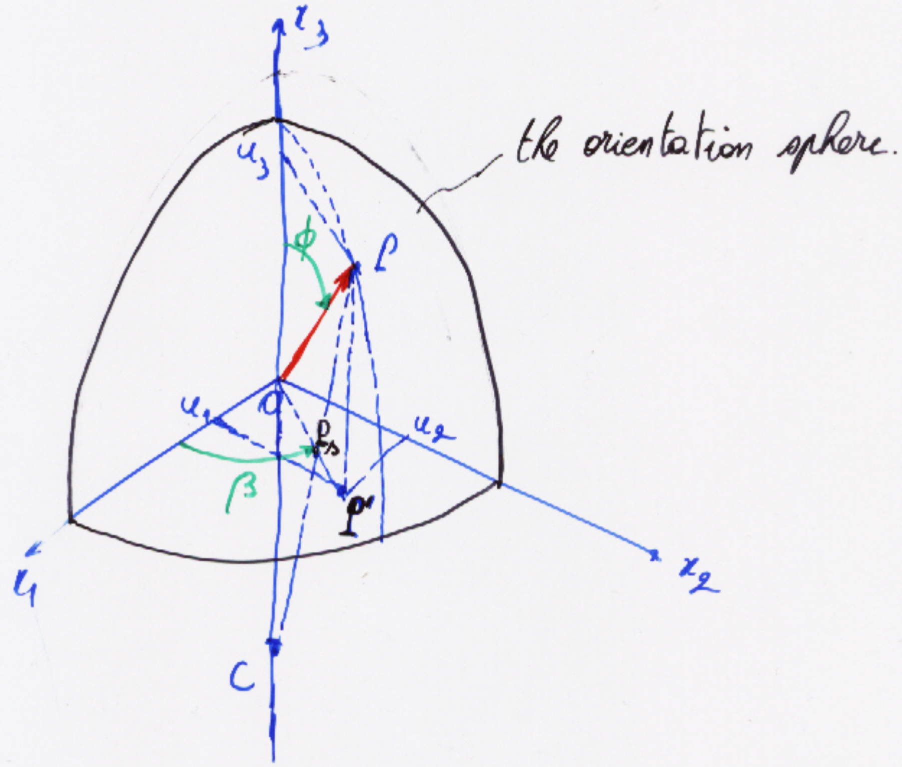
Parte 1

Directions in space.

Directions are described with respect to a reference system.

Convention:
right-handed orthogonal + normal (= orthonormal) reference system
x_1, x_2, x_3.



* The direction OP is described by a unit vector $\vec{OP}$. All unit vectors describing all directions in space are on a sphere = the unit sphere.

* The direction OP is uniquely characterized by the direction cosines of $\overline{OP}$

u_i = cosine of the angle between OP and the reference axis x_i.

with $\sum_i u_i^2 = 1$.

($\rightarrow$ 2 degrees of freedom)

* The direction OP is uniquely characterized by the spheric coordinates ϕ, β

ϕ = angle (OP, x_3) $\quad 0 < \phi < 180°$

β = angle (OP', x_1) $\quad 0 < \beta < 360°$

It is easy to show:

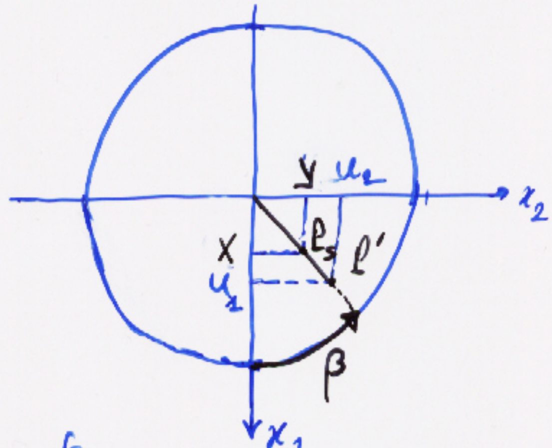
$$\begin{cases} u_3 = \cos\phi \\ u_1 = \sin\phi\cos\beta \\ u_2 = \sin\phi\sin\beta \end{cases}$$

The stereographic projection of OP

P_s = intersection of $\overline{PC}$ with $x_1 x_2$ plane
= stereographic projection of $\overline{OP}$.

$\Rightarrow$ each direction is represented by one single point, unless this direction is in the (x_1, x_2) plane

$P_s \rightarrow$ coordinates (X, Y) in the (x_1, x_2) plane
$\rightarrow$ can be expressed in terms of u_i.

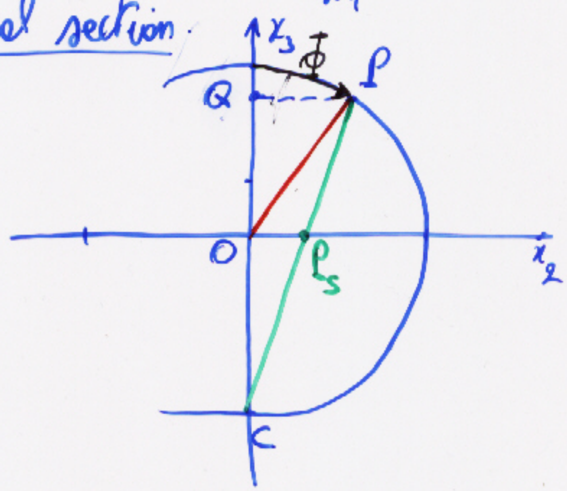


$X = OP_s \cos\beta$

$Y = OP_s \sin\beta$

$OP_s = ?$

Vertical section.



ΔQPC is congruent with $\Delta OP_s C$

$$\Downarrow$$

$$\frac{OP_s}{QP} = \frac{1}{1+OQ}$$

and $QP = \sin\phi$

$OQ = \cos\phi$

$$\Rightarrow OP_s = \left(\frac{1}{1+\cos\phi}\right)\sin\phi = \frac{\sin\phi}{1+\cos\phi}$$

$$X = \frac{\cos\beta \sin\phi}{1+\cos\phi} \Rightarrow \boxed{X = \frac{u_1}{1+u_3}}$$

$$Y = \frac{\sin\beta \sin\phi}{1+\cos\phi} \Rightarrow \boxed{Y = \frac{u_2}{1+u_3}}$$

<u>Remark</u>

If $u_3 < 0 \Rightarrow$ point P is on the "southern hemisphere"

$\Rightarrow$ stereographic projection P_s falls outside the unit circle in the (x_1, x_2) plane

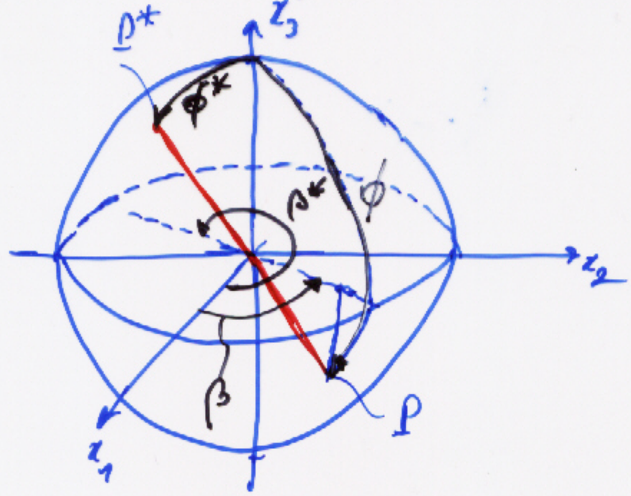
$\rightarrow$ is "inconvenient"

$\rightarrow$ these southern points will be transferred to northern hemisphere.

<u>How?</u> By considering the direction $-OP$

= point symmetry through O

The result of this symmetry operation

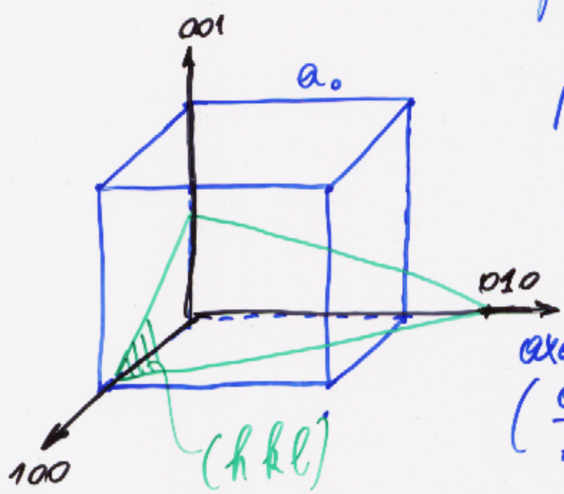


$$u_i^* = -u_i$$

$$\begin{cases} \phi^* = 180° - \phi \\ \beta^* = \beta + 180° \end{cases}$$

Example.

Given: a cubic crystal with lattice cte a_0
$\langle 100 \rangle$ axes = reference axes.



plane with Miller-indices $(h\,k\,l)$
↓
intersects (x_1, x_2, x_3)-axes at
$$\left(\frac{a_0}{h}, \frac{a_0}{k}, \frac{a_0}{l}\right)$$

A direction $[u, v, w]$ has coordinates
$$[a_0 u, a_0 v, a_0 w]$$

- The unit vector // $[u, v, w]$ has coordinates

$$\frac{[u, v, w]}{\sqrt{u^2+v^2+w^2}}$$

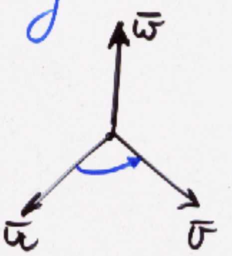
- For a cubic crystal:

(h, k, l) = Miller indices of the plane

$\Downarrow$

$[h, k, l]$ = direction normal to that plane.

- Suppose $\bar{u}[u_1, u_2, u_3]$ and $\bar{v}[v_1, v_2, v_3]$ are two directions $\Rightarrow$ direction $\bar{w} \perp \bar{u}, \bar{v}$ is given by: $\bar{w} = \bar{u} \otimes \bar{v}$



$$\begin{vmatrix} u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix}$$

$$\begin{cases} w_1 = u_2 v_3 - v_2 u_3 \\ w_2 = -u_1 v_3 + v_1 u_3 \\ w_3 = u_1 v_2 - v_1 u_2 \end{cases}$$

<u>Question</u>

Draw the pole of plane $(1\bar{1}1)$ on a stereographic projection.

<u>Answer</u>

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

$\rightarrow$ $[1\bar{1}1] \perp$ to $(1\bar{1}1)$ plane

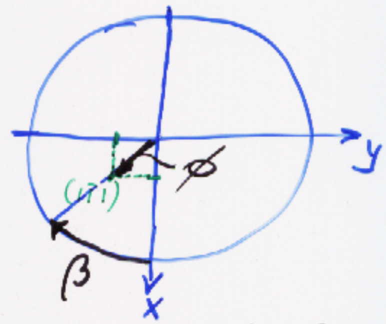
$$u_1 = \frac{1}{\sqrt{1+1+1}} = 1/\sqrt{3}$$

$$u_2 = -1/\sqrt{3} \; ; \; u_3 = 1/\sqrt{3}$$

Stereographic projection:

$$X = \frac{u_1}{1+u_3} = 0.366$$

$$Y = \frac{u_2}{1+u_3} = -0.366$$



What are the polar coordinates (ϕ, β) of the pole $(1\bar{1}1)$

$$u_3 = \cos\phi \Rightarrow \phi = \arccos u_3 \Rightarrow \phi = 54.7°$$

$$\cos\beta = \frac{u_1}{\sin\phi} = \frac{0.366}{\sin 54.7°} \quad (>0)$$

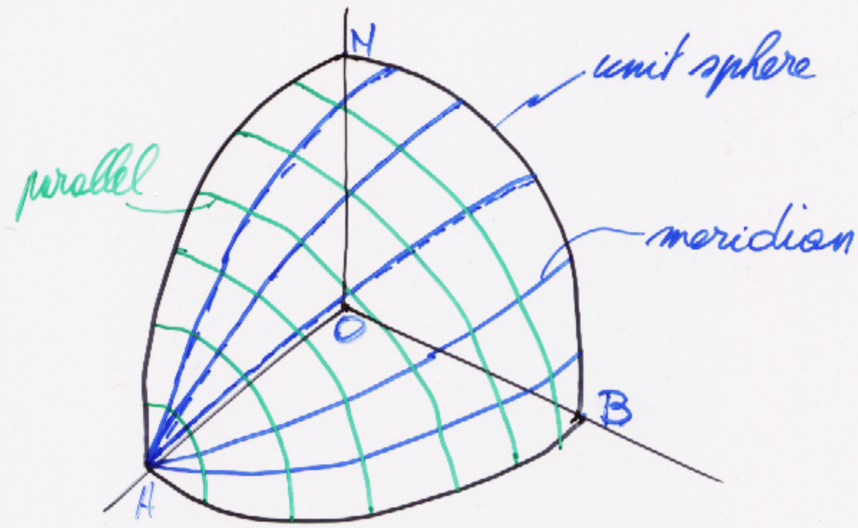
$$\sin\beta = \frac{u_2}{\sin\phi} = \frac{-0.366}{\sin 54.7°} \quad (<0)$$

$\rightarrow \beta \in [0, -90°]$

$\rightarrow \beta = -45°$

The Wulff net.

= Geometric construction, based on a unit sphere and a stereographic projection which allows to execute geometric operations on planes and directions



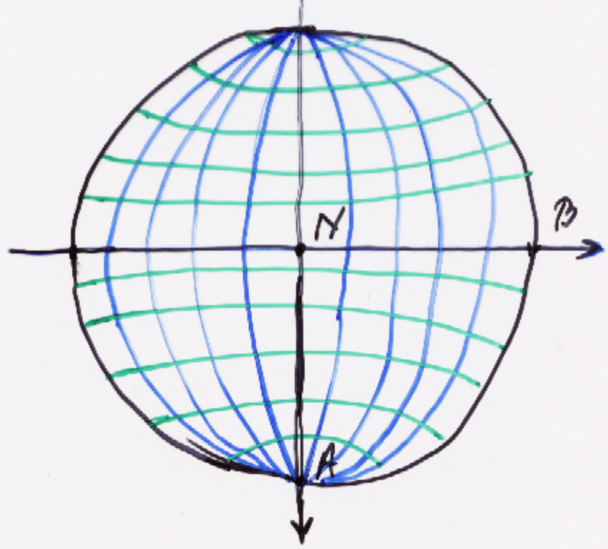
Unit sphere is covered with meridians and parallels

- Large circle = cross-section of the unit sphere with a plane through O
- Small circle = cross-section of the unit sphere with a plane not through O

→ meridian = large circles

→ parallels = small circles.

Wulff net = stereographic projection of all parallels and meridians.



- Angles between directions (and planes) can be truefully observed along large circles
- Rotations can be truefully executed around N-axis (⊥ sheet) and around axis NA.

Exercises.

1) Draw the directions $[1\bar{1}1]$ and $[1\bar{2}1]$
Determine the angle between those 2 axes
(on stereographic projection + analytical)

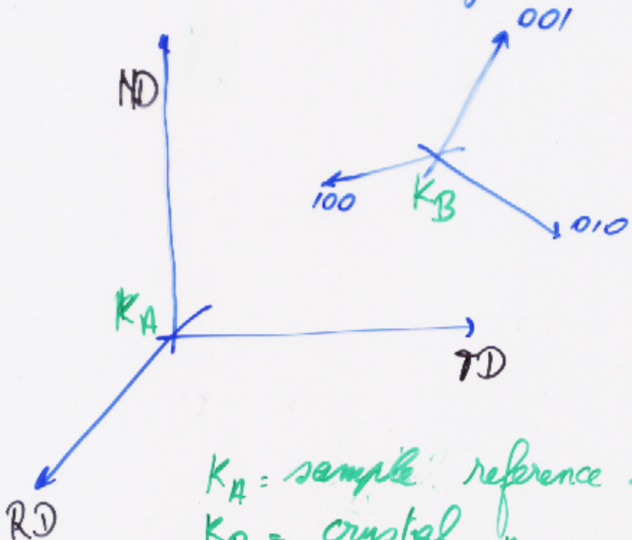
2) All directions ⊥ on a given direction = Zone circle and given direction = zone axis
Draw the zone circle of the $[1\bar{1}1]$ direction.

3) Rotate the $[1\bar{1}1]$ pole $+30°$ around x_3

4) Rotate the $[1\bar{1}1]$ pole $+30°$ around the $[110]$ axis

5) Rotate the $[1\bar{1}1]$ pole $+30°$ around the $[\bar{1}21]$ axis.

Matrix representation of orientations



K_A = sample reference system
K_B = crystal " "

Suppose a_{ij} = direction cosine of sample axis x_j with respect to crystal axis x_i'

→ we can construct the following table:

	RD	TD	ND
[100]	a_{11}	a_{12}	a_{13}
[010]	a_{21}	a_{22}	a_{23}
[001]	a_{31}	a_{32}	a_{33}

This is the transformation matrix $[a_{ij}]$

x_j = point with coordinates in K_A
x_i' = " " " " K_B

$$\boxed{x_i' = \sum_{j=1}^{3} a_{ij}\, x_j}$$

Matrix $[a_{ij}]$ = orthonormal matrix

$$\sum_{i=1}^{3} a_{ij}\, a_{ik} = \delta_{jk} \quad (*)$$

$[a_{ij}] \rightarrow 9$ elements but $(*) \rightarrow 6$ eq^s
$\Rightarrow$ 3 degrees of freedom.

Property of orthonormal matrices.

$$[a_{ij}]^{-1} = [a_{ji}]$$

$$\Rightarrow \underbrace{x_j}_{K_A} = \sum_i a_{ji} \underbrace{x_i'}_{K_B}$$

Advantage of the matrix representation:

→ two successive rotations → product of the two corresponding matrices!

$$\underbrace{x_k'' = \sum_{i=1}^{3} a^2_{ki}\, x_i'}_{\text{rotation } 1} \; ; \; \underbrace{x_i' = \sum_{j=1}^{3} a^1_{ij}\, x_j}_{\text{rotation } 2}$$

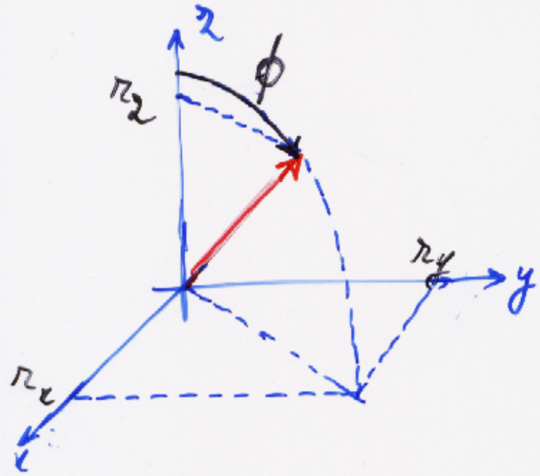
$$\Rightarrow x_k'' = \sum_{i=1}^{3} \left[\sum_{j=1}^{3} a^2_{ki}\, a^1_{ij}\right] x_j$$

$$x_k'' = \sum_{j=1}^{3} a_{kj}\, x_j$$

with $a_{kj} = \sum_{i=1}^{3} a^2_{ki}\, a^1_{ij}$

Relations between different orientation representations.

1] Polar coordinates (ϕ, β) vs. direction cosines (r_x, r_y, r_z)



$$\begin{cases} r_x = \sin\phi \cos\beta \\ r_y = \sin\phi \sin\beta \\ r_z = \cos\phi \end{cases}$$

2] Orientation matrix expressed in terms of spherical polar coordinates :

$$g = \begin{array}{c} \left[\begin{array}{c|c|c} \sin\phi_{RD}\cos\beta_{RD} & \sin\phi_{TD}\cos\beta_{TD} & \\ \sin\phi_{RD}\sin\beta_{RD} & \sin\phi_{TD}\sin\beta_{TD} & ND \\ \cos\phi_{RD} & \cos\phi_{TD} & \end{array}\right] \\ \begin{array}{ccc} RD \quad\quad\quad & TD \quad\quad & ND \end{array} \end{array}$$

3] Miller indices vs. polar coordinates.

$$\begin{cases} h = n \sin\phi_{ND} \cos\beta_{ND} \\ k = n \sin\phi_{ND} \sin\beta_{ND} \\ l = n \cos\phi_{ND} \end{cases} \quad \text{with } n = \sqrt{h^2+k^2+l^2}$$

$$\begin{cases} u = n' \sin\phi_{RD} \cos\beta_{RD} \\ v = n' \sin\phi_{RD} \sin\beta_{RD} \\ w = n' \cos\phi_{RD} \end{cases} \quad \text{with} \quad n' = \sqrt{u^2+v^2+w^2}$$

For the inverse relation :

$$\phi = \arccos r_z \quad (0 < \phi < 180^\circ)$$

$$\beta = \arcsin \frac{r_y}{\sqrt{1-r_z^2}} = \arccos \frac{r_x}{\sqrt{1-r_z^2}}$$

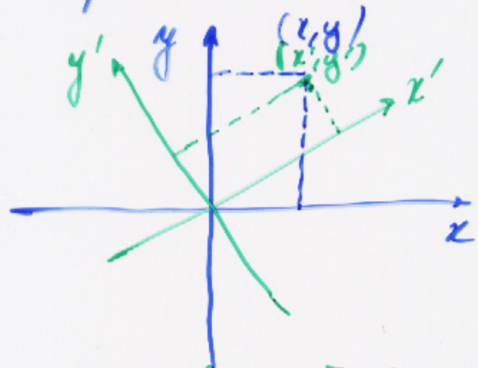
and hence :

$$\begin{cases} \phi_{ND} = \arccos \left[\dfrac{l}{\sqrt{h^2+k^2+l^2}} \right] \\ \beta_{ND} = \arcsin \left[\dfrac{k}{\sqrt{h^2+k^2}} \right] = \arccos \left[\dfrac{h}{\sqrt{h^2+k^2}} \right] \end{cases}$$

$$\begin{cases} \phi_{RD} = \arccos \left[\dfrac{w}{\sqrt{u^2+v^2+w^2}} \right] \\ \beta_{RD} = \arcsin \left[\dfrac{v}{\sqrt{u^2+v^2}} \right] = \arccos \left[\dfrac{u}{\sqrt{u^2+v^2}} \right] \end{cases}$$

4] Relation between matrix representation and Euler angles:

simple rotation



$$\begin{bmatrix} x' \\ y' \\ z' \end{bmatrix} = \begin{bmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix}$$

Hence, the 3 Euler rotations:

$$g_{\varphi_1}^{z} = \begin{bmatrix} \cos\varphi_1 & \sin\varphi_1 & 0 \\ -\sin\varphi_1 & \cos\varphi_1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$g_{\phi}^{x} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & \sin\phi \\ 0 & -\sin\phi & \cos\phi \end{bmatrix}$$

$$g_{\varphi_2}^{z} = \begin{bmatrix} \cos\varphi_2 & \sin\varphi_2 & 0 \\ -\sin\varphi_2 & \cos\varphi_2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$g = g_{\varphi_2}^{z} \cdot g_{\phi}^{x} \cdot g_{\varphi_1}^{z} =$$

$$g(\varphi_1, \phi, \varphi_2) =$$

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

5] Axis-angle pair vs. matrix representation.

Axis-angle pair $(\vec{d}, \omega) \longleftrightarrow$ matrix $[a_{ij}]$

$$g(\vec{d}, \omega) =$$

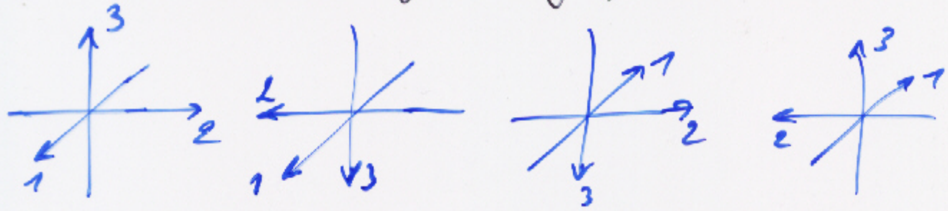
$$\begin{bmatrix} (1-d_1^2)\cos\omega + d_1^2 & d_1 d_2 (1-\cos\omega) + d_3 \sin\omega & d_1 d_3 (1-\cos\omega) - d_2 \sin\omega \\ d_1 d_2 (1-\cos\omega) - d_3 \sin\omega & (1-d_2^2)\cos\omega + d_2^2 & d_2 d_3 (1-\cos\omega) + d_1 \sin\omega \\ d_1 d_3 (1-\cos\omega) + d_2 \sin\omega & d_2 d_3 (1-\cos\omega) - d_1 \sin\omega & (1-d_3^2)\cos\omega + d_3^2 \end{bmatrix}$$

$$\rightarrow \cos\omega = \frac{\mathrm{Tr}[a_{ij}] - 1}{2} \qquad (0 < \omega < 180^\circ)$$

6] Relation between Euler angles and axis-angle pair
→ via orientation matrix.

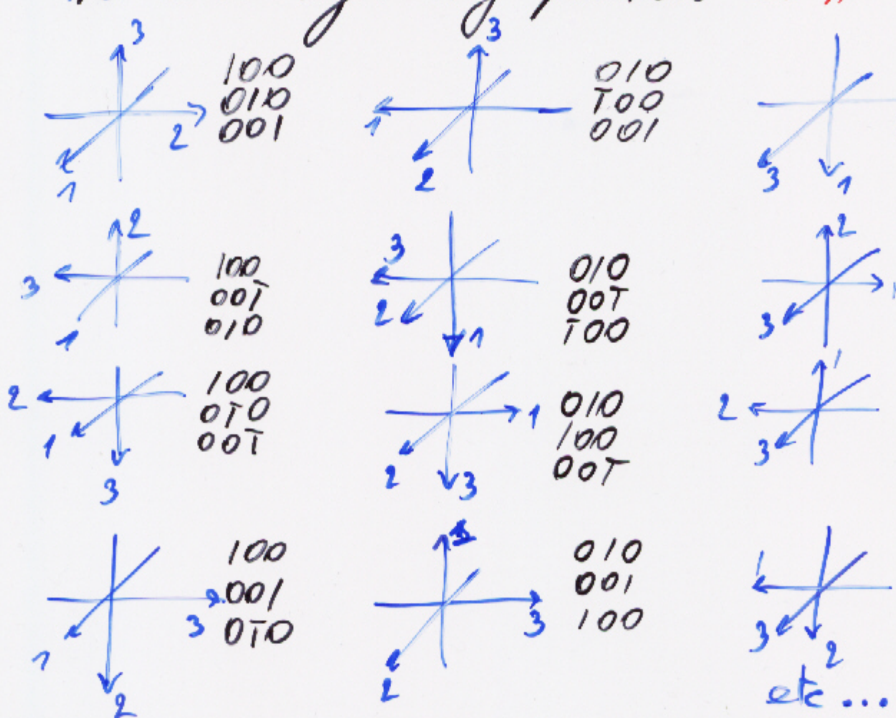
Symmetry Operators

The orthorhombic symmetry operators. → # = 4



$$\begin{matrix}100\\010\\001\end{matrix}\qquad\begin{matrix}100\\0\bar{1}0\\00\bar{1}\end{matrix}\qquad\begin{matrix}\bar{1}00\\010\\00\bar{1}\end{matrix}\qquad\begin{matrix}\bar{1}00\\0\bar{1}0\\001\end{matrix}$$

The cubic symmetry operators → # = 24



$$\begin{matrix}100\\010\\001\end{matrix}\qquad\begin{matrix}010\\\bar{1}00\\001\end{matrix}\qquad\begin{matrix}001\\010\\\bar{1}00\end{matrix}$$

$$\begin{matrix}100\\00\bar{1}\\010\end{matrix}\qquad\begin{matrix}010\\00\bar{1}\\\bar{1}00\end{matrix}\qquad\begin{matrix}001\\100\\010\end{matrix}$$

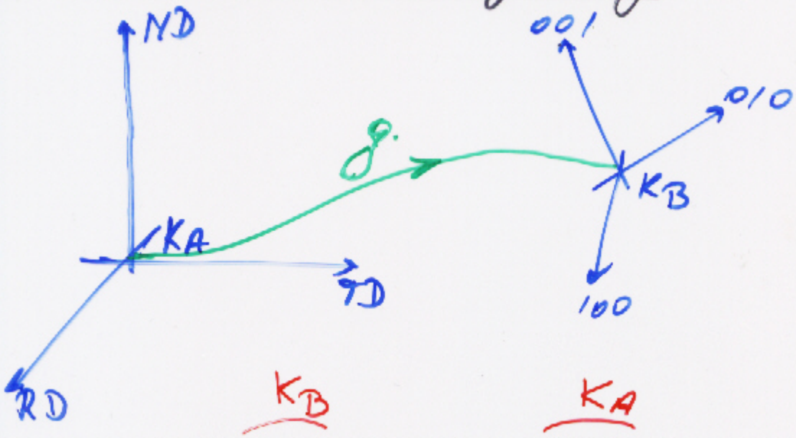
$$\begin{matrix}100\\0\bar{1}0\\00\bar{1}\end{matrix}\qquad\begin{matrix}010\\100\\00\bar{1}\end{matrix}\qquad\begin{matrix}001\\0\bar{1}0\\100\end{matrix}$$

$$\begin{matrix}100\\001\\0\bar{1}0\end{matrix}\qquad\begin{matrix}010\\001\\100\end{matrix}\qquad\begin{matrix}001\\\bar{1}00\\0\bar{1}0\end{matrix}$$

etc...

How to deal with symmetric equivalent orientations?

① Orthorombic - Cubic symmetry.



$$\overbrace{[x']}^{K_B} = [g]\overbrace{[x]}^{K_A}$$

Suppose $[x']^{eq}$ and $[x]^{eq}$ are symm. equivalents to $[x']$ and $[x]$, respectively.

$$\Rightarrow [x']^{eq} = [Sym]_{cub}[x']$$

$$[x]^{eq} = [Sym]_{ort}[x]$$

with $[Sym]_{cub}$ and $[Sym]_{ort}$, the cubic and orthorombic symm. operators, respectively.

$$\Rightarrow [x']^{eq} = [g]^{eq}[x]^{eq}$$

$$[Sym]_{cub}[x'] = [g]^{eq}[Sym]_{ort}[x]$$

$$[x'] = [Sym]_{cub}^{-1}[g]^{eq}[Sym]_{ort}[x]$$

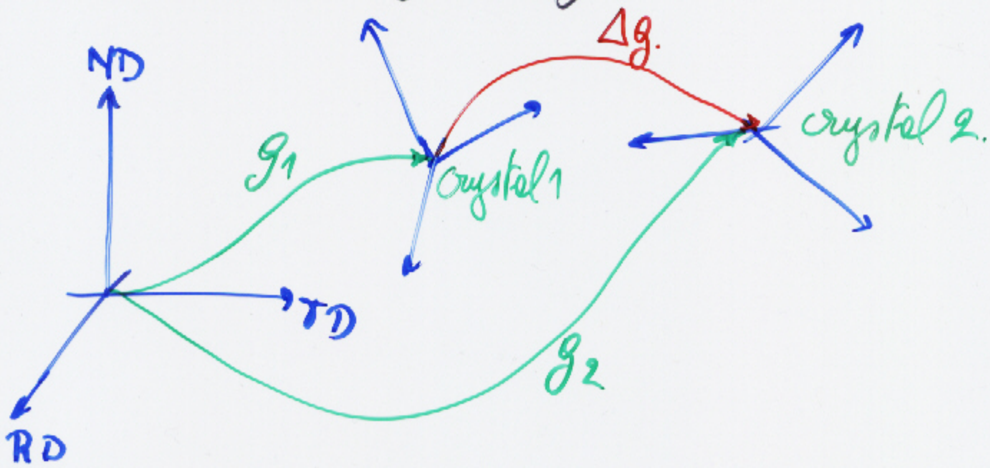
$$[g]\cancel{[x]} = [Sym]^{-1}_{cub}\,[g]^{eq}\,[Sym]_{ort}\,\cancel{[x]}$$

$$\Rightarrow \boxed{[g]^{eq} = \underbrace{[Sym]_{cub}}_{24}\,[g]\,\underbrace{[Sym]_{ort.}}_{4}}$$

In case there is cubic crystal symm. + orthorombic sample symm.

$\Rightarrow$ there are $24 \times 4 = 96$ symm. equivalent orientations for each given orient.

② Cubic - Cubic Symmetry.



$$\Delta g = g_2\,(g_1)^{-1}$$

$$\Rightarrow \Delta g^{eq} = g_2^{eq}\,(g_1^{eq})^{-1}$$

$$\Delta g^{eq} = [Sym]_{cub}\,[g_2]\,[Sym]_{ort} \times \left([Sym]_{cub}\,[g_1]\,[Sym]_{ort}\right)^{-1}$$

$$\Delta g^{eq} = [Sym]_{cub} [g_2] \cancel{[Sym]_{ort}} \cancel{[Sym]_{ort}^{-1}} [g_1]^{-1} [Sym]_{cub}^{-1}$$

$$\Delta g^{eq} = [Sym]_{cub} [g_2][g_1]^{-1} [Sym]_{cub}^{-1}$$

$$\boxed{\Delta g^{eq} = \underbrace{[Sym]_{cub}}_{24} \Delta g \underbrace{[Sym]_{cub}^{-1}}_{24}}$$

There are $24^2 = 576$ symmetric equivalent

In terms of axis-angle pairs:

24 axes $(d_1, d_2, d_3)^i$ with $i = 1, \dots, 24$

24 angles ω_i with $0 < \omega_i < 180°$

$(d_1\ d_2\ d_3)^i$ $(d_2\ d_1\ d_3)^i$

$(\bar{d}_1\ d_2\ d_3)^i$ $(\bar{d}_2\ d_1\ d_3)^i$ etc.

$(d_1\ \bar{d}_2\ d_3)^i$ $(d_2\ \bar{d}_1\ d_3)^i$ 24 combinations.

$(d_1\ d_2\ \bar{d}_3)$ $(d_2\ d_1\ \bar{d}_3)^i$

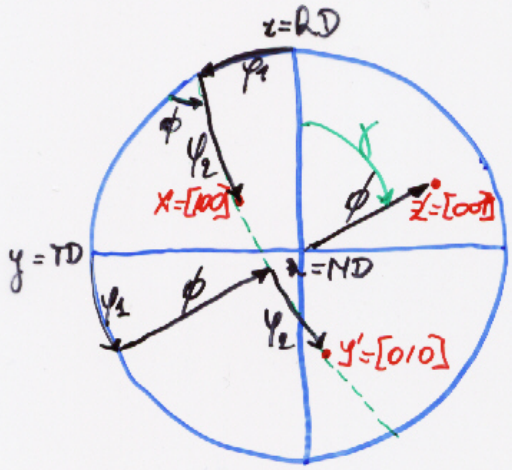
- 24 angles are paired 2 by 2 with 24 axes.
- There is always at least one angle ω_i for which $0 < \omega_i < 63°$

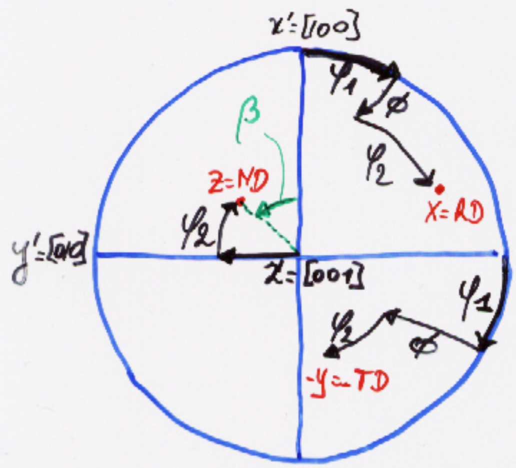
↳ the min. angle representation of the misorientation

= The orientation distance between g_1 and g_2

Euler angles represented on a pole figure.

Euler angle rotations bring the [RD, TD, ND] ref. system in coincidence with crystal ref. system





Relation between polar coordinates of arbitrary crystal direction $\vec{n}$ // ND and Euler angles

$$\vec{n} = \{\phi, \beta\} \rightarrow \phi_{Euler} = \phi$$

$$\beta = \frac{\pi}{2} - \varphi_2$$

Relation between polar coordinates of arbitrary sample direction $\bar{y}$ // [001] and Euler angles

$$\bar{y} = \{\phi, \gamma\} \rightarrow \quad \phi_{Euler} = \phi$$

$$\gamma = \varphi_1 - \pi/2$$

Orientation Distributions.

The orientation distribution function is defined by:

$$f(g)\,dg = \frac{dV}{V}$$

with

dV = totality of all volume elements of the sample which possess the orientation $g \in [g \pm dg]$.

V = total volume of the sample.

Problem:

How to represent the ODF ?
How to determine the ODF ?

→ the series expansion method by H.-J. Bunge.

$$f(g) = \sum_{\ell=0}^{+\infty} \sum_{m=-\ell}^{+\ell} \sum_{n=-\ell}^{+\ell} C_\ell^{mn}\, T_\ell^{mn}(g) \quad [1]$$

with $T_\ell^{mn}(g) = T_\ell^{mn}(\varphi_1, \phi, \varphi_2)$

$$= e^{im\varphi_2}\, P_\ell^{mn}(\cos\phi)\, e^{in\varphi_1}$$

and $P_\ell^{mn}(\cos\phi)$ = generalized associated Legendre functions.

$T_\ell^{mn}(\varphi_1, \Phi, \varphi_2)$ = generalized spherical harmonics.

⇒ Eq. [1] is a series expansion of $f(g)$ in generalized spherical harmonics.

Symmetry conditions

- crystal symmetry operators g_B

$$\rightarrow f(g_B\, g) = f(g) \qquad [2]$$

- sample symm. operators g_A

$$\rightarrow f(g\, g_A) = f(g) \qquad [3]$$

A new type of series expansion is introduced in which each term of the series expansion seperately fulfils eq^s [2] and [3]

$$f(g) = \sum_{\ell=0}^{+\infty} \sum_{\mu=1}^{M(\ell)} \sum_{\nu=1}^{N(\ell)} C_\ell^{\mu\nu}\, \dot{\dot{T}}_\ell^{\mu\nu}(g) \qquad [3]\text{ bis}$$

The dots signify that we are dealing with <u>symmetric</u> generalized spherical harmonics.

The symmetric functions are all linear comb^s of the usual functions:

$$\dot{\dot{T}}_\ell^{\mu\nu}(g) = \sum_{m=-\ell}^{+\ell} \sum_{n=-\ell}^{+\ell} \dot{A}_\ell^{m\mu}\, \dot{A}_\ell^{n\nu}\, T_\ell^{mn}(g)$$

The coeff^{ts} $\dot{A}_\ell^{m\mu}$ and $\dot{A}_\ell^{n\nu}$ must be chosen so that crystal and sample symmetry are fulfilled.

- The symmetric generalized spherical harmonics $\dot{\dot{T}}_\ell^{\mu\nu}$
$\rightarrow$ orthonormal function system:

$$\oint \dot{\dot{T}}_\ell^{\mu\nu}(g)\, \dot{\dot{T}}_{\ell'}^{*\mu'\nu'}(g)\,dg = \frac{1}{2\ell+1}\,\delta_{\ell\ell'}\,\delta_{\mu\mu'}\,\delta_{\nu\nu'} \quad [4]$$

with $\delta_{\ell\ell'} = 1$ if $\ell = \ell'$
$\delta_{\ell\ell'} = 0$ if $\ell \neq \ell'$

- The orientation element dg, expressed in Euler angles, is given by the following expression:

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

- The ODF is normalized so that:

$$\oint f(g)\,dg = 1 \quad [5]$$

- For a random texture: ODF = cte = f_r

$$\oint f_r\, dg = 1$$

$$f_r \int_0^{\pi}\int_0^{2\pi}\int_0^{2\pi} \frac{1}{8\pi^2}\sin\phi\, d\phi\, d\varphi_1\, d\varphi_2 = 1$$

$$f_r\,\frac{1}{8\pi^2}\left[-\cos\phi\right]_0^{\pi} 4\pi^2 = 1$$

$$\boxed{f_r = 1}$$

Insert the series expansion [3] bis in the normalization [5]

$$\Rightarrow \sum_{l=0}^{+\infty} \sum_{\mu=1}^{M} \sum_{\nu=1}^{M} C_l^{\mu\nu} \oint \dot{\dot{T}}_l^{\mu\nu}(g)\, dg = 1$$

Due to the orthonormality property [4]

$$\Rightarrow C_0^{11} = 1$$

- <u>Determination of the coeff^{ts} $C_l^{\mu\nu}$</u>

Suppose :

$$f(g) = \sum_{l',\mu',\nu'} C_{l'}^{\mu'\nu'} \dot{\dot{T}}_{l'}^{\mu'\nu'}(g)$$

multiply both sides with $\dot{\dot{T}}_l^{*\mu\nu}$ and integrate over all orientations :

$$\Rightarrow \oint f(g)\, \dot{\dot{T}}_l^{*\mu\nu}(g)\, dg = \sum_{l',\mu',\nu'} C_{l'}^{\mu'\nu'} \oint \dot{\dot{T}}_{l'}^{\mu'\nu'} \dot{\dot{T}}_l^{\mu\nu} dg$$

$$C_l^{\mu\nu} = (2l+1) \oint f(g)\, \dot{\dot{T}}_l^{*\mu\nu}(g)\, dg. \quad [6]$$

↳ the coeff^{ts} $C_l^{\mu\nu}$ can be calculated if the function $f(g)$ is known

· Individual orientation measurements.

Suppose : OD consists of only a single crystal g_o

$\rightarrow f(g) \neq 0$ if $g \in [g_o \pm dg]$

$$\Rightarrow \quad C_\ell^{\mu\nu} = (2\ell+1)\, \dot{\dot{T}}_\ell^{*}(g_o) \oint f(g)\, dg.$$

(normalization $\Rightarrow$ integral $= 1$)

$$\Rightarrow \quad C_\ell^{\mu\nu} = (2\ell+1)\, \dot{\dot{T}}_\ell^{*}(g_o) \qquad [7]$$

If the texture consists of several different crystals with orientation g_i and volumes V_i

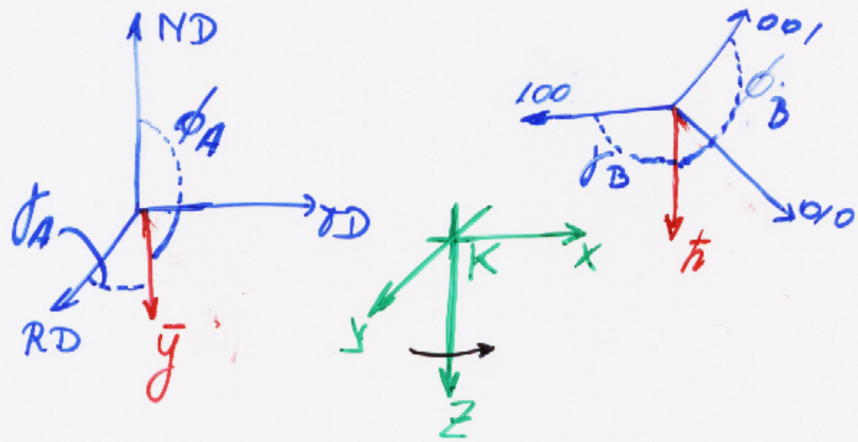
↳ one obtains the C-coeff^ts as weighted average values from eq. [7] :

$$C_\ell^{\mu\nu} = (2\ell+1)\, \frac{\sum_i V_i\, \dot{\dot{T}}_\ell^{*}(g_i)}{\sum_i V_i} \qquad [8]$$

↳ this method can be used for the determination of the coeff^ts in cases in which the texture is determined by single orientation measurements.

The general axis distribution function.

K_A = sample ref. system
K_B = crystal ref. system
K = intermediate ref. system
$\hookrightarrow Z \parallel \bar{y} \rightarrow \bar{y}\,(\phi_A, \gamma_A)$
$\rightarrow Z \parallel \bar{h} \rightarrow \bar{h}\,(\phi_B, \gamma_B)$



$g_1 = (\gamma_A + \frac{\pi}{2}, \phi_A, \psi)$ transforms K_A to K

$g_2 = (\psi', \phi_B, \frac{\pi}{2} - \beta)$ " K to K_B.

$g = g_2 g_1$ leads from K_A to K_B

Suppose we fix g_1 + ϕ_B and γ_B of g_2
→ only ψ' can rotate freely
⇒ all orientations g are described for which $\bar{h} \parallel \bar{y}$

Average value of the ODF over all these orientations → the function $A(\vec{h}, \bar{y})$

$$A(\vec{h},\bar{y}) = \frac{1}{2\pi}\int_0^{2\pi} f(g_2 g_1)\, d\gamma'$$

In symbolic notation:

$$A(\vec{h},\bar{y}) = \frac{1}{2\pi}\int_{[\vec{h}\parallel y]} f(g)\, d\gamma'$$

Substitution of the series expansion:

$$A(\vec{h},\bar{y}) = \frac{1}{2\pi}\sum_{l,\mu,\nu}^{+\infty,M,N} C_l^{\mu\nu}\int_{[\vec{h}\parallel y]} \dot{\dot{T}}_l^{\mu\nu}(g)\, d\gamma' \quad [9]$$

It can be proven that this integral can be expressed as:

$$A(\vec{h},\bar{y}) = 4\pi \sum_{l,\mu,\nu}^{+\infty,M,N} \frac{C_l^{\mu\nu}}{2l+1}\, \dot{k}_l^{*\mu}(\vec{h})\, \dot{k}_l^{\nu}(\bar{y}) \quad [10]$$

with $\dot{k}_l^{*\mu}(\vec{h})$ and $\dot{k}_l^{\nu}(\bar{y})$ =

symmetric, spherical <u>surface</u> harmonics

$A(\vec{h},\bar{y})$ → practical specifications: pole fig^s + inverse pole figures

↳ cannot be measured unequivocally by polycrystal diffraction experiments.

→ what one measures $A(+\vec{h},\bar{y}) + A(-\vec{h},\bar{y})$

→ multiplication of terms of odd l in [10]

⇒ odd C-coeff^ts cannot be obtained from pole figures.

Pole Figures $P_{\bar{h}}(\bar{y})$

We hold the crystal direction $\bar{h}_i$ fixed and choose it so that $\bar{h}_i = \{h_1, h_2, h_3\}^i$ corresponds to a low index lattice plane.

In this case:

$$A(\bar{h}_i, \bar{y}) = P_{\bar{h}_i}(\bar{y}) = \sum_{\ell=0}^{+\infty} \sum_{\mu=1}^{M} \sum_{\nu=1}^{N} \frac{4\pi\, C_\ell^{\mu\nu}}{(2\ell+1)} \dot{k}_\ell^{\mu}(\bar{h}_i) \times \dot{k}_\ell^{\nu}(\bar{y})$$

$$= \sum_{\ell=0}^{+\infty} \sum_{\nu=1}^{N} \left[\sum_{\mu=1}^{M} \frac{4\pi}{(2\ell+1)} C_\ell^{\mu\nu} \dot{k}_\ell^{\mu}(\bar{h}_i) \right] \dot{k}_\ell^{\nu}(\bar{y}) \quad [11]$$

Suppose:

$$F_\ell^{\nu}(\bar{h}_i) = \frac{4\pi}{(2\ell+1)} \sum_{\mu=1}^{M(\ell)} C_\ell^{\mu\nu} \dot{k}_\ell(\bar{h}_i) \quad [12]$$

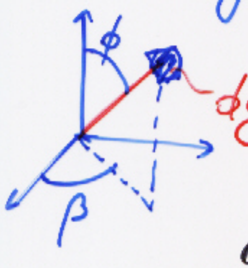
$$\Rightarrow \quad P_{\bar{h}_i}(\bar{y}) = \sum_{\ell=0}^{+\infty} \sum_{\nu=1}^{N(\ell)} F_\ell^{\nu}(\bar{h}_i)\, \dot{k}_\ell^{\nu}(\bar{y}) \quad [13].$$

$P_{\bar{h}_i}(\bar{y})$ = the volume fraction of the sample for which $\bar{h}_i \parallel \bar{y}$.
= pole figure associated with direction $\bar{h}_i$.

Normalization of pole figures?

$$\oint P_{\bar{h}_i}(\bar{y})\,d\bar{y} = \sum_{\ell,\nu}\left[\frac{4\pi}{(2\ell+1)}\sum_{\mu} C_\ell^{\mu\nu}\, k_\ell^{*\mu}(\bar{h}_i)\right] \times \oint k_\ell^{\nu}(\bar{y})\,d\bar{y} \quad [14]$$

with $d\bar{y} = \sin\phi\, d\phi\, d\beta$
= the element of solid angle



The orthonormality property is also valid for surface harmonics

$$\oint k_\ell^{\nu}(\bar{y})\, k_{\ell'}^{*\nu'}(\bar{y})\,d\bar{y} = \delta_{\ell\ell'}\,\delta_{\nu\nu'}$$

For $\ell = \ell' = 0$

$$\Rightarrow \quad k_0^{1} = \text{cte.}$$

$$\Rightarrow \quad \left(k_0^{1}\right)^2 \oint d\bar{y} = 1$$

$$\left(k_0^{1}\right)^2 \left[-\cos\phi\right]_0^{\pi} 2\pi = 1$$

$$k_0^{1} = 1/\sqrt{4\pi}$$

And thus:

$$\oint P_{\bar{h}_i}(\bar{y})\,d\bar{y} = 4\pi\, C_0^{11}\, k_0^{1} \oint k_0^{1}\, d\bar{y}$$

$$\oint P_{\bar{h}_i}(\bar{y}) = 4\pi \quad [15].$$

which is exactly the normalization which one obtains if $P^{r}_{\bar{h}}(\bar{y}) = 1$ was set for a random texture.

In eq. [13] → replace indices l, ν by l', ν' and multiply by $k_l^{*}(\bar{y})\,d\bar{y}$ and integrate over all directions $\bar{y}$

$$\Rightarrow \quad F_l^{\nu}(h_i) = \oint P_{h_i}(\bar{y})\, k_l^{*\nu}(\bar{y})\, d\bar{y} \quad [16]$$

For the coeff^{t} $F_0^1(h_i)$

$$F_0^1(h_i) = k_0^{*1}(\bar{y}) = \sqrt{4\pi}\,.$$

1 Normally, the pole figure $P_{h_i}(\bar{y})$ is known, <u>except</u> for an intensity factor depend^{t} on h_i

Suppose:

$$\hat{P}_{h_i}(\bar{y}) = \frac{1}{M_i} P_{h_i}(\bar{y}).$$

From the normalization condition [15]

$$\Rightarrow \quad \frac{1}{M_i} = \frac{1}{4\pi} \oint \hat{P}_{h_i}(\bar{y})\, d\bar{y}$$

$$\Rightarrow \quad F_l^{\nu}(h_i) = 4\pi \frac{\oint \hat{P}_{h_i}(\bar{y})\, k_l^{*\nu}(\bar{y})\, d\bar{y}}{\oint \hat{P}_{h_i}(\bar{y})\, d\bar{y}} \quad [17]$$

⇒ The coeff^{ts} $F_l^{\nu}(h_i)$ can be obtained from <u>not</u> normalized pole figures.

Normally, pole figures are only known in individual points.

Assume: pole figure $\neq 0$ in one point $\bar{y} = \bar{y}_0$

$$\Rightarrow F_\ell^\nu(h_i) = k_\ell^{*\nu}(\bar{y}_0) \oint P_h(\bar{y})\, d\bar{y}$$

$$F_\ell^\nu(h_i) = k_\ell^{*\nu}(\bar{y}_0)\, 4\pi$$

Assume pole figure $\neq 0$ in points y_j and to each point the weight factor V_j (e.g. the X-ray intensities)

$$\Rightarrow F_\ell^\nu(h_i) = 4\pi \frac{\sum_j k_\ell^{*\nu}(y_j)\, V_j}{\sum_j V_j}, \quad [18]$$

<u>Alternatively</u>

Calculate the coeff^{ts} $F_\ell^\nu(h)$ of the pole figure h_i from the values of $P_{h_i}(\bar{y}_j)$ which the pole figure assumes in points $\bar{y}_j$.

To be applied when the number of coeff^{ts} is small compared to the number of points $\bar{y}_j$.

We introduce an approximation function

$$P'_h(\bar{y}_j) \approx \sum_{\ell=0}^{L} \sum_{\nu=1}^{N(\ell)} F_\ell^\nu(h_i)\, \dot{k}_\ell^\nu(\bar{y}_j) \quad [19]$$

We then require the condition:

$$\sum_j \omega_j \left[P(\bar{y}_j) - P'(\bar{y}_j) \right]^2 = \min.$$

Derivative w.r.t. the unknown coeff^{ts} $F_\ell^\nu(\hbar) = 0$

$$\sum_j \omega_j \left[P(\bar{y}_j) - P'(\bar{y}_j) \right] \dot{k}_{\ell'}^{\nu'}(\bar{y}_j) = 0 \quad [20]$$

Substitute Eq. [19] in [20]

$$\Rightarrow \sum_{\ell=0}^{L} \sum_{\nu=1}^{N(\ell)} F_\ell^\nu(\hbar_i) \sum_j \omega_j \dot{k}_\ell^\nu(\bar{y}_j) \dot{k}_{\ell'}^{\nu'}(\bar{y}_j) = \sum_j \omega_j P(\bar{y}_j) \dot{k}_{\ell'}^{\nu'}(\bar{y}_i)$$

Suppose:

$$\sum_j \omega_j \dot{k}_\ell^\nu(\bar{y}_j) \dot{k}_{\ell'}^{\nu'}(\bar{y}_j) = \kappa_{\ell\ell'}^{\nu\nu'}$$

$$\sum_j \omega_j P(\bar{y}_j) \dot{k}_{\ell'}^{\nu'}(\bar{y}_j) = \gamma_{\ell'}^{\nu'}$$

$$\Rightarrow \boxed{\sum_{\ell=0}^{L} \sum_{\nu=1}^{N(\ell)} F_\ell^\nu(\hbar_i) \kappa_{\ell\ell'}^{\nu\nu'} = \gamma_{\ell'}^{\nu'}}$$

Linear system of eq^s with as many unknowns $F_\ell^\nu(\hbar)$ as equations $\Rightarrow$ unique solution!