Crystal Mechanics

Lecture 5 – Orientation of Crystallites

Ref : Texture and Related Phenomena, D. N. Lee, 2006
Quantitative Texture Analysis, H.J. Bunge & C. Esling, 1979
Texture and Anisotropy, U.F. Kocks, C.N. Tome H.-R. Wenk, 1998

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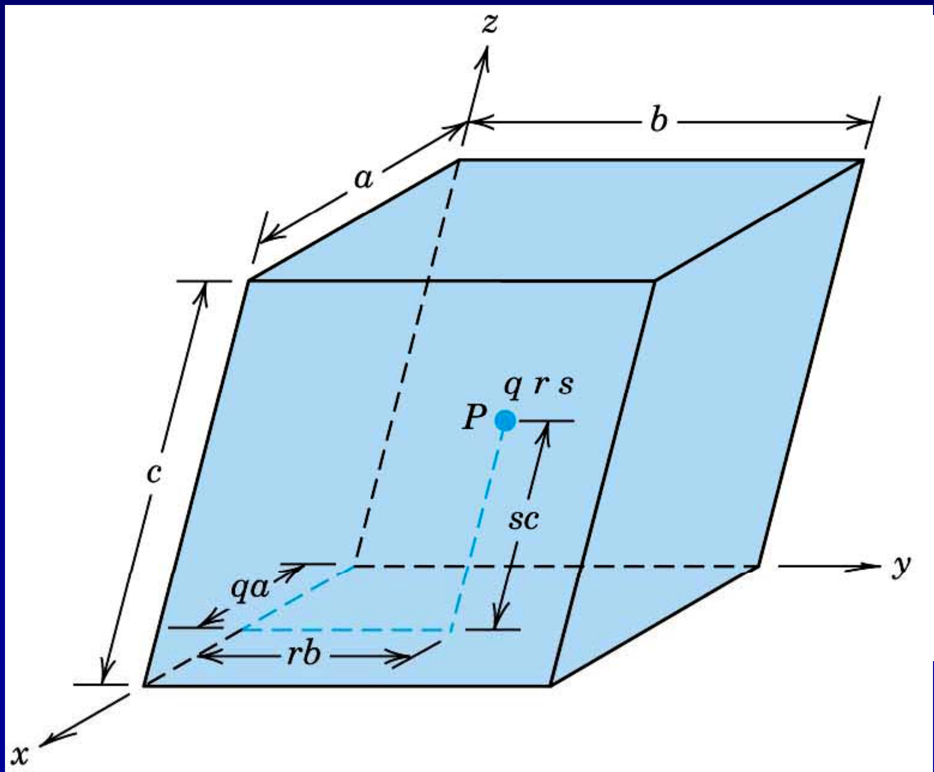
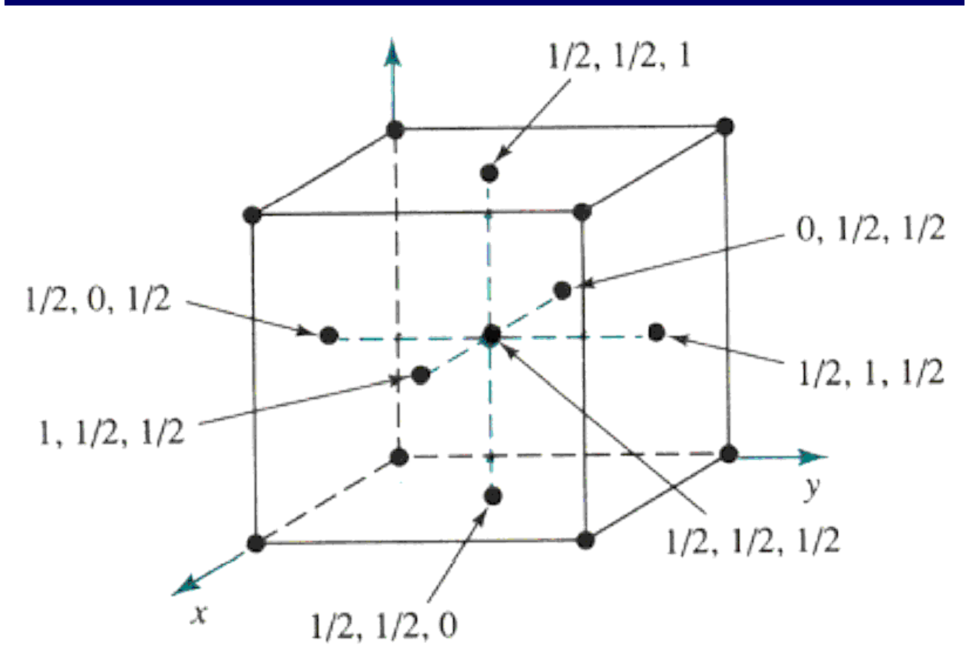
Crystallographic Coordinates

• position: fractional multiples of the unit cell edge lengths
ex) P: q,r,s

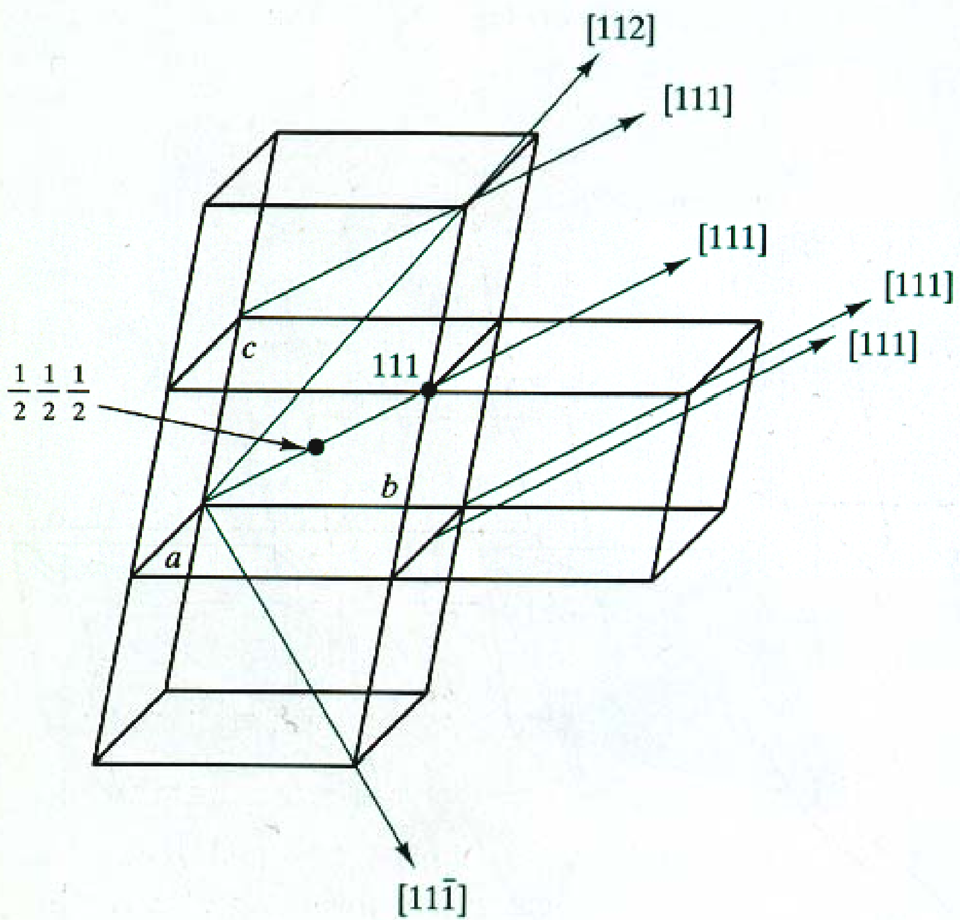




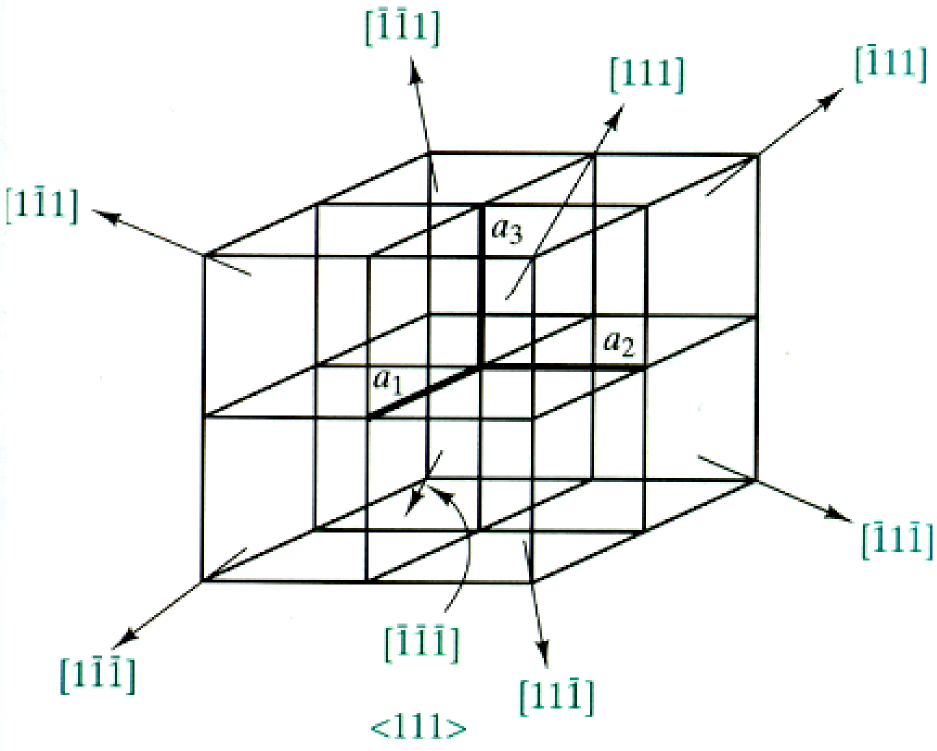
cubic unit cell

Crystallographic Directions

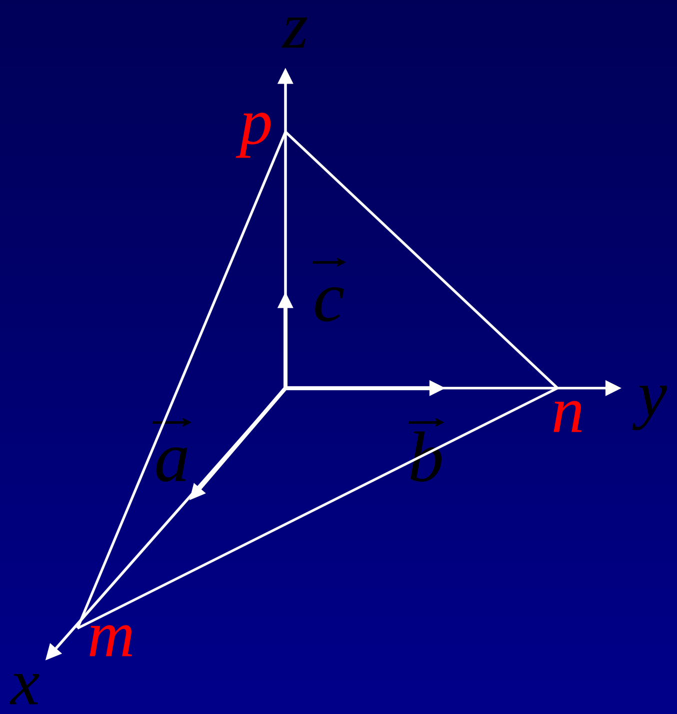
- a line between two points or a vector
- [uvw] square bracket, smallest integer
- families of directions: <uvw> angle bracket



cubic



Crystallographic Planes (Miller Index)



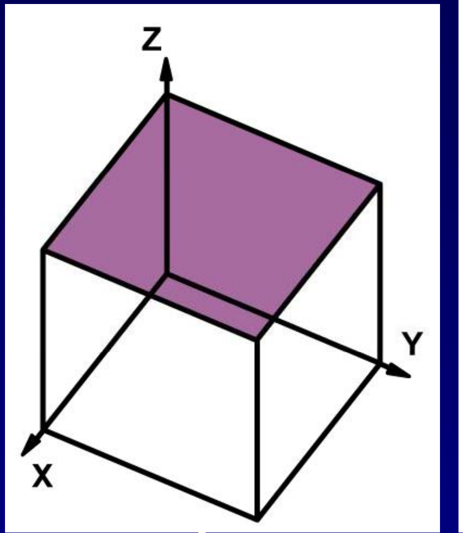
Plane (hkl)
Family of planes {hkl}

m00, 0n0, 00p: define lattice plane

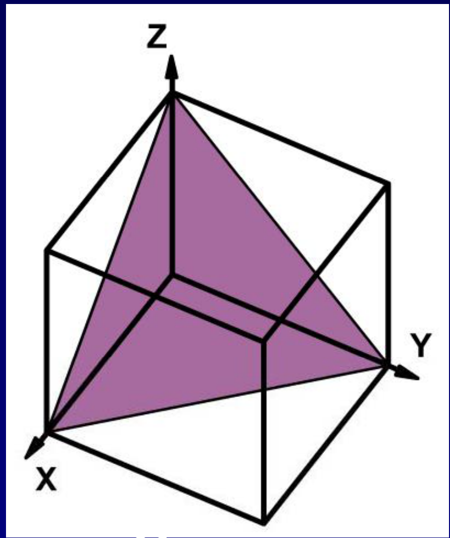
m, n, ∞ : no intercepts with axes

Miller indicies ; defined as the smallest integral multiples of the reciprocals of the plane intercepts on the axes

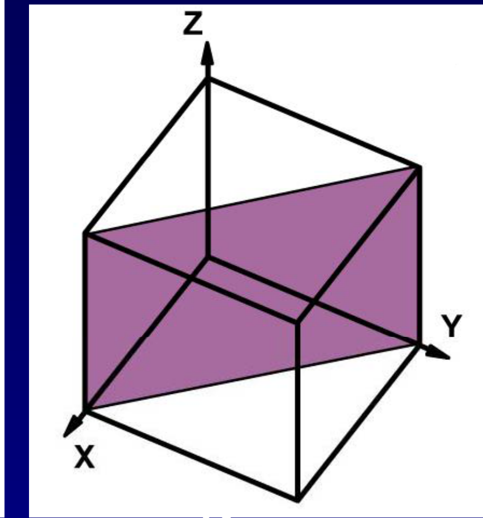
Crystallographic Planes



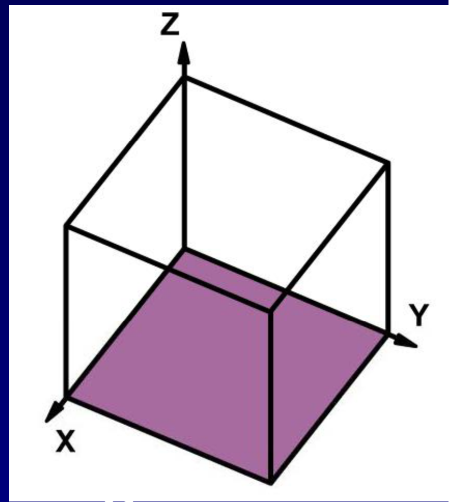
A



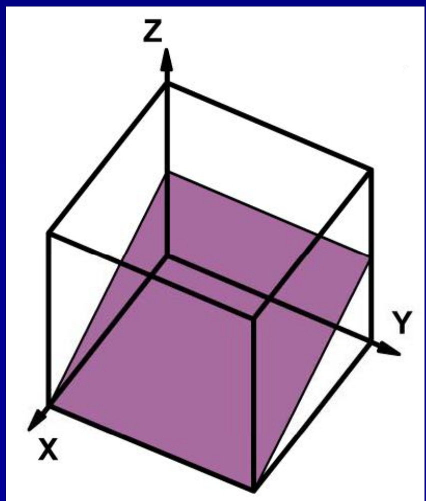
B



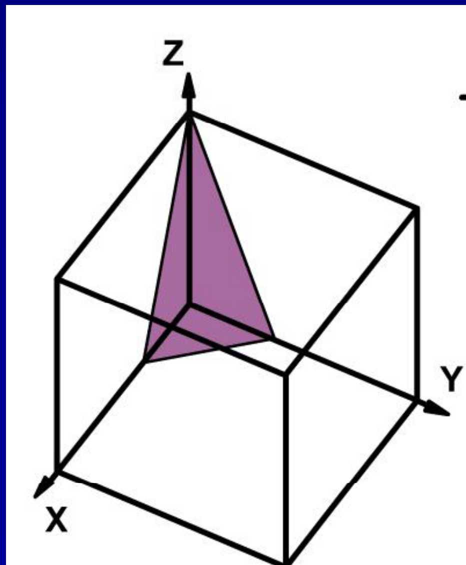
C



D



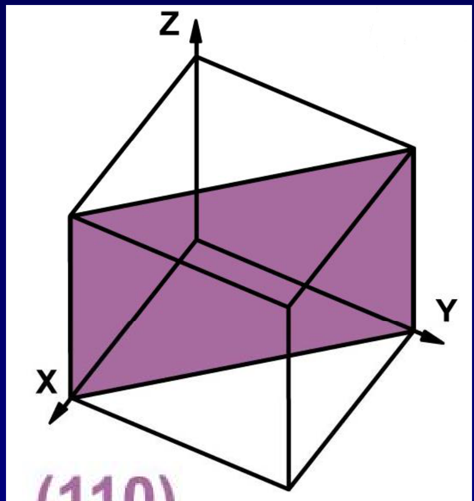
E



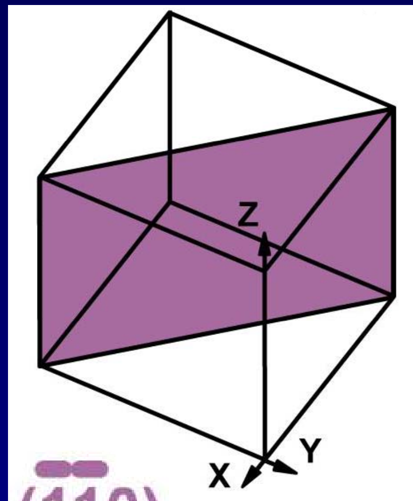
F

Plane	Intercepts	Indices
A	$\infty, \infty, 1$	(001)
B	1, 1, 1	(111)
C	$1, 1, \infty$	(110)
D	$\infty, \infty, -1$	$(00\bar{1})$
E	$1, \infty, 1/2$	( )
F	1/3, 1/3, 1	( )

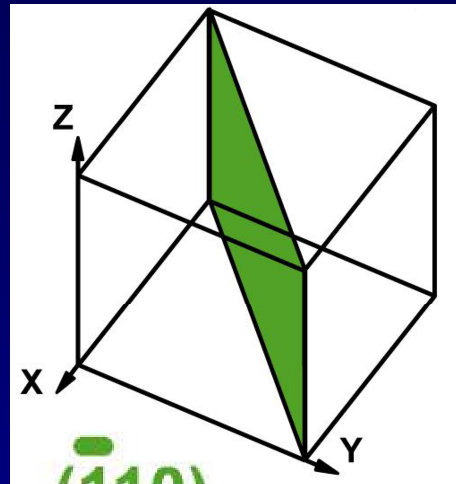
{110} Family



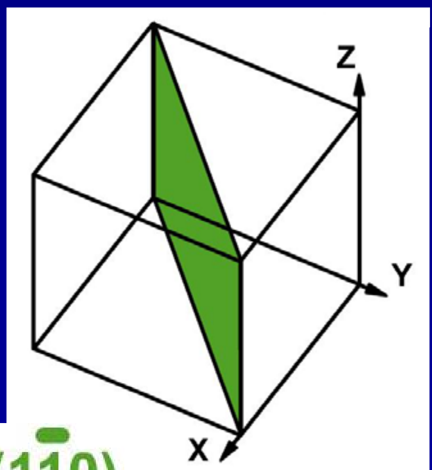
(110)



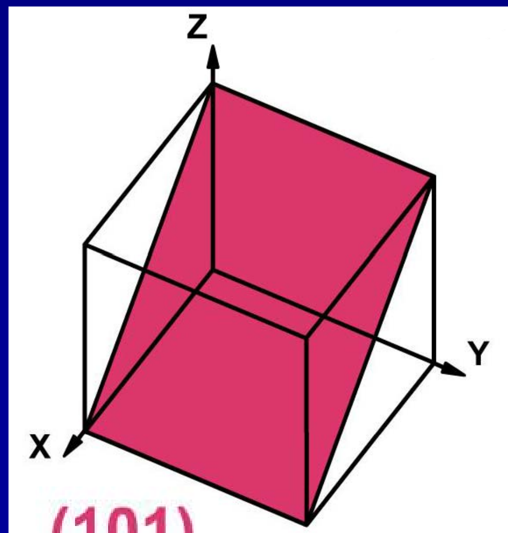
($\bar{1}\bar{1}0$)



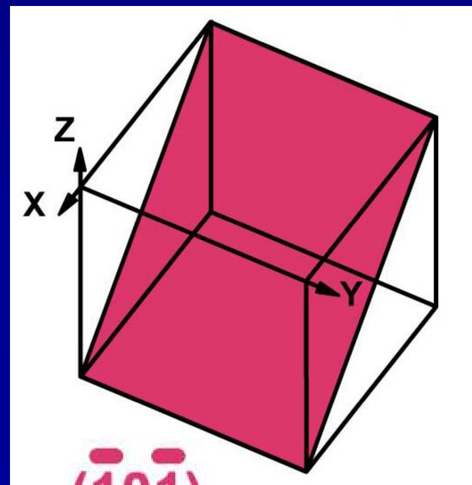
($\bar{1}10$)



($1\bar{1}0$)

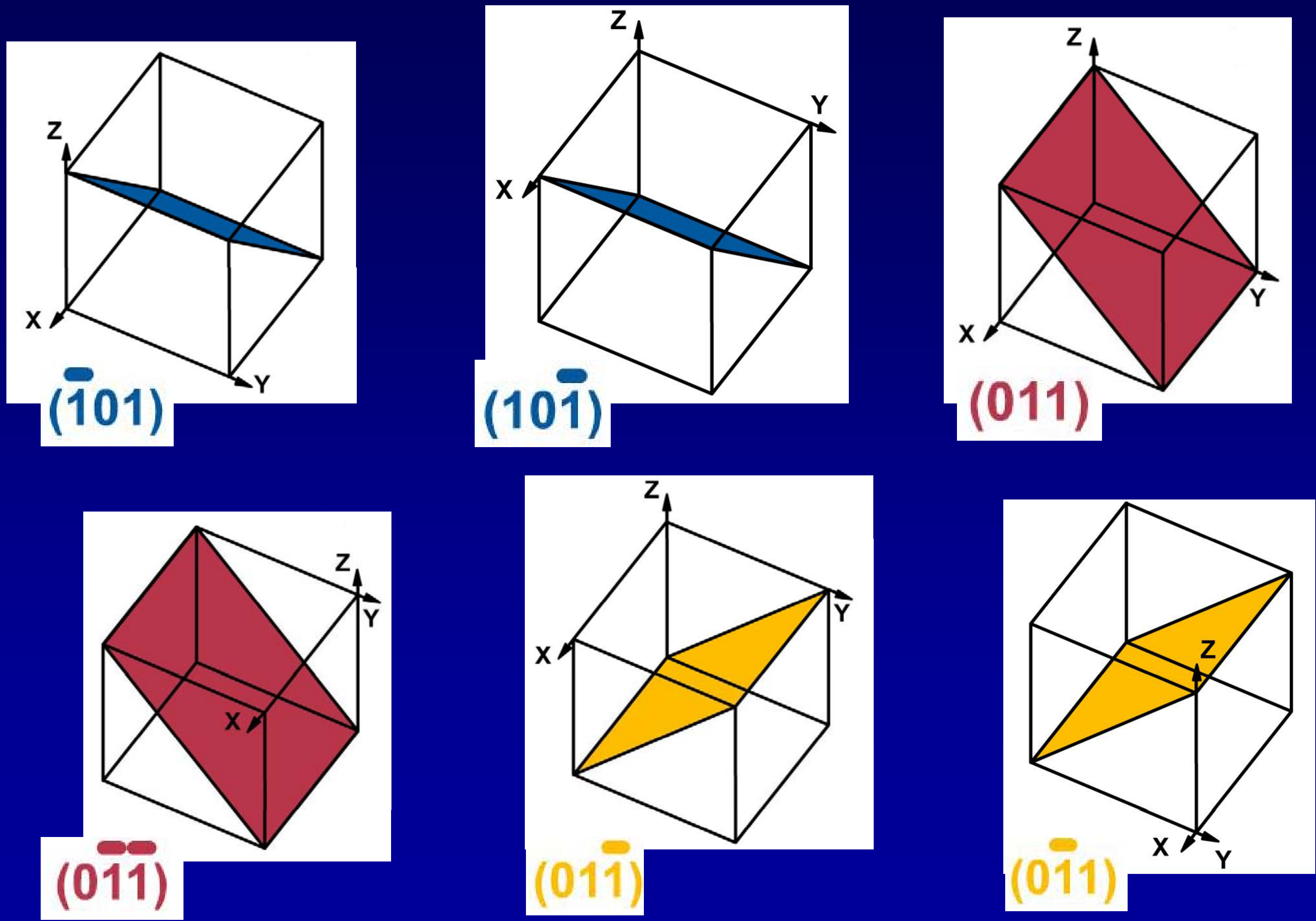


(101)



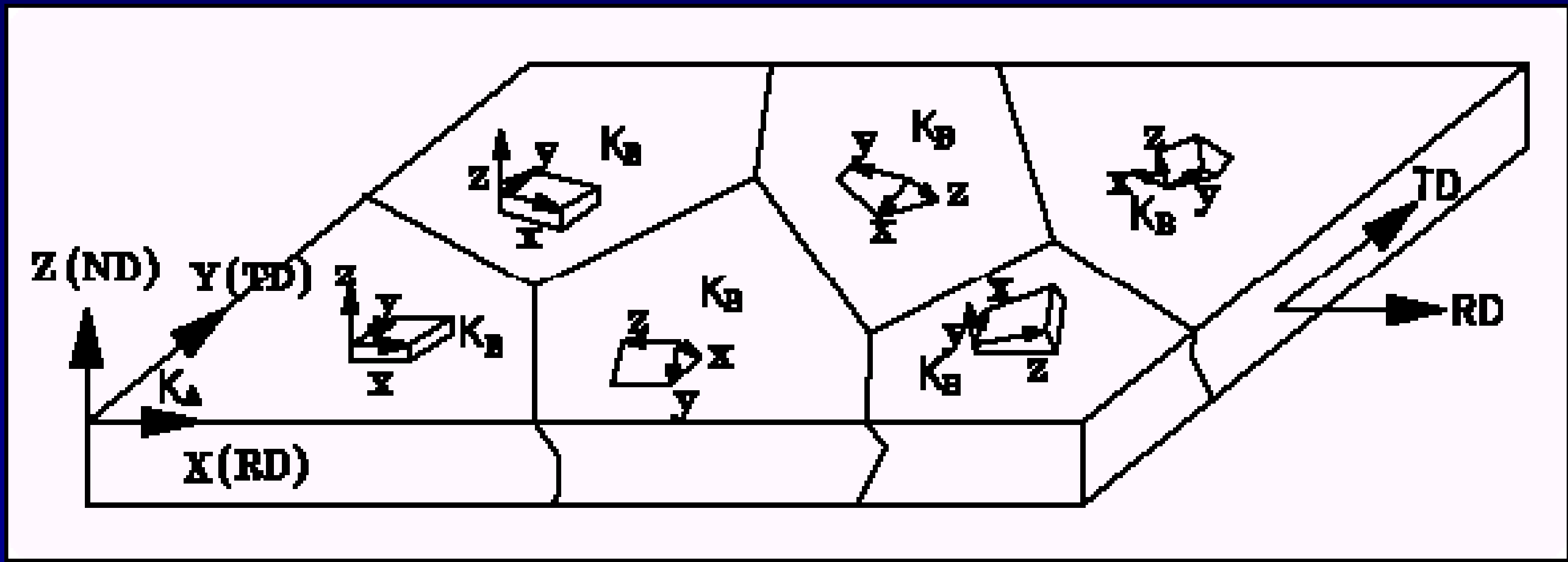
($\bar{1}0\bar{1}$)

{110} Family



Z
X
Y
$(\bar{1}01)$
Z
Y
X
$(10\bar{1})$
Z
Y
X
(011)
Z
Y
X
$(0\bar{1}\bar{1})$
Z
Y
X
$(01\bar{1})$
Z
X
Y
$(0\bar{1}1)$

Definite of crystal orientation

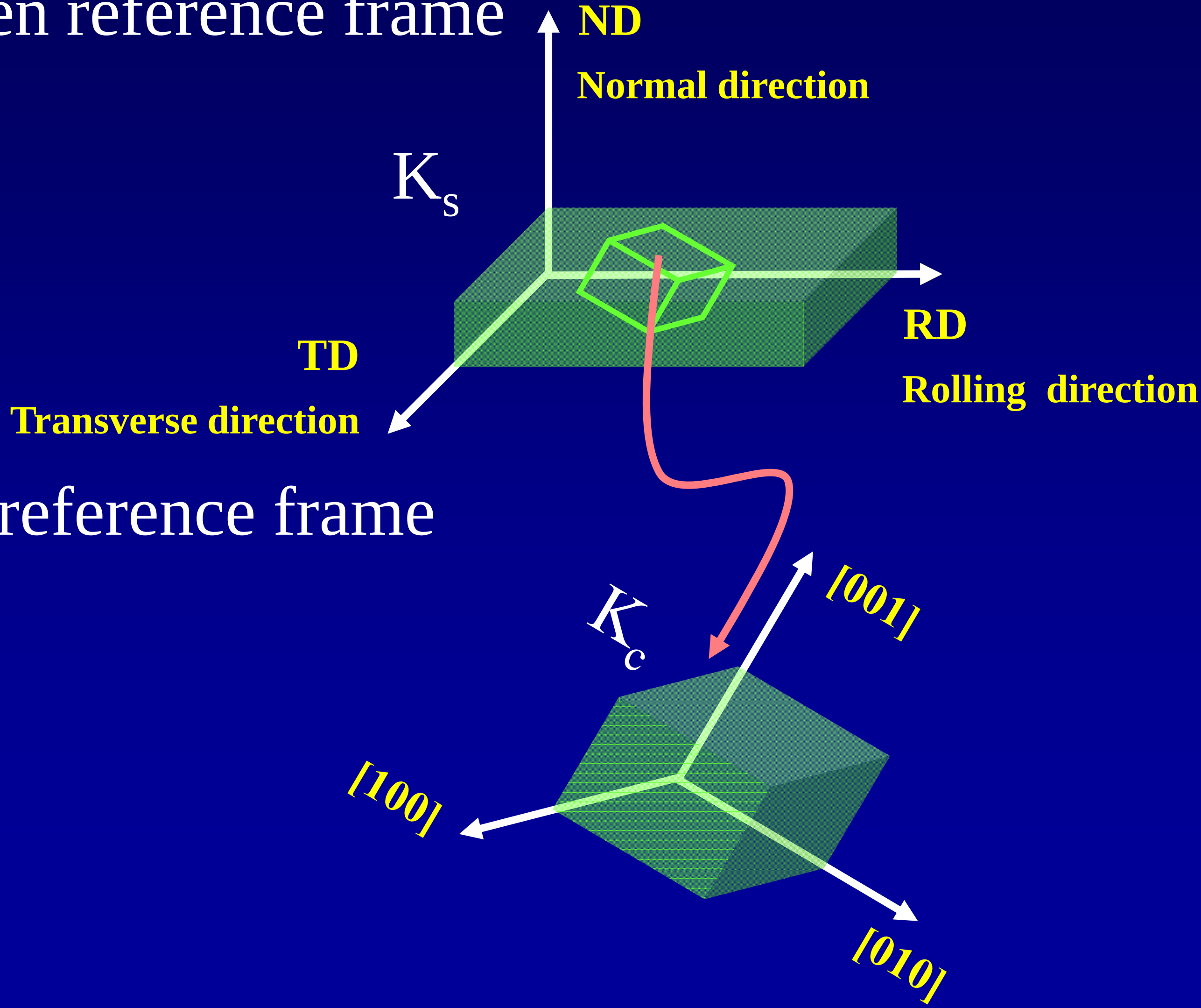


Specimen coordinate $K_A = K_S$ and crystal coordinate $K_B = K_C$

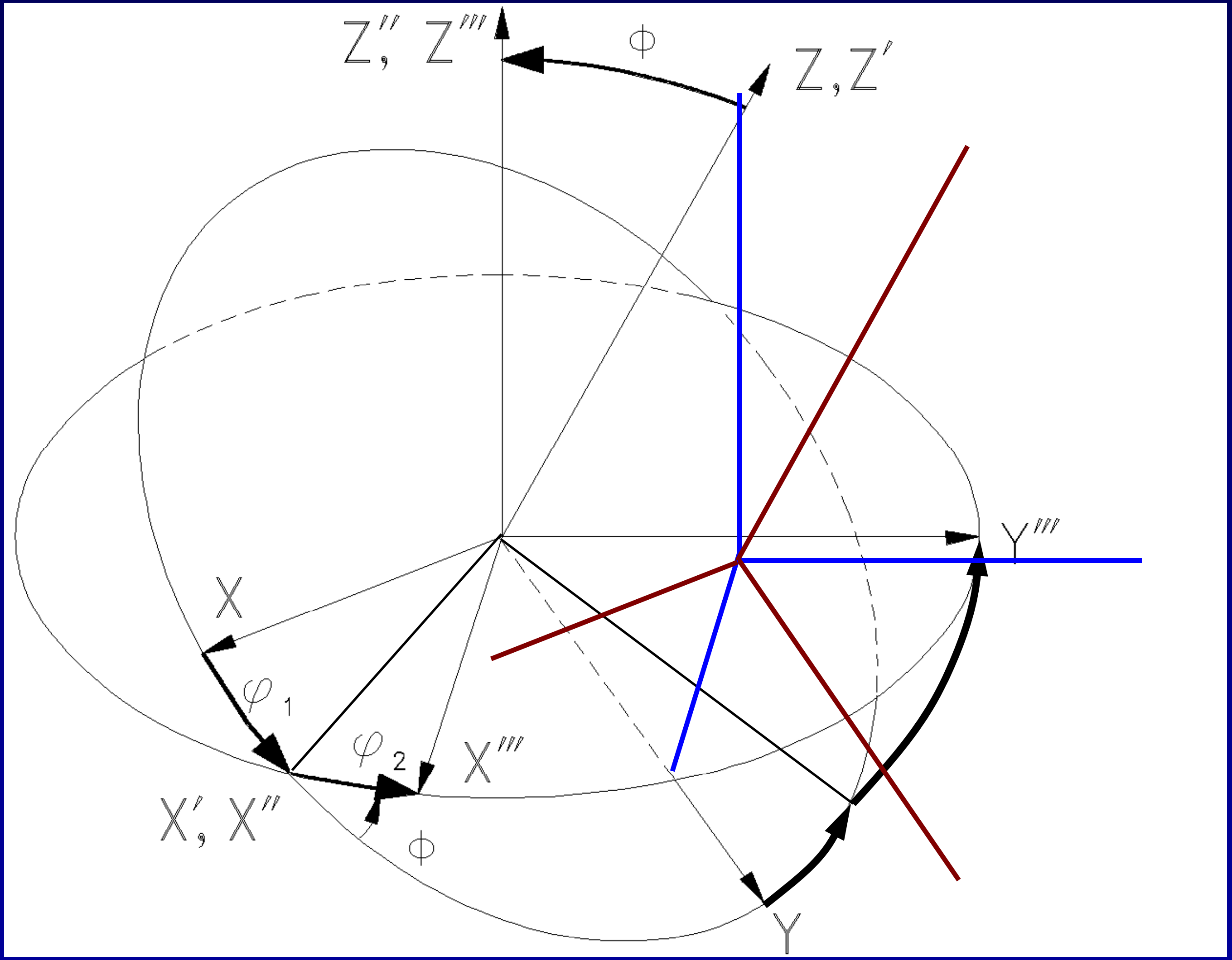
Crystal orientation

❖ Specimen reference frame

❖ Crystal reference frame



Crystal orientation Euler angles

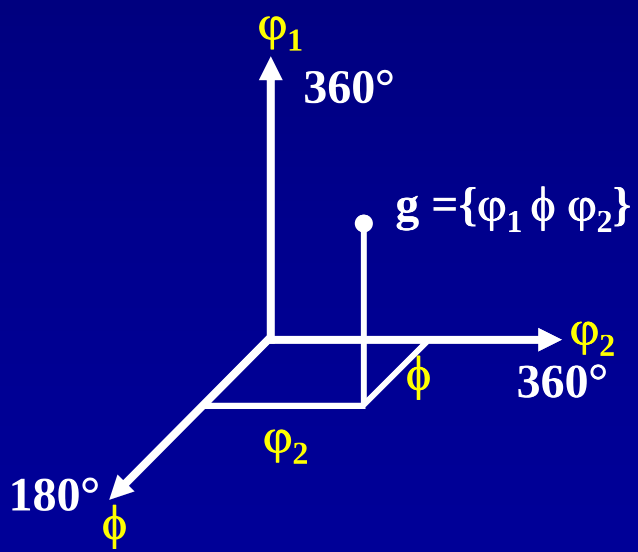


$$g = \{\varphi_1\ \phi\ \varphi_2\}$$

Crystal orientation

Euler angles and Euler space

- Each point in this space represents a specific choice of the parameters φ_1 ϕ φ_2 and hence a specific crystal orientation.

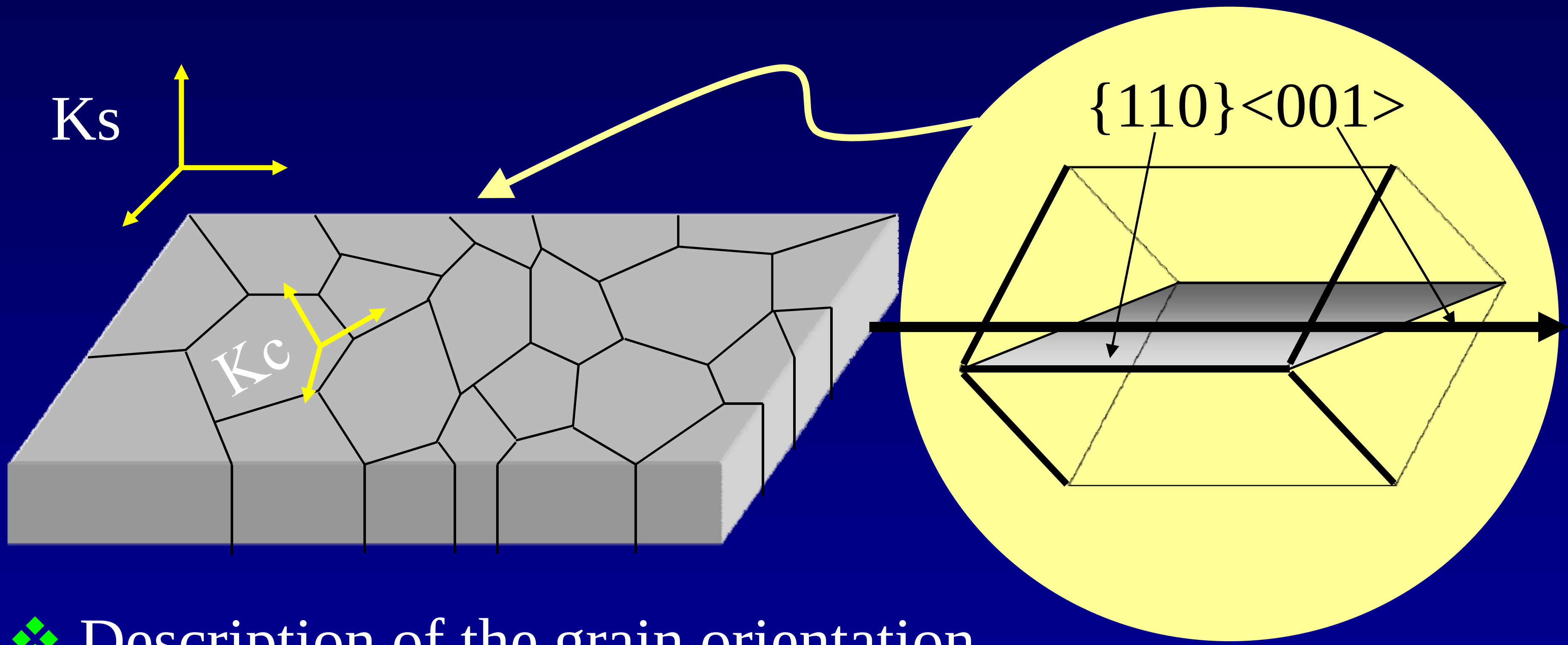


φ_1 [0 -360 °]

ϕ [0 -180 °]

φ_2 [0 -360 °]

Crystal orientation Miller Indices

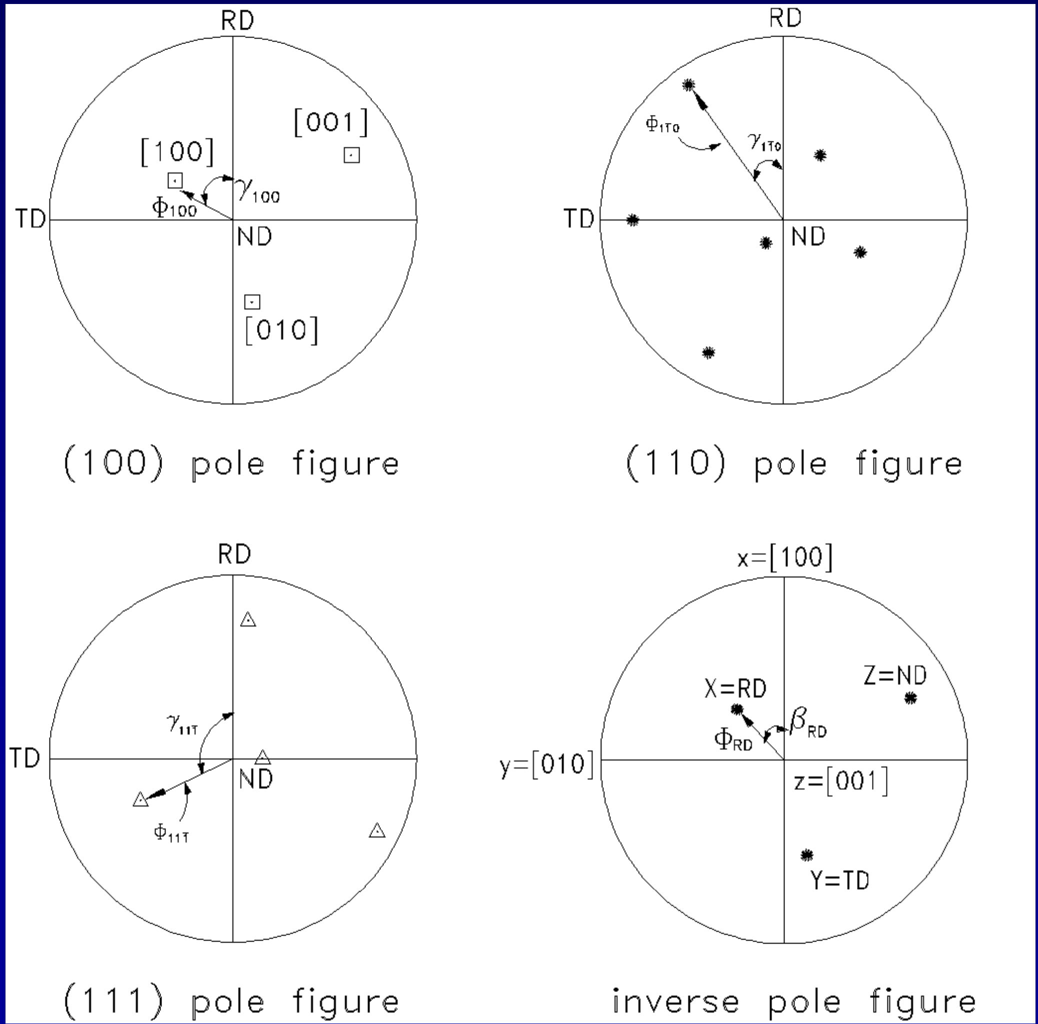


- Description of the grain orientation

  g= (hkl)[uvw]

  g={hkl}<uvw>

Definition of the Pole Figure and Inverse Pole Figure



Crystal orientation Matrix Representation

$$\begin{array}{cccc} & \mathrm{RD} & \mathrm{TD} & \mathrm{ND} \\ g = & \left[\begin{array}{c} u' \\ v' \\ w' \end{array}\right. & \begin{array}{c} r' \\ s' \\ t' \end{array} & \left.\begin{array}{c} h' \\ k' \\ l' \end{array}\right] \end{array}$$

❖ Representation of orientation g by ND, TD, RD parallel to [hkl], [rst], [uvw] respectively.

Crystal orientation Matrix Representation

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} u' & r' & h' \\ v' & s' & k' \\ w' & t' & l' \end{pmatrix} \begin{pmatrix} X \\ Y \\ Z \end{pmatrix}$$

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} u' & v' & w' \\ r' & s' & t' \\ h' & k' & l' \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

- **[XYZ] in specimen coord.**
- **[x,y,z] in crystal coord.**

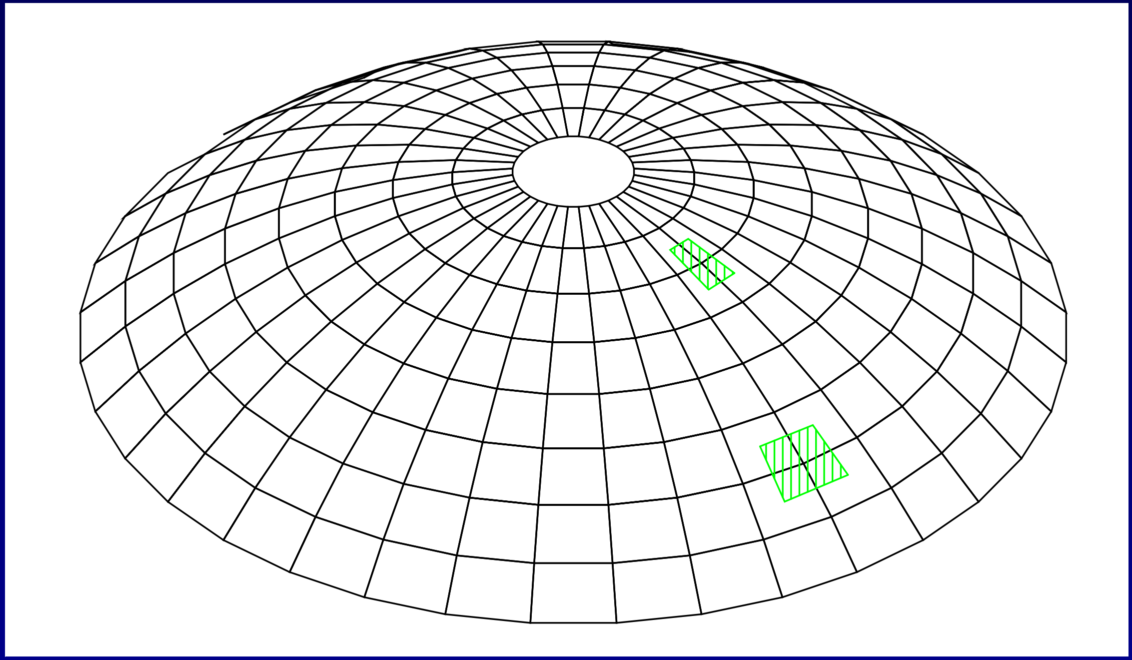
Crystal orientation

$$g_{\varphi_2}^{Z'} \quad \bullet \quad g_{\phi}^{X'} \quad \bullet \quad g_{\varphi_1}^{Z'}$$

$$g = \begin{bmatrix} \cos\varphi_2 & \sin\varphi_2 & 0 \\ -\sin\varphi_2 & \cos\varphi_2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \bullet \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & \sin\phi \\ 0 & -\sin\phi & \cos\phi \end{bmatrix} \bullet \begin{bmatrix} \cos\varphi_1 & \sin\varphi_1 & 0 \\ -\sin\varphi_1 & \cos\varphi_1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

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

Invariant measure



The invariant measure is introduced because the orientation transformation is combined with a distortion. For the Euler angles, the invariant measure is

$$\mathbf{I}(\varphi_1\ \phi\ \varphi_2) = \sin\phi$$

Normalization factor

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} \sin\phi \; d\varphi_1 d\phi d\varphi_2 = 8\pi^2$$

$$dg = \frac{1}{8\pi^2}\sin\phi \; d\varphi_1 d\phi d\varphi_2$$

If we add the normalization factor and invariant measure for the orientation element in Euler space, the orientation can be transformed without a distortion.

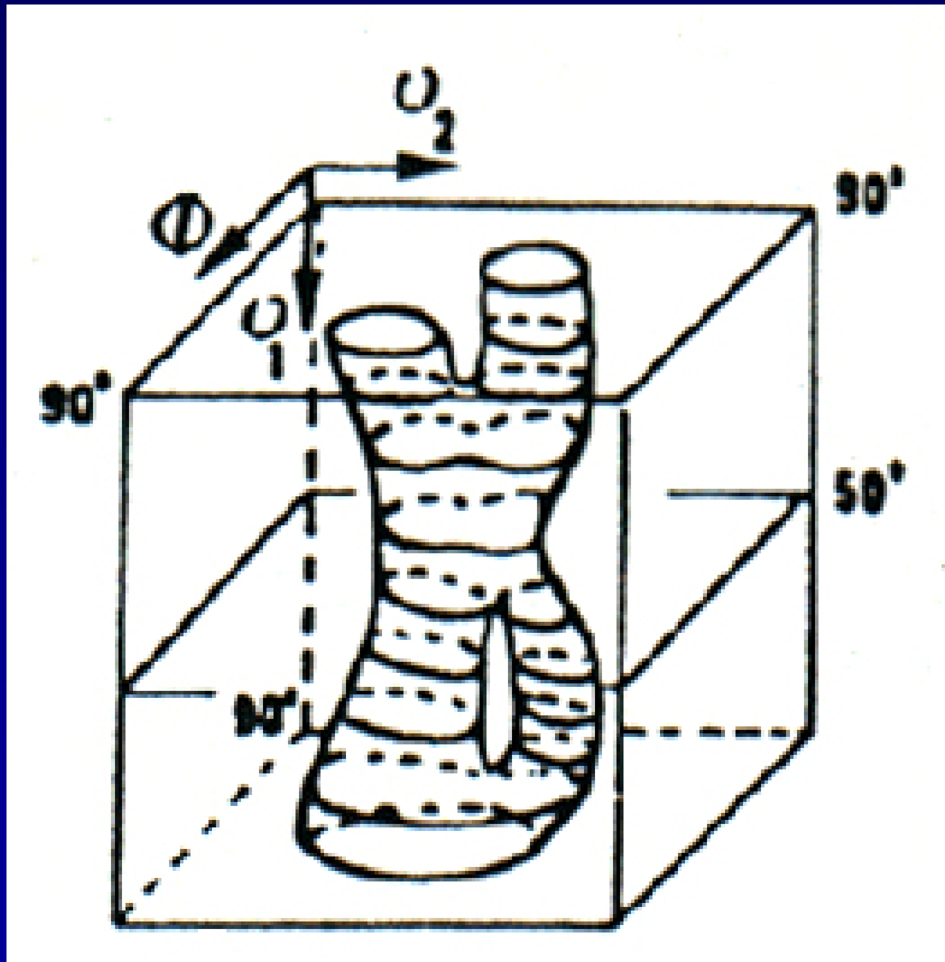
How can Orientation Distributions (Texture) be represented?

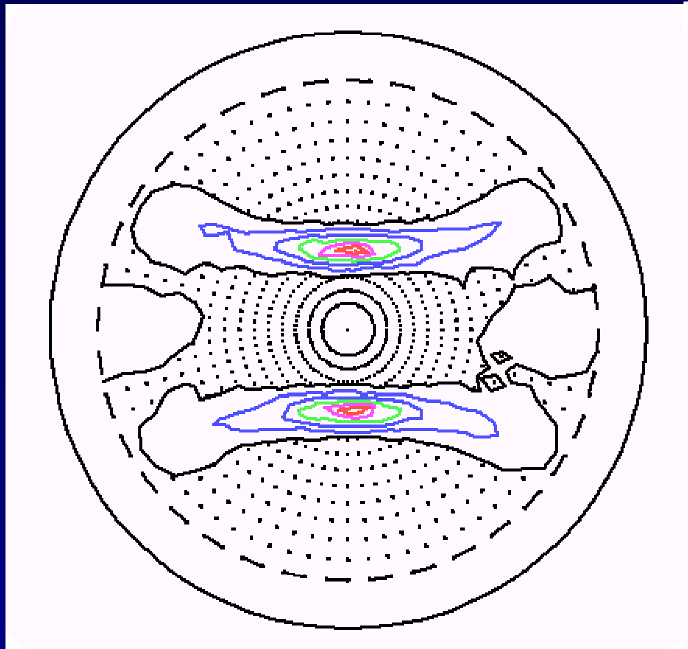
$$\frac{d\mathrm{V}}{\mathrm{V}} = f(g)dg$$

f(g) : the orientation distribution function

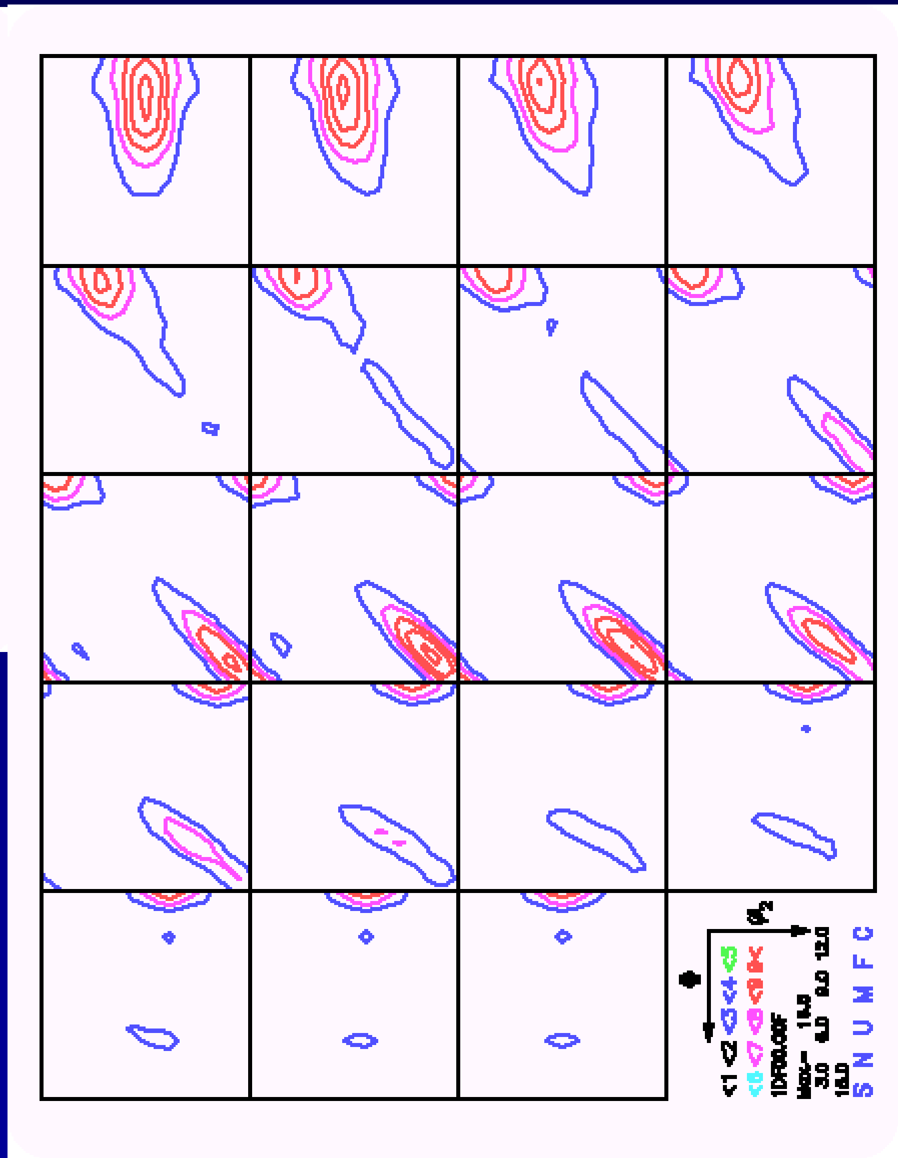
f(g)=1 for random distribution.

How Texture is represented?





(110) Pole Figure



ODF :
Orientation
Distribution
Function

Random orientation distribution