Determination of the coefficients $C_\ell^{\mu\nu}$

Pole figures $P_{\hbar_i}(\vec{y})$ are developed in a series of spherical surface harmonics.

$$P_{\hbar_i}(\vec{y}) = \sum_{\ell=0}^{+\infty} \sum_{\nu=1}^{M(\ell)} F_\ell^\nu(\hbar_i) \dot{k}_\ell^\nu(\vec{y}) \qquad [21]$$

with the coefficients:

$$F_\ell^\nu(\hbar_i) = \frac{4\pi}{(2\ell+1)} \sum_{\mu=1}^{M(\ell)} C_\ell^{\mu\nu} \dot{k}_\ell^{*\mu}(\hbar_i) \qquad [22]$$

Coefficients $F_\ell^\nu(\hbar_i)$ are known for a certain number I_p of pole figures

→ [22] represents a system of I_p linear equations with $M(\ell)$ unknowns.
(only even values of ℓ)

In order to have a (unique) solution:

$$M(\ell) \leq I_p$$

If there are more equations than unknowns
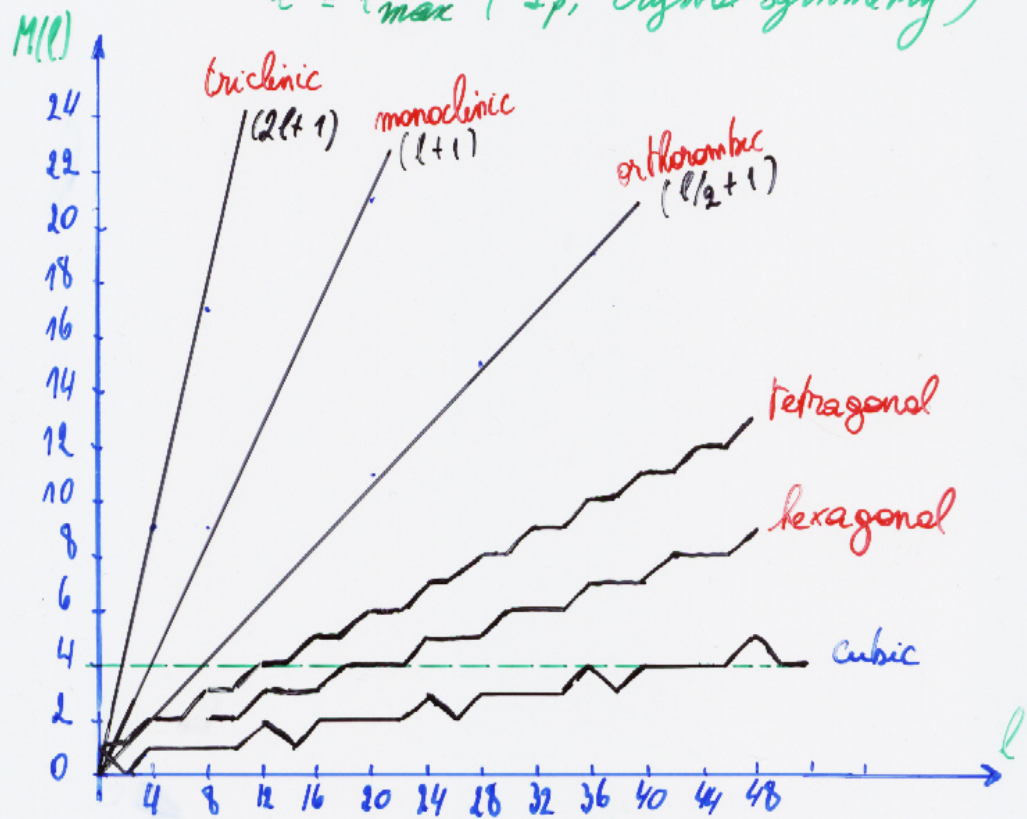→ it can occur there is no solution?

However! physics of the phenomenon
→ $F_\ell^\nu(\hbar_i)$ must be conditioned such that [g [22]
has a unique solution because some ODF $f(g)$
and thus a set of C coeff^{ts} must exist.

→ if Eg. [22] has more equations than unknowns ⇒ equations are not linear independent ⇒ # eqs can be reduced
→ unique solution.

$M(\ell)$ is increasing function of ℓ (depending on crystal symmetry)

⇒ For a given number of pole figures the system of eqs [22] can only be solved uniquely up to a certain degree

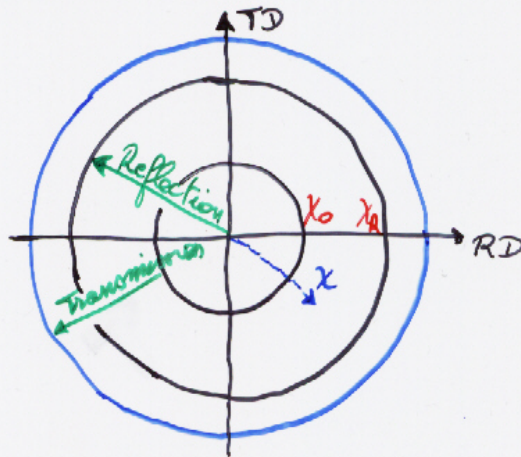$$\ell = \ell_{max}(I_p, \text{crystal symmetry})$$

triclinic $(2\ell + 1)$
monoclinic $(\ell + 1)$
orthorombic $(\ell/2 + 1)$
tetragonal
hexagonal
cubic

ℓ_{max} = the resolving power

2

Determination of the coefficients $C_\rho^{\mu\nu}$ from incompletely measured pole figures.

In practice (e.g. due to the defocusation effect) pole figures can only be measured over a limited range: $\chi_{min} < \chi < \chi_{max}$

(for the backreflection method with X-ray-diffraction: $\chi_{min} = 0$ and $\chi_{max} \approx 80°$).

Suppose: pole figure can only measured over an area B for which: $\chi_0 < \chi < \chi_R$

→ previous method for calculating coeff^{ts} can no longer be used because orthogonality relations are no longer valid:

$$\oint \dot{k}_\ell^\mu \dot{k}_{\ell'}^\nu (\bar{y}) \, d\bar{y} = \delta_{\ell\ell'} \delta_{\nu\nu'}$$

↳ integration over the entire surface of the pole figure.

Alternative method:

Suppose $C_l^{\mu\nu}$ are known

$\rightarrow$ we can calculate pole fig.² $P_{h_i}(\bar{y})_{cal}$ using

$$P_{h_i}(\bar{y})_{cal} = \sum_{l,\nu} \left[\frac{4\pi}{2l+1} \sum_{\mu} C_l^{\mu\nu} \dot{k}_l^{*\mu}(h_i) \right] \dot{k}_l^{\nu}(\bar{y}) \qquad [23]$$

Suppose: measured (and normalized) pole figures $P_{h_i}(\bar{y})_{obs}$

Now, we set as a condition:

$$\sum_i w_i \int_B \left[P_{h_i}(\bar{y})_{obs} - P_{h_i}(\bar{y})_{cal} \right]^2 d\bar{y} = min \qquad [24]$$

w_i = weight factors which reflect the accuracy of the pole figure measurement.

In general: measured pole figure

$\rightarrow$ unknown normalization

$$\hat{P}_{h_i}(\bar{y})_{obs} = \frac{1}{N_i} P_{h_i}(\bar{y})_{obs} \qquad [25]$$

with N_i = the unknown normalization factor.

Substituting eq. [23] in condition [24], considering eq. [25]

$$\sum_i w_i \int_B \left[N_i \hat{P}_{h_i}(\bar{y})_{obs} - \sum_{l,\mu,\nu} \frac{4\pi}{(2l+1)} C_l^{\mu\nu} \dot{k}_l^{*\mu} \dot{k}_l^{\nu}(\bar{y}) \right]^2 \times d\bar{y} = \underline{min} \qquad [26]$$

Expression [26] must be minimized w.r.t. the unknowns $C_\ell^{\mu\nu}$ and N_i

→ differentiation w.r.t. $C_\ell^{\mu\nu}$

$$\sum_i w_i \int_B \ell_\ell^{i*\mu}(\hat{n}_i)\,\ell_{\ell'}^{\nu'}(\bar{y}) \qquad [27]$$

$$\times \left[N_i\,\hat{P}_{\hat{n}_i}(\bar{y})_{obs} - \sum_{\ell,\mu,\nu} \frac{4\pi}{2\ell+1} C_\ell^{\mu\nu}\ell_\ell^{i*\mu}(\hat{n}_i)\,\ell_\ell^{\nu}(\bar{y}) \right] d\bar{y}$$
$$= 0$$

→ differentiation w.r.t. N_i :

$$\int_B \hat{P}_{\hat{n}_i}(\bar{y}_{obs}) \left[N_i\,\hat{P}_{\hat{n}_i}(\bar{y})_{obs} - \sum_{\ell=0}^{L}\sum_{\mu=1}^{M(\ell)}\sum_{\nu=1}^{N(\ell)} \frac{4\pi}{(2\ell+1)} C_\ell^{\mu\nu} \times \right.$$
$$\left. \ell_\ell^{i*\mu}(\hat{n}_i)\,\ell_\ell^{i\nu}(\bar{y}) \right] d\bar{y} = 0$$
$$[28]$$

We introduce the following quantities :

$$\int_B \left[\hat{P}_{\hat{n}_i}(\bar{y})_{obs} \right]^2 = P_i$$

$$\ell_\ell^{i*\mu}(\hat{n}_i) \int_B \hat{P}_{\hat{n}_i}(\bar{y})_{obs}\,\ell_\ell^{i\nu}(\bar{y})\,d\bar{y} = a_\ell^{\mu\nu}(\hat{n}_i)$$

$$\int_B \ell_\ell^{i\nu}(\bar{y})\,\ell_{\ell'}^{i\nu'}(\bar{y})\,d\bar{y} = \xi_{\ell\ell'}^{\nu\nu'}$$

$$\sum_i w_i \frac{4\pi}{2\ell+1}\,\ell_\ell^{i*\mu}(\hat{n}_i)\,\ell_{\ell'}^{i*\mu'}(\hat{n}_i) = \alpha_{\ell\ell'}^{\mu\mu'}$$

⇒ the equations [27] and [28] can be written as

$$\sum_{l=0}^{L} \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} C_l^{\mu\nu} \, \alpha_{ll'}^{\mu\mu'} \, \zeta_{ll'}^{\nu\nu'} = \sum_i \omega_i \, N_i \, a_{l'}^{\mu'\nu'}(h_i)$$

[29]

$$\sum_{l=0}^{L} \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} C_l^{\mu\nu} \, \frac{4\pi}{2l+1} \, a_l^{\mu\nu}(h_i) = N_i \, P_i$$

[30]

If the normalization factor N_i is expressed according to eq. [30] and substituted in eq [29]

$$\sum_{l=0}^{L} \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} C_l^{\mu\nu} \left[\alpha_{ll'}^{\mu\mu'} \zeta_{ll'}^{\nu\nu'} - \frac{4\pi}{2l+1} \sum_i \frac{\omega_i}{P_i} \times \right.$$

[31]

$$\left. a_l^{\mu\nu}(h_i) \, a_{l'}^{\mu'\nu'}(h_i) \right] = 0$$

This is a system of linear eq^s with as many eq^s as unknowns.

Eq. [31] is a homogeneous system $\Rightarrow$ the coeff^{ts} are only determined up to a common factor.
$\rightarrow$ can be derived from the normalization cond.

$$C_0^{11} = 1$$

The texture index

$$J = \oint \left[f(g) \right]^2 dg \quad = \text{texture index}$$

Because of the orthogonality rules:

$$J = \sum_{l,\mu,\nu} \frac{1}{(2l+1)} \left| C_l^{\mu\nu} \right|^2$$

For a random texture : $\quad J_r = 1$

For a single crystal texture : $\quad J_{g_0} \longrightarrow +\infty$

Ghost Correction.

Pole figures are independent of $C_l^{\mu\nu}$ coeff^{ts} of odd (uneven) rank because of the centro-symmetry property of pole figures.

$\Rightarrow$ classical pole figure inversion only yields even $C_l^{\mu\nu}$ coeff^{ts}.

However, it does NOT mean that the uneven C coeff^{ts} are zero!

$$f(g) = \sum_{l=0}^{L} \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} C_l^{\mu\nu} \dot{T}_l^{\mu\nu}(g) \quad [1]$$

If uneven C coeff^{ts} are ignored
$\downarrow$
$f(g) =$ the reduced ODF.

The reduced ODF may contain peaks (positive + negative) which do not represent real existing texture comp^{ts}
$\Rightarrow$ GHOST peaks.

In literature: various ghost correction procedures:
- positivity method (Bunge and Dahms)
- quadratic method (Van Houtte)
- exponential method (Van Houtte).

All these methods use the positivity property
$f(g) \geqslant 0$ of the texture function.

The ODF is a statistical distribution function
→ physical it must be non-negative
everywhere.

Construction of a general algorithm.

Suppose: $f_{true}(g)$ = the true texture function.

In reality we only know an approximation $f'(g)$ of $f_{true}(g)$.

⌐→ represented by a finite nr. of parameters such as:

1) $C_l^{\mu\nu}$ coeff^{as}

2) $f_{true}(g)$ on a 5° grid in Euler space.

Suppose:

x_i $(i = 1, .., n)$ is one set of values to reconstruct $f_{true}(g)$

y_j $(j = 1, .., m)$ is another set.

Obviously, there must exist a relation between both sets of parameters:

$$y_j = Y_j(x_i) \text{ and } x_i = X_i(y_j)$$

Assume x_i's are known, and y_j's not but we know y_{oj} as a first estimate for y_j.

$$\Rightarrow x_{oi} = X_i(y_{oj}) \quad [2]$$

We can now expand the function $y_j(x_i)$ as a Taylor series:

$$y_j(x_i) = y_{oj} + \sum_{i=1}^{n} \frac{\partial y_j}{\partial x_i}(x_{ok})(x_i - x_{oi}) + \cdots \quad [3]$$

If we neglect the higher order terms:
a new estimate of y_j can now be made:

$$y_{1j} = y_{oj} + \sum_{i=1}^{n} \frac{\partial y_j}{\partial x_i}(x_{ok})(x_i - x_{oi}) \quad [4]$$

The old y_{oj} are replaced by the new y_{1j} and the algorithm can be executed again starting with Eq. [2].

These algorithms can only be used if the functions $x_i(y_j)$ are known and if the values $\frac{\partial y_j}{\partial x_i}(x_{ok})$ can be evaluated.

The positivity method.

The two parameter sets are chosen as follows:

$$\begin{cases} y_j = \text{odd} \;\; C\text{-coeff}^{ts} \;\; (\# = m) \\ x_i = \text{values of the complete ODF on a } 5° \\ \qquad \text{grid in Euler space.} (\# = n) \end{cases}$$

The function $x_i(y_j)$ is given by:

$$x_i = X_i(y_j) = \tilde{f}(g_i) + \sum_{\ell=1(2)}^{L} \sum_{\mu,\nu} \dot{T}_\ell^{\mu\nu}(g_i) y_j \quad [5]$$

with g_i = crystal orientations at the grid points
and $\tilde{f}$ = the reduced ODF (even C-coeff^{ts})

9

Relation between C coeff^{ts} and $f(g)$:

$$C_\ell^{\mu\nu} = (2\ell+1) \oint f(g) \overset{\cdots}{T}_\ell^{\mu\nu}(g)\, dg.$$

In a discrete way:

$$C_\ell^{\mu\nu} = (2\ell+1) \sum_{i=1}^n w_i \, f(g_i) \overset{\cdots}{T}_\ell^{\mu\nu}(g_i) \quad [6]$$

with w_i = weight factors suitable for numerical integration.

With above conventions for z_i and y_j:

$$y_j(z_i) = (2\ell+1) \sum_{i=1}^n w_i \, \overset{\cdots}{T}_\ell^{\mu\nu}(g_i)\, z_i \quad [7]$$

$$\Rightarrow \frac{\partial y_j}{\partial z_i} = (2\ell+1)\, w_i \, \overset{\cdots}{T}_\ell(g_i) \quad [8]$$

The initial estimate y_{oj} of the odd C-coeff$^{ts} = 0$
$\Rightarrow$ the z_{oi} coeff^{ts} = the reduced ODF $\tilde{f}$

In certain negative regions (i.e. regions for which $\tilde{f}(g_i) < 0$) $\longrightarrow$ the true value should be zero.

$\Rightarrow$ we assume :

[7 bis]
$$z_i = z_{oi} = \tilde{f}(g_i) \text{ if } z_{oi} \geq \alpha \quad \longrightarrow \text{range } Z_+$$
$$z_i = 0 \text{ if } z_{oi} \leq \alpha \quad \longrightarrow \text{range } Z_-$$

Using eq. [4] and eq. [8]

$$y_{1j} = y_{oj} - (2\ell+1) \sum_{g_i \in Z_-} w_i \, \overset{\cdots}{T}_\ell^{\mu\nu}(g_i)\, z_{oi}$$

- In the next iteration step → values y_{oj} are substituted by values y_{1j} in eq. [4] and eq. [5] is used to calculate the new x_{oi} being x_{1i}, whereas [7bis] is used to find the new values for x_i.

- The algorithm can be repeated as often as necessary. At each stage x_{oi} is the current estimate of the complete ODF.

- Convergence can be monitored by some error criterion:

$$-\int_Z f(g) < \varepsilon \quad \hookrightarrow \text{small positive value.}$$

Exponential Method.

Idea to produce a strictly non-negative ODF with C-coeffts $C_{sl}^{\mu\nu}$.

→ even C-coeffts should be equal to those obtained after classical pole figure inversion $C_l^{\mu\nu}$

$$[8] \quad \Delta = \sum_{\ell=0(2)}^{L} \sum_{\mu,\nu} \frac{1}{(2\ell+1)} \left[C_{s\ell}^{\mu\nu} - C_{\ell}^{\mu\nu} \right]^2 \to 0$$

Strictly positive ODF: $f_s(y) = e^{h(g)}$ [9]

Choice of parameter sets:

$y_j = h(g_j)$ on grid points g_j in E.S.

$x_i = C_{sl}^{\mu\nu}$ (even + uneven).

y_{oj} is estimated from other method (e.g. positivity).

$$X_i(y_j) = (2\ell+1) \sum_{j=1}^{m} \omega_j \, \ddot{T}_\ell^{\mu\nu}(g_j) \, e^{y_j}$$

and using eq. [1] and eq. [9]

$$\Rightarrow \quad e^{y_j} = \sum_{\ell=0}^{L} \sum_{\mu,\nu} x_i \, \ddot{T}_\ell^{\mu\nu}(g_j)$$

i corresponds to a comb. of ℓ, μ, ν

Differentiation w.r.t. x_i

$$e^{y_j} \frac{\partial y_j}{\partial x_i} = \ddot{T}_\ell^{\mu\nu}(g_j)$$

$$\frac{\partial y_j}{\partial x_i} = e^{-y_j} \ddot{T}_\ell^{\mu\nu}(g_j)$$

The general algorithm can now be
applied with eq. [8] as convergence criterion.

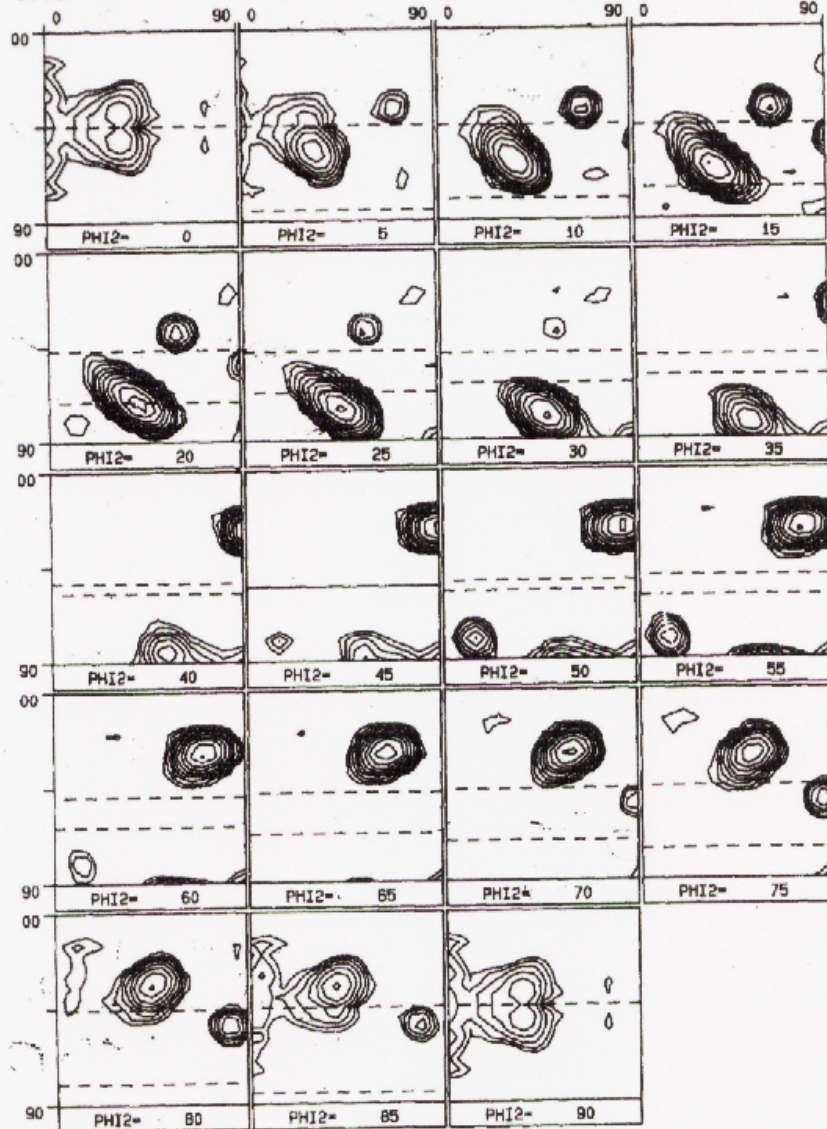# Texture before ghost correction

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1.00   1.40   2.00   2.80   4.00   5.60   8.00   11.0   16.0   22.0

Texture after ghost correction

Discretization of continuous ODFs.

Literature : L. S. Tóth and P. Van Houtte,
Textures and Microstructures, Vol. 19, pp. 229-244.

Approximation of the ODF by a discrete set
of orientations is required in many
modelling studies of texture dependent physical
properties.

1. Discretization on the basis of a random set of
   orientations.

Suppose: g_i = set of N orientations randomly
distributed in orientation space
(N can be chosen freely).

With each orientation a volume v_i of Euler
space is associated such that:

$$\sum_{i=1}^{N} v_i = \text{the total volume of E.S}$$
$$= 1 \quad (\text{if the Bunge normalization is accepted})$$

$f(g)$ is specified by its set of $C_l^{\mu\nu}$ coeff[ts]

$$\Rightarrow \quad f(g_i) = \sum_{l,\mu,\nu}^{L,M,N} C_l^{\mu\nu} \dot{T}_l^{\mu\nu}(g_i)$$

can be calculated for any arbitrary orientation.

and $v_i f(g_i) =$ an approximation of the volume fraction of orientation g_i

$\Rightarrow$ The set of orientations g_i with volume fractions ω_i given by

$$\omega_i = v_i \, f(g_i)$$

can be regarded as a discrete representation of $f(g)$.

_____

2. Discretization on the basis of the "cumulative" ODF statistical technique.

For some applications it is desirable to produce a discrete grain orientation distribution in which each grain has the same volume fraction.

$\hookrightarrow$ Can be obtained by employing the cumulative distribution function.

The cumulative ODF is defined by:

$$F(G) = \int_{G_0}^{G} f(g)\, dg \qquad [1]$$

with $G =$ an arbitrary crystal orientation the integral follows an arbitrary integration path that covers the whole orientation space.

The integration of eq. [1] will be carried out in a discrete way over a number of boxes in Euler space.

Suppose, we use the 5°- grid in E.S.
→ partitions E.S. in N boxes with sequence numbers i (i = 1, ..., N).
The centre of such a box is orient. g_i.
⇒ the discrete version of integral [1] is given by :

$$F_j = \sum_{i=1}^{d} f_i \qquad [2]$$

with f_i = the integral of $f(g)$ over box i :
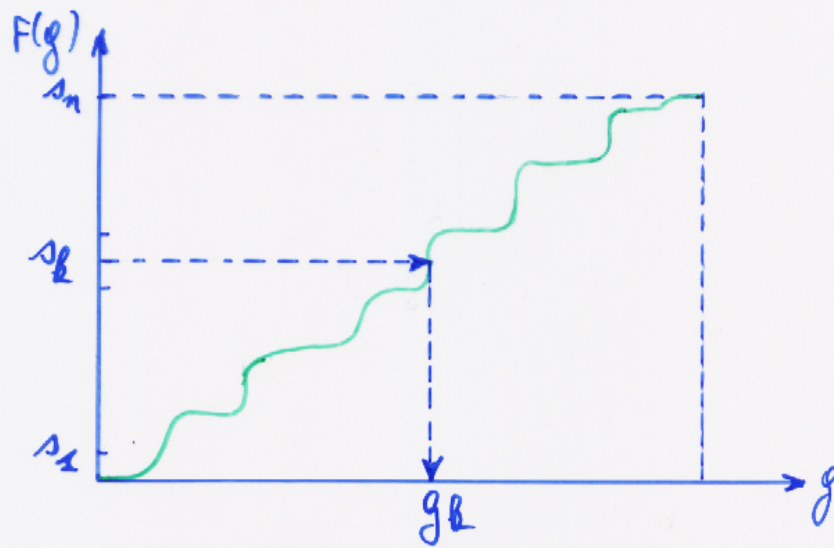
$$f_i = \int_{box\,i} f(g)\, dg$$

and because of the normalization condition
$$\sum_{c=1}^{N} f_i = 1$$
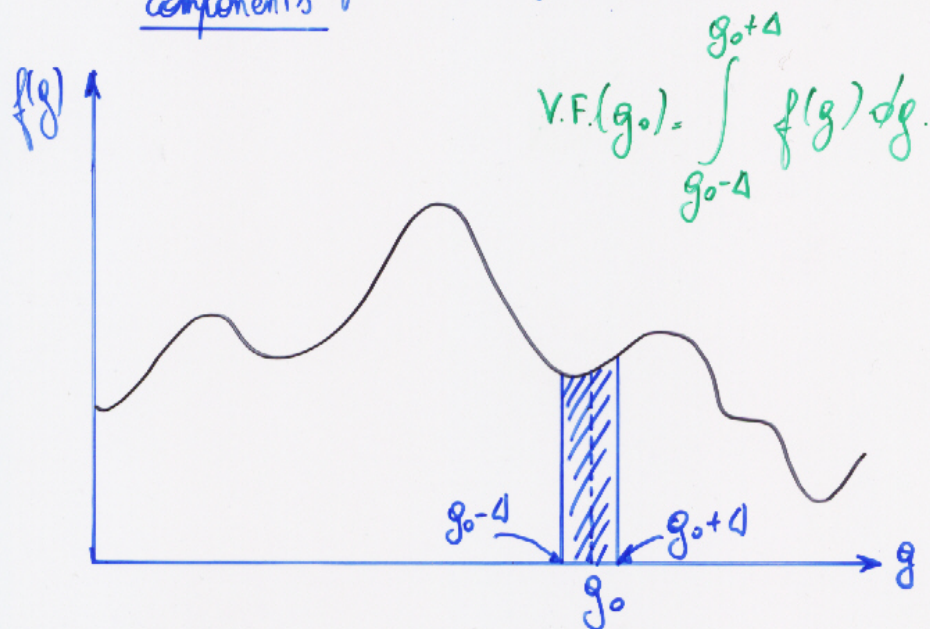
Eq. [2] defines a kind of "staircase" function.

A discrete set of orientations is produced in the following way !

1) a set of n number ("selectors") is generated in a range between 0 and 1

2) One discrete orientation will be generated for each selector by using the inverse function of the staircase function.

The volume fraction of individual texture components

$$V.F.(g_0) = \int_{g_0-\Delta}^{g_0+\Delta} f(g)\, dg.$$

How to chose Δ ?

Method, proposed by Bunge :

• Consider a Gaussian spread function
around g_0 with max S and spread ϕ :

$$\omega_{g_0}(g) = S \exp\left[-\left(\phi/\phi_0\right)^2\right]$$

with ϕ_0 = the angular width
(typical $\phi_0 = 16.5°$ or $11°$).

• The volume fraction $VF(g_0)$ of the comp^t g_0
is estimated by :

$$V.F(g_0) = \frac{1}{S} \oint \omega_{g_0}(g) f(g) dg.$$

(cfr. Bunge, "Texture Analysis in Materials Science",
   p. 171).

Disadvantage of this method

1] Vol. fractions are not normalized to 1
(there is always the contribution from the
tail of the Gaussian spread function)

2] Strong dependence from the choice of ϕ_0.

Modelling of texture dependent physical properties!

Each orientation dependent physical property of the single crystal

$\Downarrow$

Texture dependent physical property of the polycrystal !

Suppose : E = an orientation dependent physical property.

$$E = E(g).$$

e.g. E = elastic modulus

= magnetization energy of a cubic crystal

= thermal expansion of non-cubic crystals

= ....

Most often : E is a tensorial property $\bar{\bar{E}}$

$\bar{\bar{E}}$ will exhibit the symmetry of both crystal and sample

$$\Rightarrow \qquad E(g) = \sum_{\ell=0}^{L} \sum_{M,N} e_\ell^{\mu\nu} \ddot{\ddot{T}}_\ell^{\mu\nu}(g)$$

$E(g)$ can be expanded in a series of symmetrical spherical harmonics.

with $e_\ell^{\mu\nu}$ given by:

$$e_\ell^{\mu\nu} = (2\ell+1) \oint E(g)\, \dot{T}_\ell^{*\mu\nu}(g)\, dg.$$

If mutual grain interaction can be ignored the polycrystalline average of $E(g)$ of a material with ODF $f(g)$ is given by:

$$\bar{E} = \oint f(g)\, E(g)\, dg.$$

$$\bar{E} = \frac{1}{(2\ell+1)} \sum_{\ell=0}^{L} \frac{1}{(2\ell+1)} \sum_{\mu,\nu}^{M,N} e_\ell^{\mu\nu}\, C_\ell^{\mu\nu}$$

Example : the elastic anisotropy.

Problem: How to obtain the effective elastic moduli of a polycrystalline material from the single crystal ones, taking the texture into account

For a single crystal : Hooke's law is formulated as follows:

$$\varepsilon_{ij} = \Lambda_{ijkl}\, \sigma_{kl}$$

$$\text{or } \sigma_{ij} = C_{ijkl}\, \varepsilon_{kl}$$

S_{ijkl} = elastic compliance tensor
C_{ijkl} = " stiffness tensor.

$$[S_{ijkl}] = [C_{ijkl}]^{-1}$$

These tensors depend on the crystallite orientation g

→ S_{ijkl} and C_{ijkl} are expressed in the sample ref. system x_1, x_2, x_3.

Literature data on stiffness or compliance are normally expressed in the cryst. ref. system x_1^c, x_2^c, x_3^c → S_{ijkl}^c, C_{ijkl}^c

According to the tensor transformation laws:

$$S_{ijkl} = a_{im} a_{jn} a_{ko} a_{lp} S_{mnop}^c$$

According to Bunge the product $a_{im} a_{jn} a_{ko} a_{lp}$ can be expressed by means of a series expansion of harmonic functions in which $L_{max} = 4$.

→ S_{ijkl} (and C_{ijkl}) can be written as a series expansion of order 4.

The polycrystalline averages of stiffness and compliance tensors are given by:

$$\bar{S}_{ijkl} = \int S_{ijkl}(g)\, f(g)\, dg =$$