frame

$$g_1 = \begin{bmatrix} \cos\varphi_1 & \sin\varphi_1 & 0 \\ -\sin\varphi_1 & \cos\varphi_1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Rotation 2 (Φ): rotation around axis 1 (*x*) of the newly formed reference frame

$$g_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\Phi & \sin\Phi \\ 0 & -\sin\Phi & \cos\Phi \end{bmatrix}$$

Rotation 3 (φ_2): rotation around axis 3 (*z*) of the newly formed reference frame

$$g_3 = \begin{bmatrix} \cos\varphi_2 & \sin\varphi_2 & 0 \\ -\sin\varphi_2 & \cos\varphi_2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$g(\varphi_1, \Phi, \varphi_2) = g_3 \cdot g_2 \cdot g_1$$

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

Geometric interpretation

Crystal *x* axis in the sample reference frame

Crystal *y* axis in the sample reference frame

Crystal *z* axis in the sample reference frame

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

Sample *x* axis in the crystal reference frame

Sample *y* axis in the crystal reference frame

Sample *z* axis in the crystal reference frame

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

2- Grain orientation
c- Graphical representation – Pole figures

Issue with 3D rotation matrices

(Almost) no-one can visualize 3D Euler angles.

Most figures in science use 2D projections. This is what people are used to. How to represent rotations in 3D projected onto a 2D figure?

A true material is made of thousands of crystallites: nearly impossible to look at all Euler angles individually.

Crystals have symmetries. Not easy (at all) to account for crystal symmetries with Euler angles.

Solution: *pole figures*.

What is a pole?

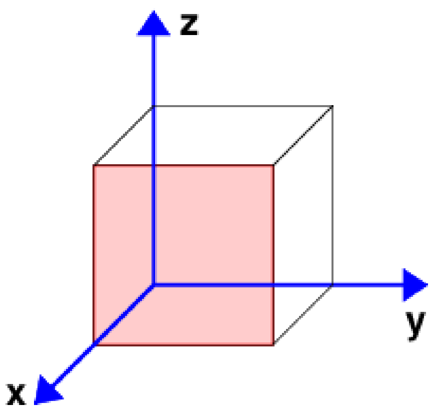
Crystallography reminders

- (hkl) is the plane of *Miller indices* *h*, *k*, and *l*
- [hkl] is the direction of *direction indices* *h*, *k*, and *l*
- {hkl} is a family of planes which are equivalent due to symmetry operations
- <hkl> is a family of directions which are equivalent due to symmetry operations
- *hkl* indices (with no parenthesis) indicate Bragg reflection from the (hkl) planes. They are called Laue indices.

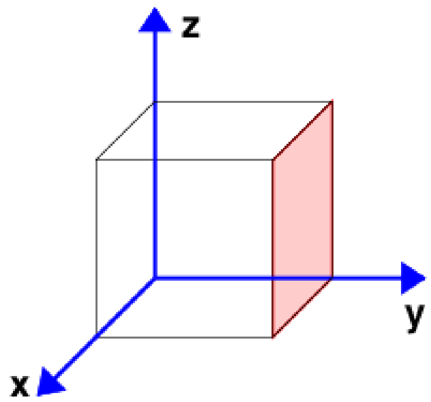
Pole = intersection between a line and a sphere around the crystal

- Planes: line perpendicular to a diffracting plane. Defined with Laue indices (i.e. no parenthesis) as we are very often referring to diffraction.
- Directions: line parallel to a crystal direction. Better use <hkl> pole in this case.

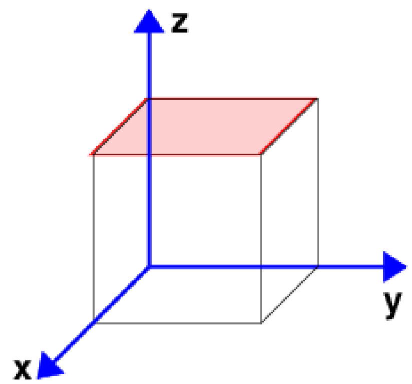
In a cubic structure



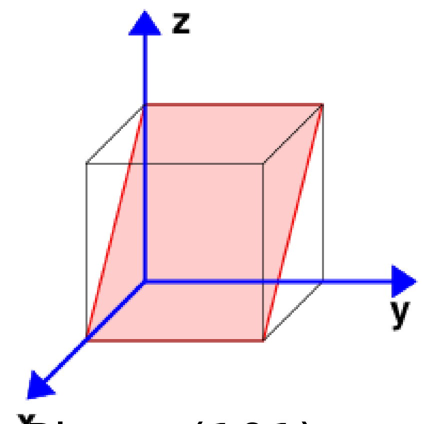
Plane: (100)
Normal : [100]



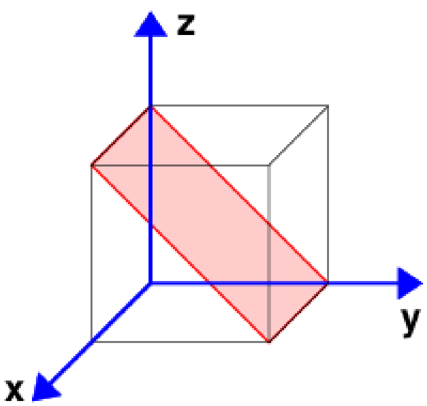
Plane: (010)
Normal: [010]



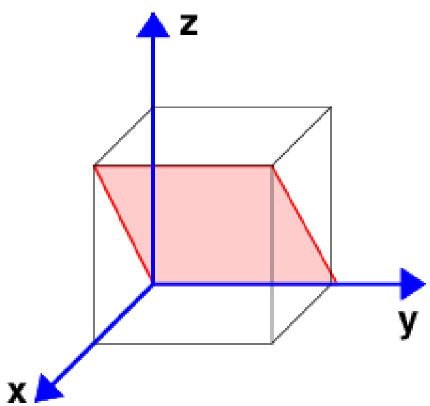
Plane: (001)
Normal: [001]



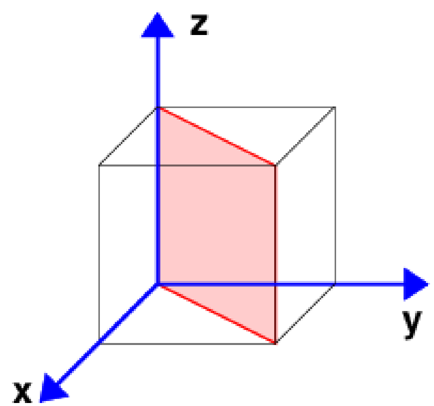
Plane: (101)
Normal: [101]/√2



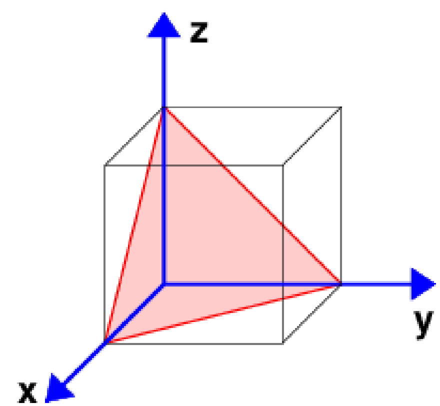
Plane: (011)
Normal: [011]/√2



Plane: (-101)
Normal: [-101]/√2



Plane: (-110)
Normal : [-110]/√2



Plane: (111)
Normal: [1,1,1]/√3

Tips and tricks

Pole = intersection between a line and a sphere around the crystal

- Planes: line perpendicular to a diffracting plane. Defined with Laue indices (i.e. no parenthesis) as we are very often referring to diffraction.
- Directions: line parallel to a crystal direction. Better use <hkl> pole in this case.

For a cubic crystal

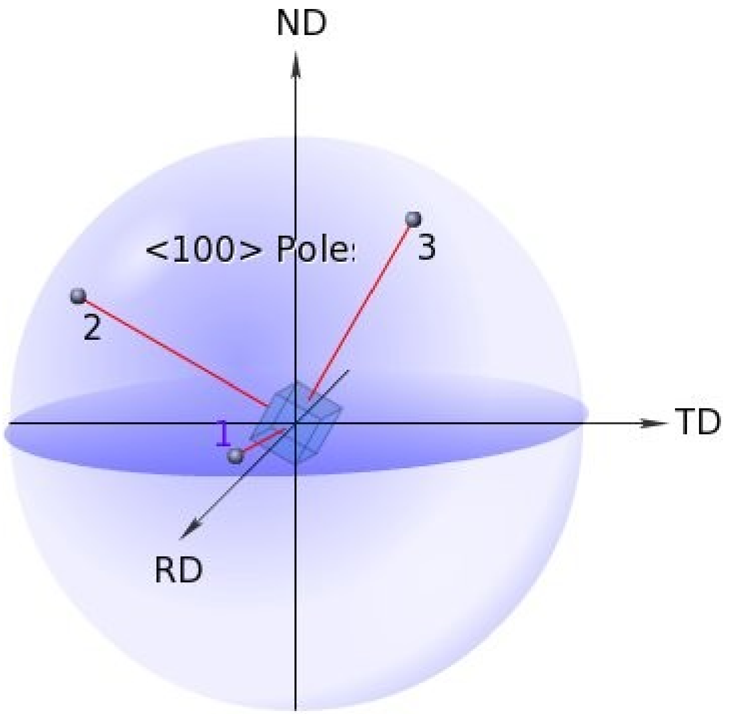
- (hkl) plane is orthogonal to [hkl] direction
- Whatever pole definition you use, it will be the same direction

Pay attention !!!

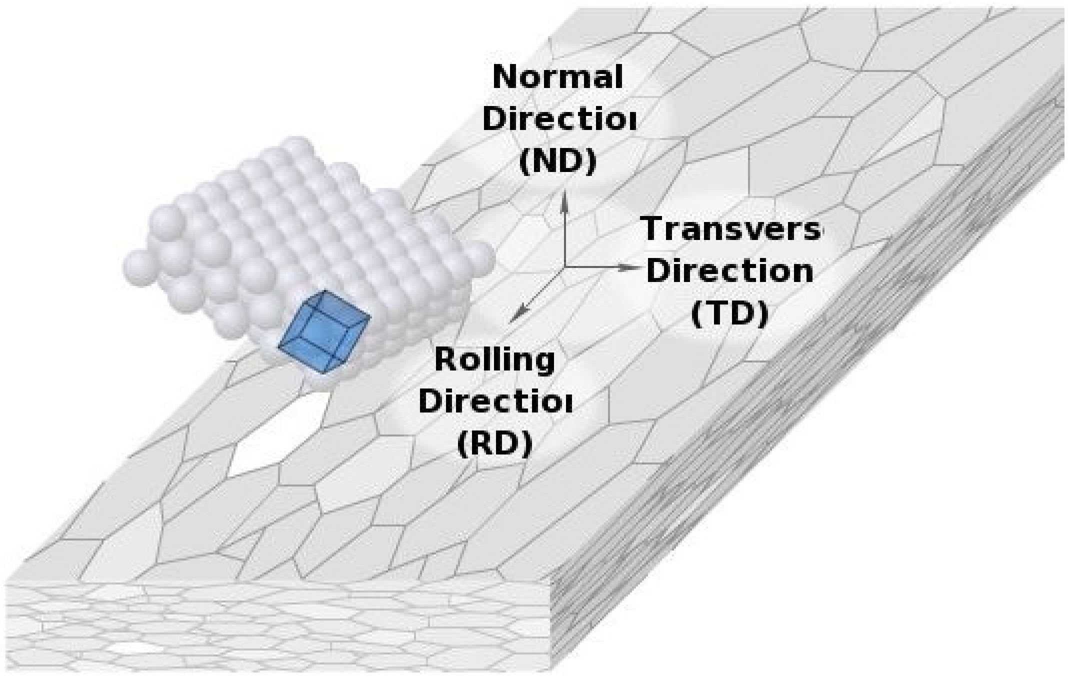
This is not true for other symmetries than cubic.

The [kkl] direction is not always perpendicular to (hkl).

The hkl Laue indices refer to a Bragg reflection, it is perpendicular to (hkl).



Orientation of poles [100], [010], [001] : <100> poles



Cubic-structured crystallite in a deformed sample

Illustrations : aluMatter

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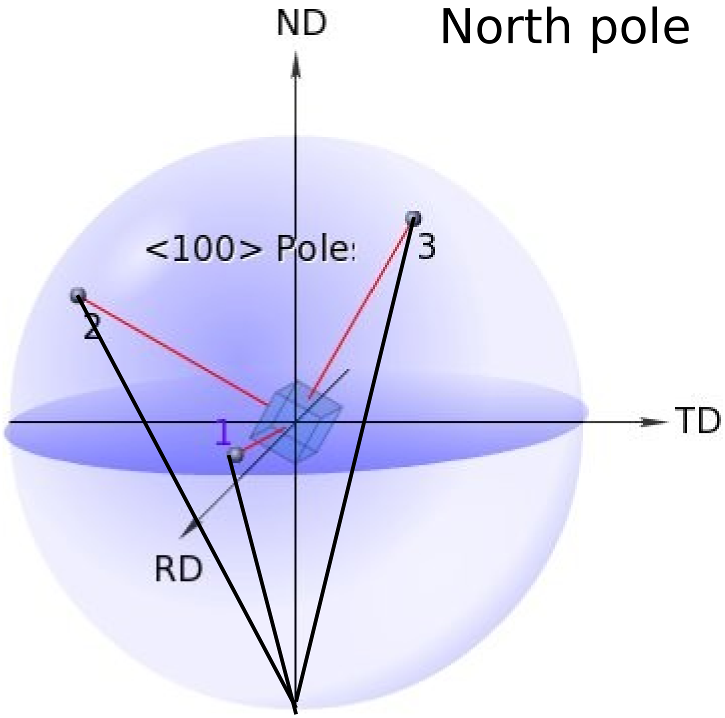
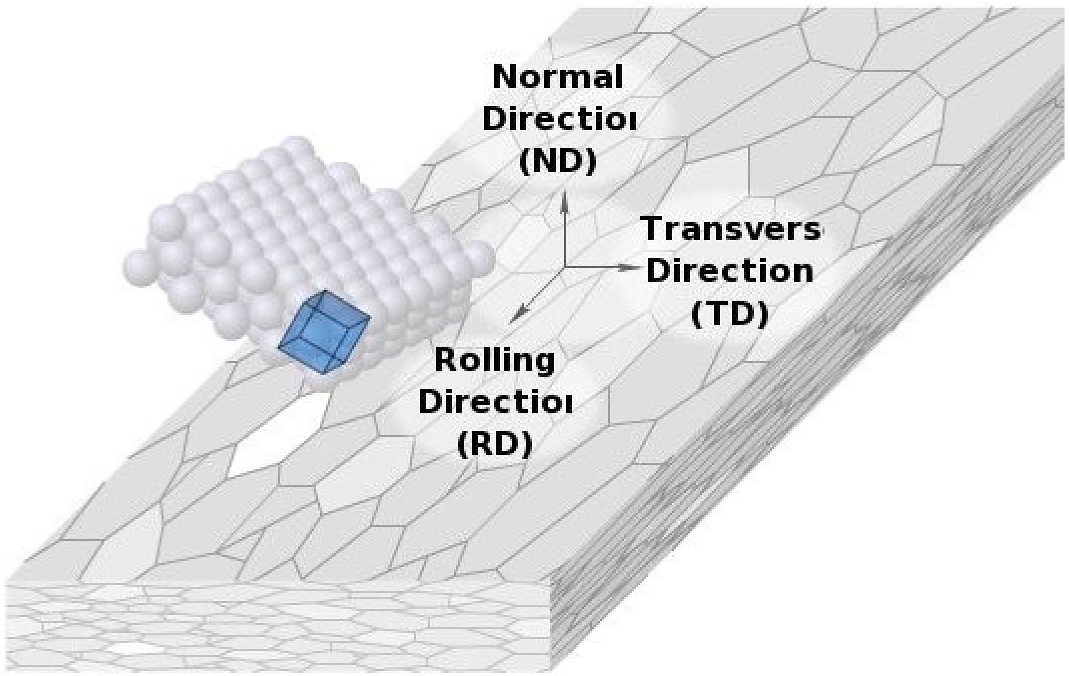
Pole figure

North pole



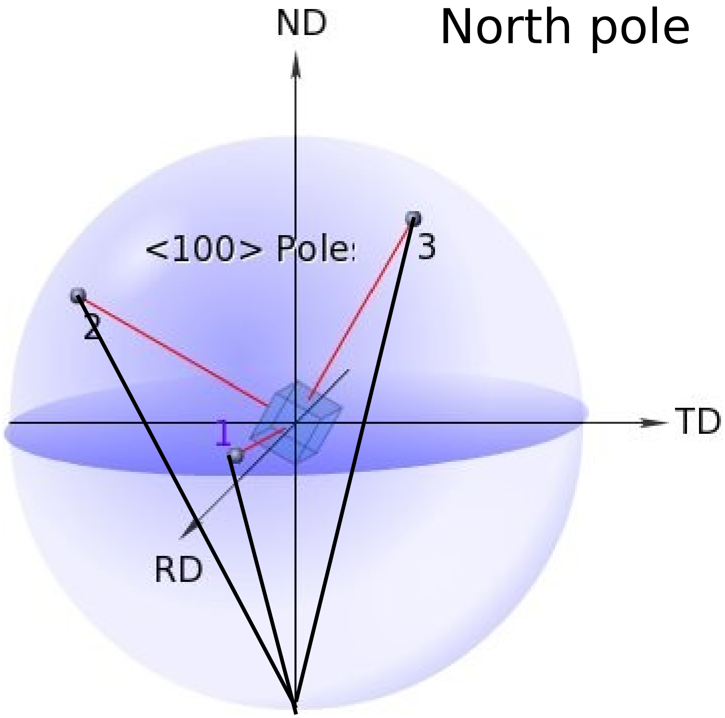
South pole

Lines between <100> poles and south pole
Intersection with equatorial plane



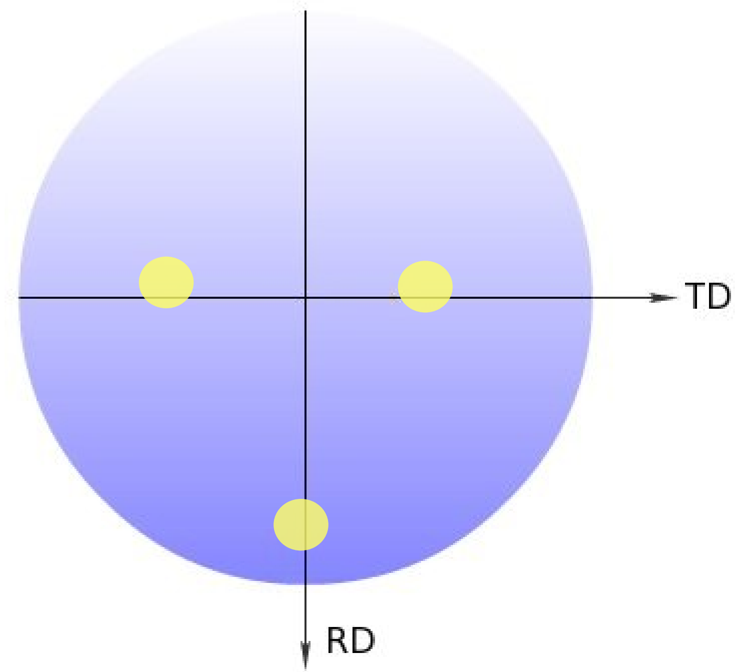
Cubic-structured crystallite in
a deformed sample

Illustrations : aluMatter



South pole

<100> pole figure



Lines between <100> poles and south pole
Intersection with equatorial plane

View from North pole

Illustrations : aluMatter

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PF training 1

Take a cubic crystal with
- [100] // RD
- [010] // TD
- [001] // ND

Plot the <100> pole figure
Plot the <111> pole figure

Illustrations : aluMatter

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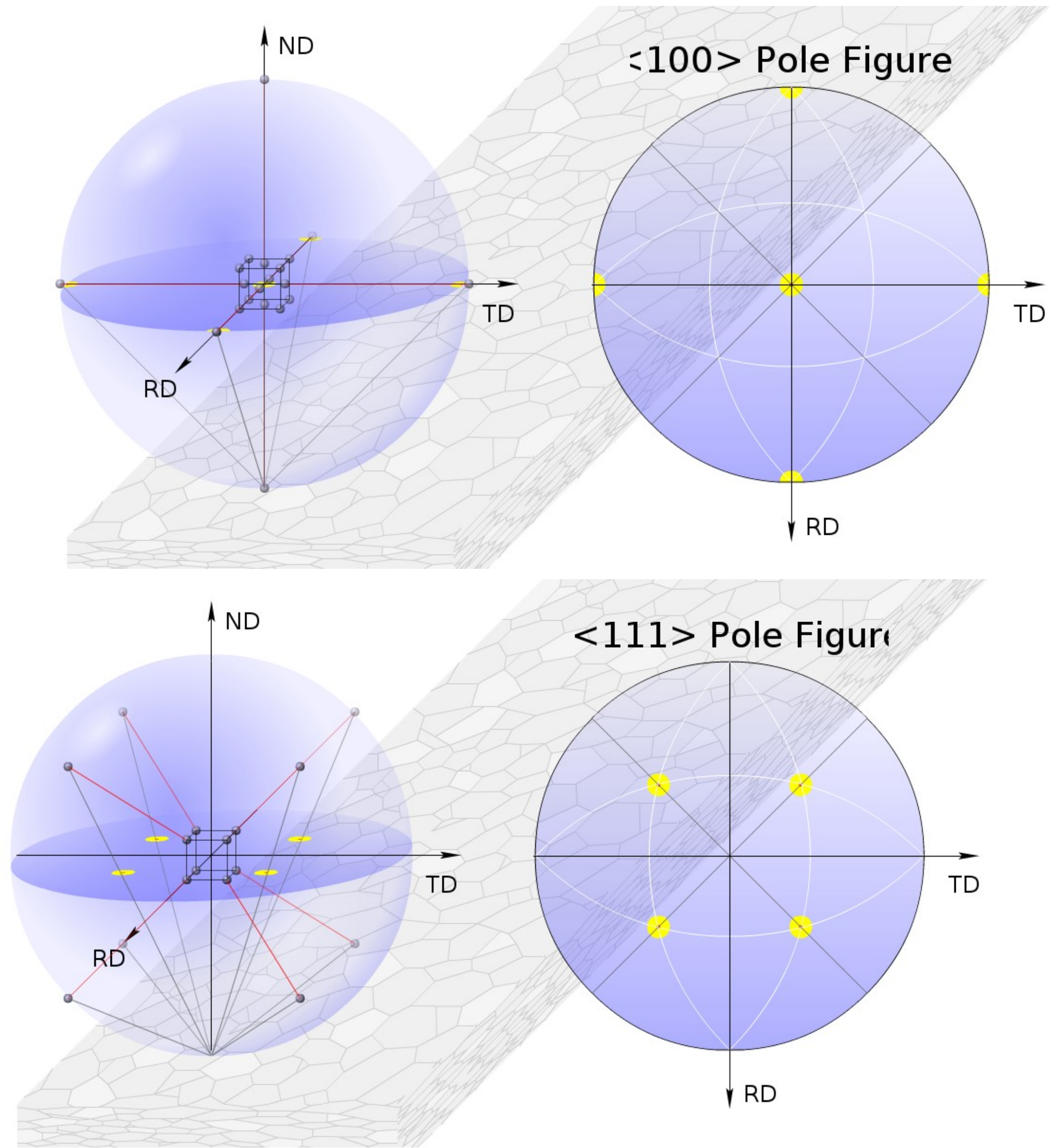
PF training 1

Take a cubic crystal with
- [100] // RD
- [010] // TD
- [001] // ND

Plot the <100> pole figure
Plot the <111> pole figure



Illustrations : aluMatter

PF training 2

Take a cubic crystal with
- [100] // RD
- [010] // TD
- [001] // ND

Rotate it by 45° around ND

Plot the <100> pole figure
Plot the <111> pole figure

Illustrations : aluMatter

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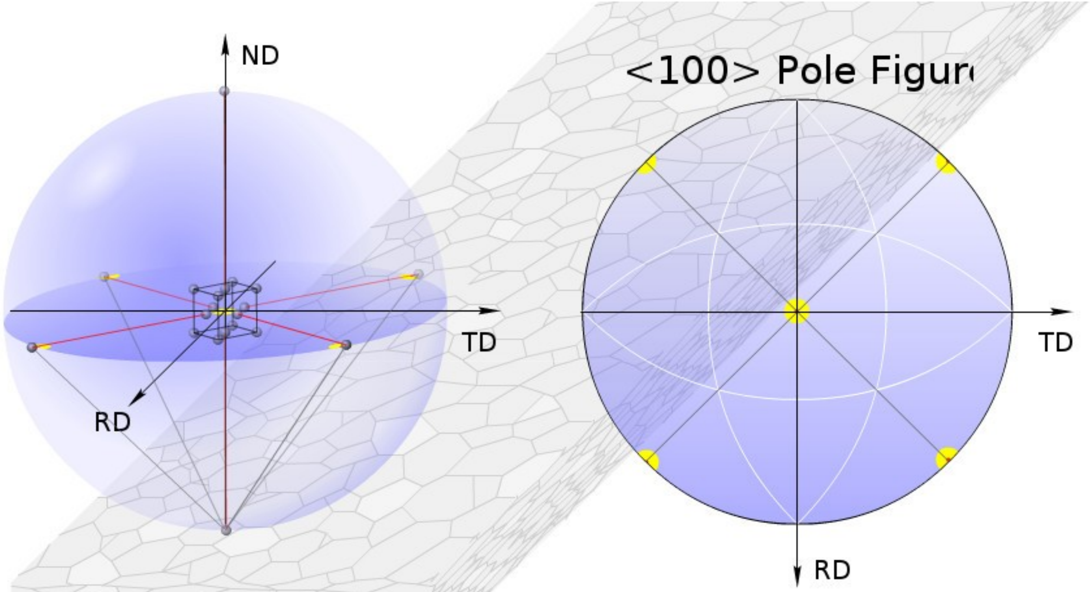
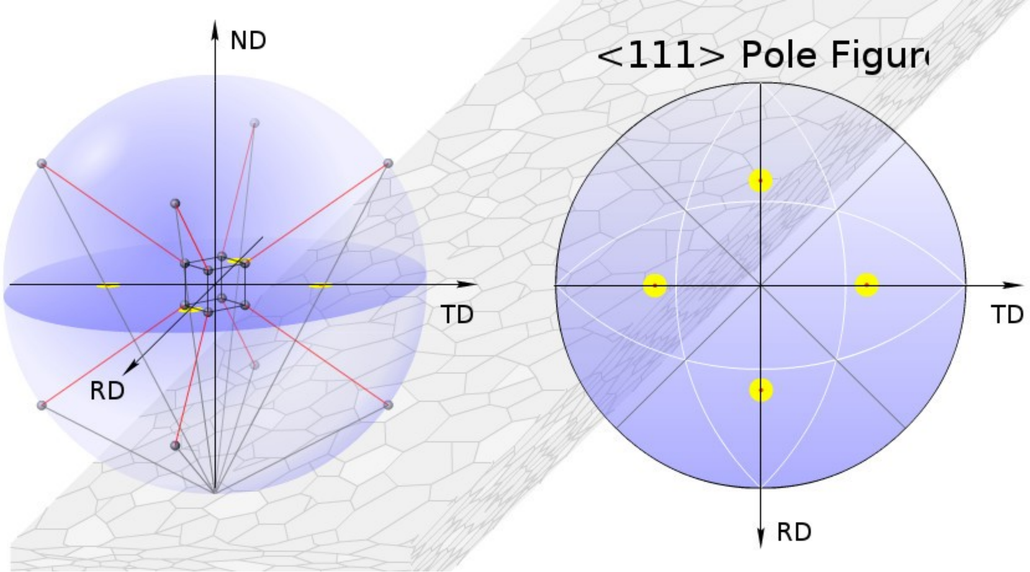
PF training 2

Take a cubic crystal with
- [100] // RD
- [010] // TD
- [001] // ND

Rotate it by 45° around ND

Plot the <100> pole figure
Plot the <111> pole figure





Illustrations : aluMatter

PF training 3

Take a cubic crystal with

- [100] // RD
- [010] // TD
- [001] // ND

Rotate it by 45° around TD

Plot the <100> pole figure
Plot the <111> pole figure

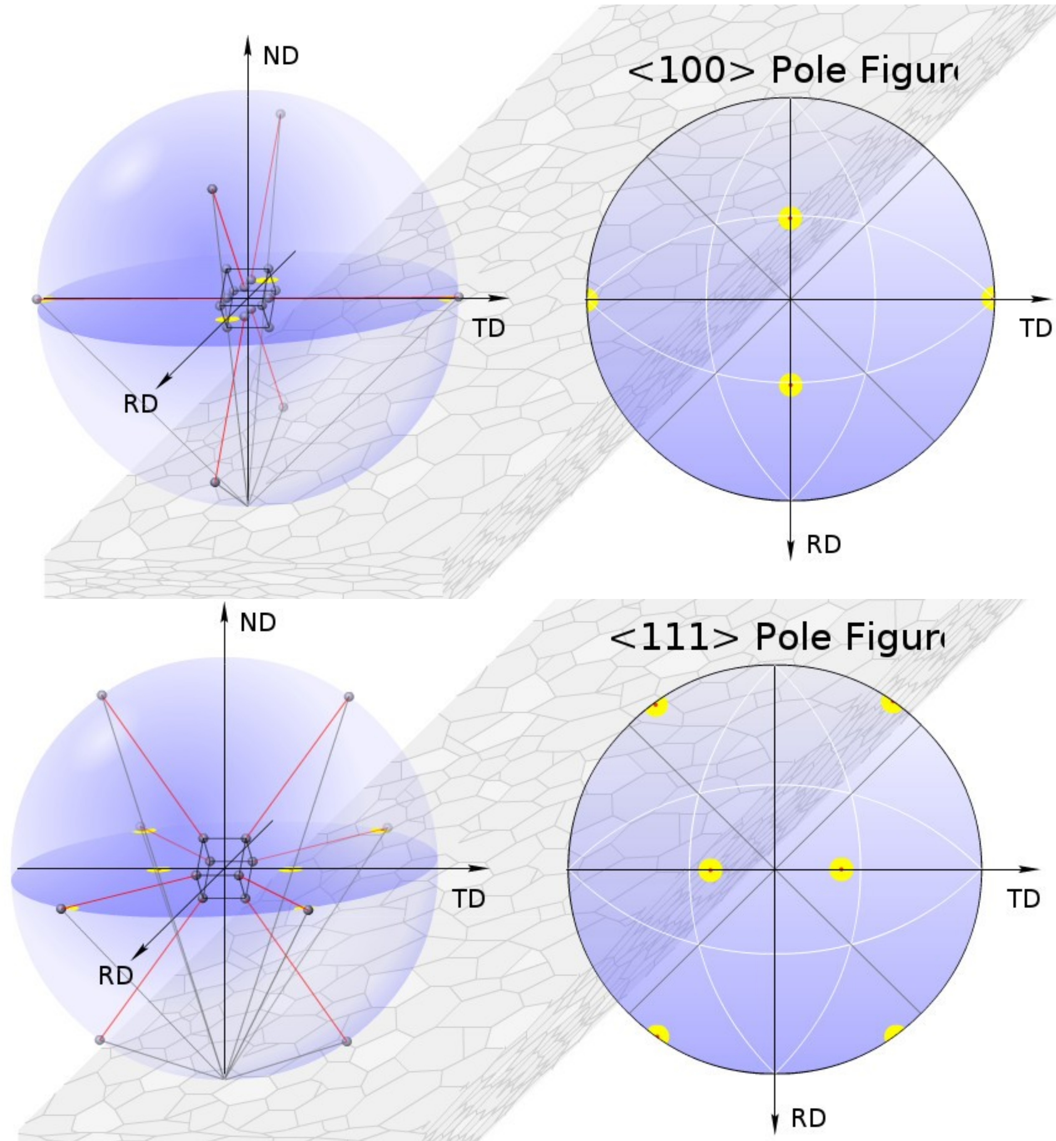
Illustrations : aluMatter

PF training 3

Take a cubic crystal with
- [100] // RD
- [010] // TD
- [001] // ND

Rotate it by 45° around TD

Plot the <100> pole figure
Plot the <111> pole figure



Illustrations : aluMatter

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Unité Matériaux et Transformations