



# *OD Calculation from Pole Figure Data*

27-750

Texture, Microstructure & Anisotropy

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# Notation

$p$  Intensity in pole figure

$\alpha, \beta$  angles in pole fig.

$\Psi, \Theta, \phi$  Euler angles (Roe/Kocks)

$\Gamma$  integration variable

$Y_{lmn}$  Spherical harmonic function

$P$  Associated Legendre polynomial

$Q$  Coefficient on Legendre polynomial

$l, m, n$  integer indices for polynomials

$Z_{lmn}$  Jacobi polynomials

$W$  Coefficient on Jacobi polynomial

$\xi, \eta$  polar coordinates pole (hkl) in crystal coordinates

$\tilde{f}_{odd}$  odd part of the orientation distribution function

$\tilde{f}_{even}$  even part of the orientation distribution function

## *Notation: 2*

$I$  = no. pole figures

$M$  = multiplicity

$N$  = normalization

$y$  = connectivity matrix between pole figures and orientation distribution space

$f$  = intensity in the orientation distribution

$p$  = pole figure intensity

$m$  = pole figure index

## *Objectives*

- To explain what is being done in popLA, Beartex, and other software packages when pole figures are used to calculate Orientation Distributions
- To explain how the two main methods of solving the “fundamental equation of texture” that relates intensity in a pole figure,  $p$ , to intensity in the OD,  $f$ .

$$P_{(hkl)}(\alpha, \beta) = \frac{1}{2\pi} \int_0^{2\pi} f(\Psi, \Theta, \phi) d\Gamma$$

## *In-Class Questions*

- Does the WIMV method fit a function to pole figure data, or calculate a discrete set of OD intensity values that are compatible with the input? Answer: discrete ODs.
- Why is it necessary to iterate with the harmonic method with typical reflection-method pole figures? Answer: because the pole figures are incomplete and iteration is required to fill in the missing parts of the data.
- What is the significance of the “order” in harmonic fitting? Answer: the higher the order, the higher the frequency that is used. In general there is a practical limit around  $l=32$ .
- What is a “WIMV matrix”? Answer: this is a set of relationships between intensities at a point in a pole figure and the corresponding set of points in orientation space, all of which contribute to the intensity at that point in the pole figure.
- What is the “texture strength”? This is the root-mean-square value of the OD.

## *Methods*

- Two main methods for reconstructing an orientation distribution function based on pole figure data.
- Standard *harmonic method* fits coefficients of spherical harmonic functions to the data.
- Second method calculates the OD directly in discrete representation via an iterative process (e.g. *WIMV method*).

# History

- Original proposals for harmonics method:  
Purseley & Cox (1954), *Phil. Mag.* **45** 295-302;  
also Viglin (1960), *Fiz. Tverd. Tela* **2** 2463-2476.
- Complete methods worked out by Bunge and Roe: “Zur Darstellung Allgemeiner Texturen”, Bunge (1965), *Z. Metall.*, **56** 872-874; “Description of crystallite orientation in polycrystalline materials. III. General solution to pole figure inversion”, Roe (1965): *J. Appl. Phys.*, **36** 2024-2031.
- WIMV method:  
Matthies & Vinel (1982): *Phys. Stat. Solid. (b)*, **112** K111-114.
- MTEX method: “A novel pole figure inversion method: specification of the MTEX algorithm”, Hielscher & Schaeben (2008): *J. Appl. Cryst.* **41** 1024–1037.

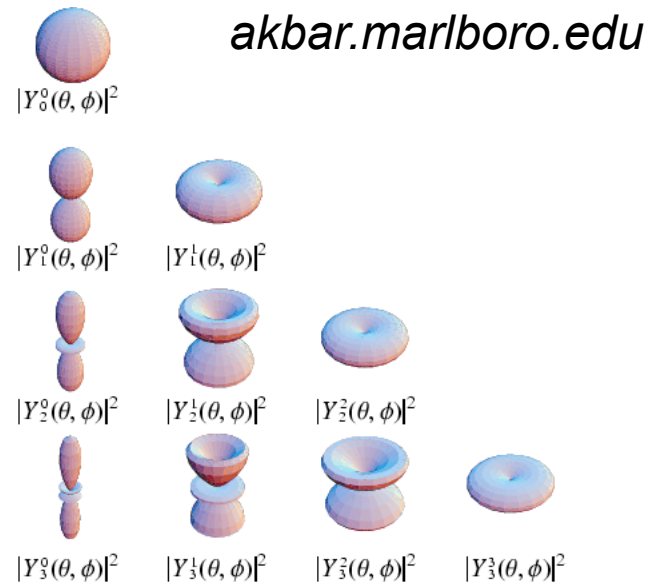
# Harmonics

- **Spherical harmonics**,  $Y_{lmn}$ :  
An infinite series of orthogonal functions that can be used to describe data (intensities) that depend on (two) spherical angles (but not radius). Analogous to Fourier series. *Legendre polynomials* are a special case of spherical harmonics. Used to fit pole figure (PF) data (intensities). Also used extensively in quantum mechanics. See [http://en.wikipedia.org/wiki/Spherical\\_harmonics](http://en.wikipedia.org/wiki/Spherical_harmonics).
- **Generalized spherical harmonics**:  
An infinite series of orthogonal functions that can be used to describe data that depend on (three) Euler angles (like spherical angles plus an extra longitude angle). Used to fit Orientation Distribution data (intensities).
- **Orthogonal functions**:  
Two functions,  $f$  and  $g$ , are orthogonal when their *inner product* is zero (analogous to the dot product between two vectors being zero when they are orthogonal/perpendicular). See [http://en.wikipedia.org/wiki/Orthogonal\\_functions](http://en.wikipedia.org/wiki/Orthogonal_functions).

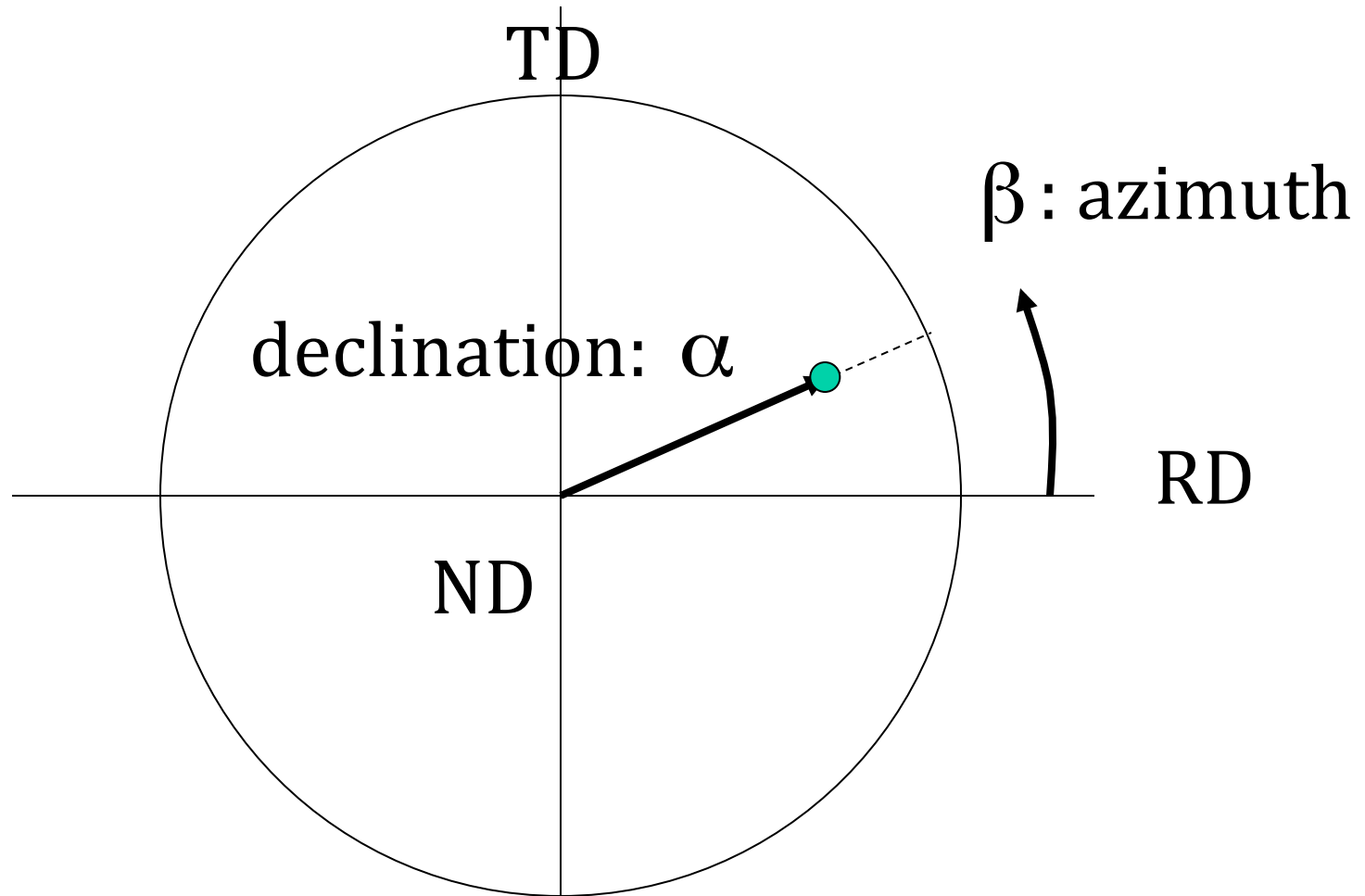


# Series Expansion Method

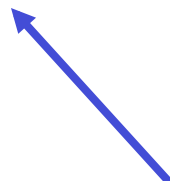
- The harmonic method is a two-step method.
- First step: fitting coefficients to the available PF data, where  $\rho$  is the intensity at an angular position;  $\alpha$ ,  $\beta$ , are the declination and azimuthal angles,  $Q$  are the coefficients,  $P$  are the associated Legendre polynomials and  $l$  and  $m$  are integers that determine the shape of the function.
- Useful URLs:
  - [geodynamics.usc.edu/~becker/teaching-sh.html](http://geodynamics.usc.edu/~becker/teaching-sh.html)
  - [http://commons.wikimedia.org/wiki/Spherical\\_harmonic](http://commons.wikimedia.org/wiki/Spherical_harmonic)



# *Pole Figure (spherical) angles*



You can also think of these angles as longitude (= azimuth) and co-latitude (= declination, i.e.  $90^\circ$  minus the geographical latitude)

$$p(\alpha, \beta) = \sum_{l=0}^{\infty} \sum_{m=-l}^l Q_{lm} P_l^m(\cos \alpha) e^{im\beta}$$


coefficients to be determined

Notes:

$p$ : intensity in the pole figure

$P$ : associated Legendre polynomial

$l$ : order of the spherical harmonic function

$l, m$ : govern shape of spherical function

$Q$ : can be complex, typically real

## *Coefficients of Sph. Harmonics*

The functions are orthogonal, which allows integration to find the coefficients. Notice how the equation for the Q values is now explicit and based on the intensity values in the pole figures!

$$Q_{lm} = \int_0^\pi \int_0^{2\pi} p(\alpha, \beta) P_l^m(\cos \alpha) e^{-im\beta} \sin \alpha d\beta d\alpha$$

“Orthogonal” has a precise mathematical meaning, similar to *orthogonality* or *perpendicularity* of vectors. To test whether two functions are orthogonal, integrate the *inner product* of the two functions over the range in which they are valid. This is a very useful property because, to some extent, sets of such functions can be treated as independent units, just like the unit vectors used to define Cartesian axes. In this case we must integrate over the applicable ranges of the angles.

$$\int_{\theta=0}^\pi \int_{\varphi=0}^{2\pi} Y_\ell^m Y_{\ell'}^{m'}{}^* d\Omega = \delta_{\ell\ell'} \delta_{mm'},$$

## *Orientation Distribution Expansion*

The expressions in Roe angles are similar, but some of the notation, and the names change.

$$f(\Psi, \Theta, \phi) =$$

$$\sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n=-l}^l W_{lmn} Z_{lmn}(\cos \Theta) e^{im\Psi} e^{im\phi}$$

Notes:

$Z_{lmn}$  are Jacobi polynomials

Objective: find values of coefficients,  $W$ , that fit the pole figure data ( $Q$  coefficients).

## *Fundamental Equation*

If, and only if  $(hkl) = (001)$ , then integrate directly over 3rd angle,  $\phi$ :

$$P_{(001)}(\alpha, \beta) = \frac{1}{2\pi} \int_0^{2\pi} f(\alpha, \beta, \phi) d\phi$$

$$P_{(hkl)}(\alpha, \beta) = \frac{1}{2\pi} \int_0^{2\pi} f(\Psi, \Theta, \phi) d\Gamma$$

For a general pole, there is a complicated relationship between the integrating parameter,  $\Gamma$ , and the Euler angles.

## *Solution Method*

coefficients to  
be determined



$$Q_{lm} = \sum_{n=-l}^l W_{lmn} P_l^n(\cos \xi) e^{-in\eta}$$

- Obtained by inserting the PF and OD equations the Fundamental Equation relating PF and OD.
- $\xi$  and  $\eta$  are the polar coordinates of the pole (hkl) in crystal coordinates.
- Given several PF data sets (sets of  $Q$ ) this gives a system of *linear simultaneous equations*, solvable for  $W$ .

## *Order of Sph. Harm. Functions*

- Simplifications: cubic crystal symmetry requires that  $W_{2mn}=0$ , thus  $Q_{2m}=0$ .
- All independent coefficients can be determined up to  $l=22$  from 2 PFs.
- Sample (statistical) symmetry further reduces the number of independent coefficients.
- Given  $W$ , other, non-measured PFs can be calculated, also Inverse Pole Figures.

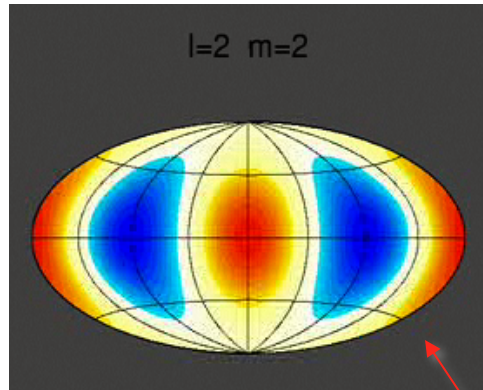


## *Incomplete Pole Figures*

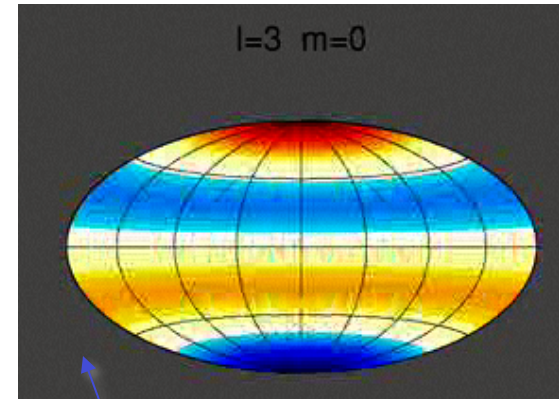
- Lack of data (from the standard reflection method for measuring PFs) at the edges of PFs requires an iterative procedure. The reason is that the integration (summation) described before only applies (directly) if the PFs are complete.
- 1: estimate PF intensities at edge by extrapolation;  
2: make estimate of  $W$  coefficients;  
3: re-calculate the edge intensities;  
4: replace negative values in the OD by zero;  
5: iterate until criterion satisfied.

## *Series Expansion Advantages*

- Set of coefficients (for each generalized spherical harmonic) is a compact representation of texture.
- Rapid calculation of anisotropic properties possible; this is particularly true of elastic anisotropy where one only needs coefficients up to  $l=4$ .
- Automatic smoothing of OD from truncation at finite order (equivalent to limiting frequency range in Fourier analysis).



## *Ghosts*



- Distribution of poles on a sphere, as in a PF, is centro-symmetric.
- Sph. Harmonic Functions are centrosymmetric for  $l=\text{even}$  but antisymmetric for  $l=\text{odd}$ . Therefore the  $Q=0$  when  $l=\text{odd}$ .
- Coefficients  $W$  for  $l=\text{odd}$  can take a range of values provided that PF intensity=0 (i.e. the intensity can vary on either side of zero in the OD).

## *Ghosts, contd.*

$$f = \tilde{f} + \tilde{\tilde{f}}$$
$$= \tilde{f}_{\text{even}} + \tilde{f}_{\text{odd}} = \tilde{f}_{l=\text{even}} + \tilde{f}_{l=\text{odd}}$$

- Need the odd part of the OD to obtain correct peaks and to avoid negative values in the OD (which is a probability density).
- Can use zero values in PF to find zero values in the OD: from these, the odd part can be estimated, Bunge & Esling, J. de Physique Lett. **40**, 627(1979).

## *Example of ghosts*

Quartz sample;  
7 pole figures;  
WIMV calculation;  
harmonic expansions

If only the even part  
is calculated, ghost  
peaks appear - fig (b)

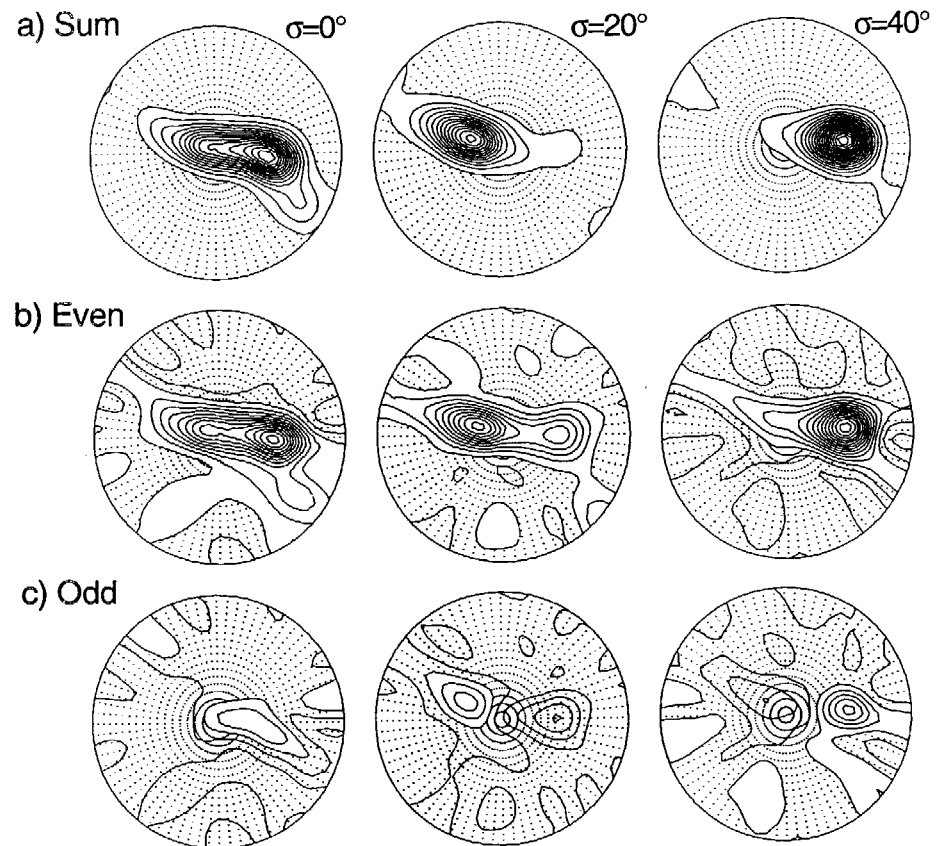


Fig. 3. Harmonic expansion of an OD that had been calculated using WIMV from seven pole figures of a quartz sample: (a) using even and odd functions (max. normalized density: 19/minimum 0); (b) even functions (14/1.8); (c) odd functions (6/-4.3). 'Ghosts' are best visible as negative regions in the odd expansion. Expansion is to order 22. Contour interval 1 m.r.d., negative regions dotted [WENK & AL. 1994b].

## *Discrete Methods: History*

- Williams (1968): *J. Appl. Phys.*, **39**, 4329.
- Ruer & Baro (1977): *Adv. X-ray Analysis*, **20**, 187-200.
- Matthies & Vinel (1982): *Phys. Stat. Solid. (b)*, **112**, K111-114.
- The idea behind the discrete methods was to construct intensity values for a discrete form of the Orientation Distribution (OD) directly from pole figure data, with no function being fitted.

## *Discrete Methods*

$$P_{(hkl)}(y) = \frac{1}{N} \sum_{i=1}^N f(y(g))$$

- Establish a grid of cells in both PF and OD space; e.g.  $5^\circ \times 5^\circ$  and  $5^\circ \times 5^\circ \times 5^\circ$ .
- Calculate a correspondence or *pointer matrix* between the two spaces, i.e.  $y(g)$ . Each cell in a pole figure is connected to multiple cells in orientation space (via the equation above). More specifically, the intensity in each pole figure cell is the summation of the intensities in the associated OD cells.
- Corrections needed for cell size, shape.

## *Initial Estimate of OD*

- Initial Estimate of the Orientation Distribution:

$$f^{(0)}(\varphi, \theta, \phi) = N \prod_{i=1}^I \prod_{m_i=1}^M p_{h_i}^{\text{exptl}}(y_{m_i})^{1/IM_i}$$

$I$  = no. pole figures;

$M$  = multiplicity;

$N$  = normalization;

$f$  = intensity in the orientation distribution;

$p$  = pole figure intensity;

$m$  = pole figure index



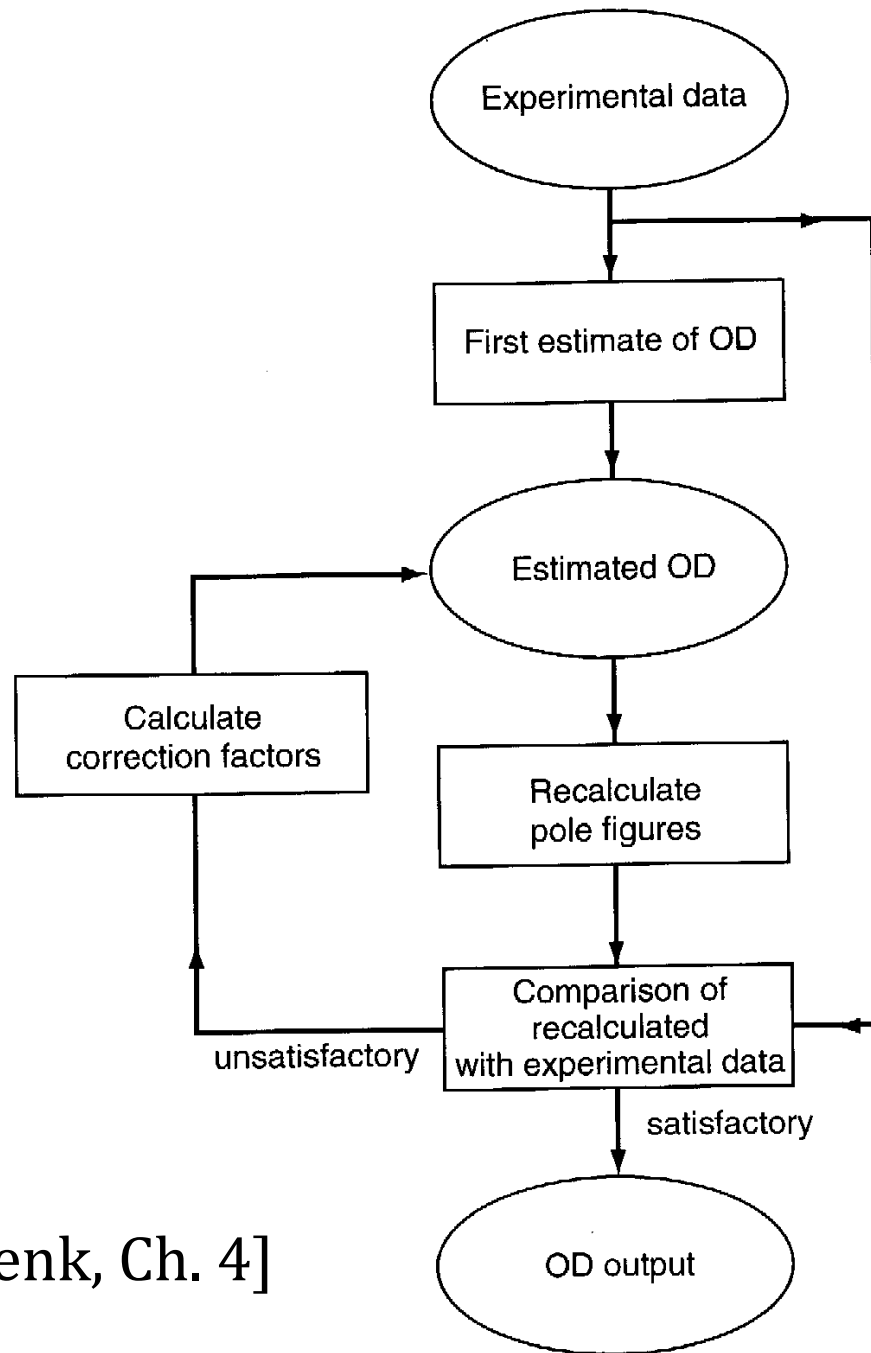
## *Iteration on OD values*

- Iteration to Refine the Orientation Distribution:

$$f^{(n+1)}(\varphi, \theta, \phi) = N^{(n)} f^{(n)}(\varphi, \theta, \phi) \frac{f^{(0)}(\varphi, \theta, \phi)}{\prod_{i=1}^I \prod_{m_i=1}^M P_{h_i}^{\text{calc}}(y_{m_i})^{1/IM_i}}$$

Note: the correction is squared in the second iteration (in the WIMV program), provided that the intensity is to be increased. This sharpens the distribution.

# Flow Chart



[Kocks Tomé Wenk, Ch. 4]

## “RP” Error

$$RP = 100\% \times \sum_g \left( \frac{f^{(0)}(g) - \text{recalc } f(g)}{f^{(0)}(g)} \right)$$

- RP: RMS value of relative error ( $\Delta P/P$ )  
- not defined for  $f=0$ .
- Note: this definition of the RP error, which is output by the WIMV code (part of popLA) in each iteration, was updated to reflect the actual code, Sept. 2011.

## *Discrete Method: Advantages*

- Ghost problem automatically avoided by requirement of  $f > 0$  in the solution.
- Zero range in PFs (i.e. an intensity value = 0) automatically leads to zero range in the OD.
- Much more efficient for lower symmetry crystal classes: useful results obtainable for only three measured PFs.

## *Discrete Method: Disadvantages*

- Susceptible to noise (filtering possible).
- Normalization of PF data is critical (harmonic analysis helps with this).
- Depending on OD resolution, large set of numbers required for representation ( $\sim 5,000$  points for  $5 \times 5 \times 5$  grid in Euler space), although the speed and memory capacity of modern PCs have eliminated this problem.
- Pointer matrix is also large, e.g.  $5 \cdot 10^5$  points required for OD  $\leftrightarrow$   $\{111\}$ ,  $\{200\}$  &  $\{220\}$  PFs.

## *MTeX method*

- From the 2008 paper, the method uses advanced numerical analysis to find a best-fit ODF from pole figure data.
- “...is the approximation by finite linear combinations of radially symmetric functions, i.e. by functions of the form:”

$$f(\mathbf{g}) = \sum_{m=1}^M c_m \psi(\mathbf{g}\mathbf{g}_m^{-1}), \quad (46)$$

where

$$\psi(\mathbf{g}) = \tilde{\psi}(\angle\mathbf{g}) = \sum_{l=0}^{\infty} \hat{\psi}(l) \mathcal{U}_{2l}[\cos(\angle\mathbf{g}/2)], \quad \mathbf{g} \in \text{SO}(3) \quad (47)$$

$\Psi$  is a non-negative radially symmetric function and  $\mathbf{g}_1, \dots, \mathbf{g}_M$  is a set of nodes in the domain of rotations.

# *Texture index, strength*

- Second moment of the OD provides a scalar measure of the randomness, or lack of it in the texture:

$$\text{Texture Index} = \langle f^2 \rangle$$

$$\text{Texture Strength} = \sqrt{\langle f^2 \rangle}$$

- Random: texture index & strength = 1.0
- Any non-random OD has texture strength  $> 1$ .
- If textures are represented with lists of discrete orientations (e.g. as in \*.WTS files) then weaker textures require longer lists.
- One can also compute the **entropy** of an OD as  $S = -\sum f(g) \ln(f(g))$ . There is an apparent problem about what to do with zero values. However, in the case of  $p(x_i) = 0$  for some  $i$ , the value of the corresponding entropy term  $[0 \log(0)]$  is taken to be 0, which is consistent with the well-known limit:  $\lim_{p \rightarrow 0^+} p \ln(p) = 0$ . Strong textures will exhibit large entropies and a perfectly uniform (random) texture will have an entropy of zero.
- Some methods of pole figure reduction are based on entropy maximization.

## Example: Rolled Cu

a) Experimental

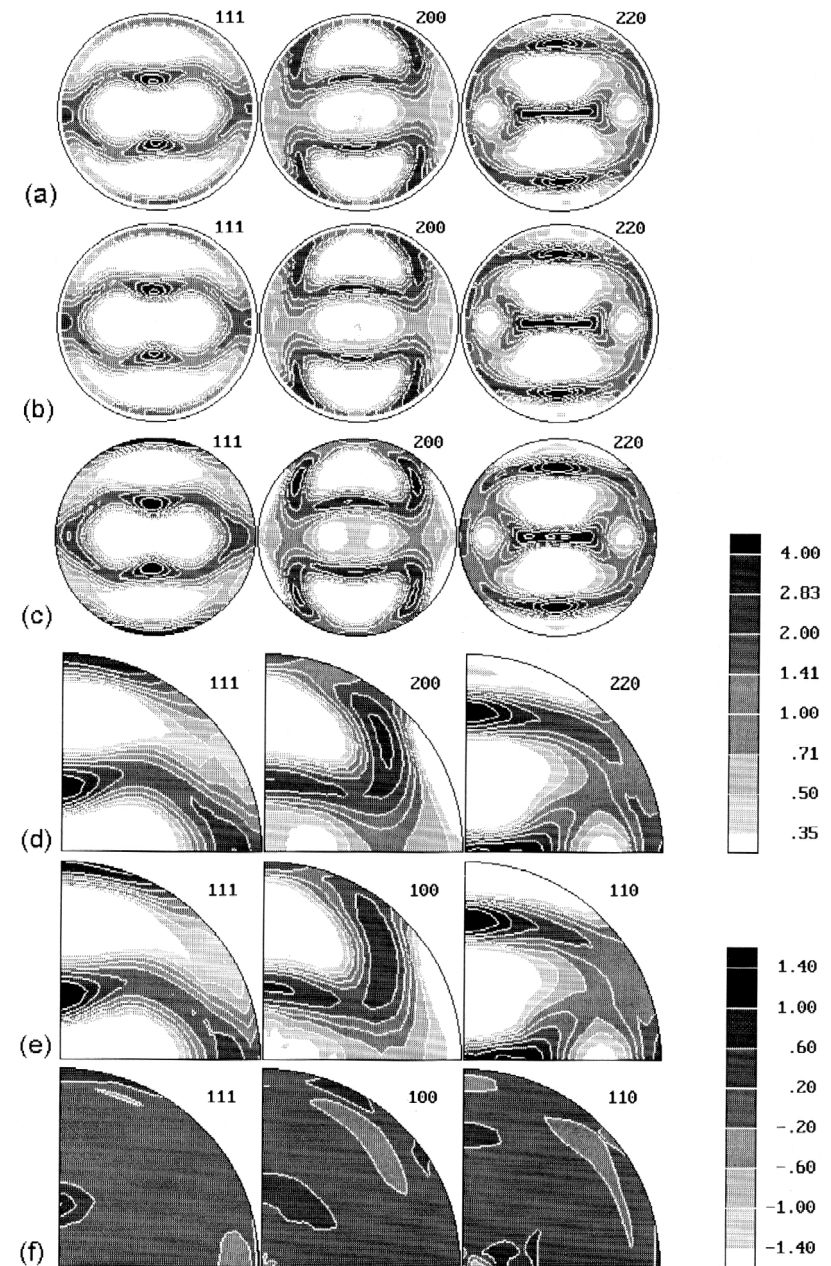
b) Rotated

c) Edge Completed  
(Harmonic analysis)

d) Symmetrized

e) Recalculated (WIMV)

f) Difference PFs





# *Summary*

- The two main methods of calculating an Orientation Distribution from Pole Figure data have been reviewed.
- Series expansion method is akin to the Fourier transform: it uses orthogonal functions in the 3 Euler angles (generalized spherical harmonics) and fits values of the coefficients in order to fit the pole figure data available.
- Discrete methods calculate values on a regular grid in orientation space, based on a comparison of recalculated pole figures and measured pole figures. The WIMV method, e.g., uses ratios of calculated and measured pole figure data to update the values in the OD on each iteration.