Mapping Texture in Thin Films

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Summary

- Introduction
  - Texture with regular scans
  - Pole figures
  - Typical pole figures
- Different approaches
  - Experimental needs
  - Choice of the detector
  - Choice of a reference frame

- Methodology
  - Pole Figure Corrections (defocusing, volumic/ absorption, location, fluorescence)
  - ODF calculation
  - Estimators of refinement quality
  - Estimators of Texture strength
  - Measurements / Orientation space coverage
- Simple objects to deal with
  - Recalculated low-indices pole figures
  - Inverse pole figures (fibre textures)
  - Volumic ratios (single-crystal like and epitaxy)
  - Deal with components in the ODF space

- Why Texture Analysis
  - Anisotropic Physical Properties
    - Elastic properties
    - Seismic wave velocities
    - Magnetic ferro or antiferro compounds
    - Anionic conductivity
    - Superconducting currents and Levitation forces
  - Anisotropic measurements
    - Polarised EXAFS
    - ESR, Raman
    - Diffraction !!!!
- Conclusions

Estimators of Refinement Quality

RP Factors:

Individual pf:

$$RP_x(h_i) = \frac{\sum_{j=1}^{J} \left| \tilde{P}^o_{h_i}(y_j) - \tilde{P}^c_{h_i}(y_j) \right|}{\sum_{j=1}^{J} \tilde{P}^o_{h_i}(y_j)} \theta\left(x, \tilde{P}^o_{h_i}(y_j)\right)$$

$$\theta(x,t) = \begin{cases} 1 \text{ for } t > x \\ 0 \text{ for } t \leq x \end{cases}$$

$$x = \varepsilon, 1, 10 \ldots$$

Averaged:

$$\overline{RP}_x = \frac{1}{I} \sum_{i=1}^{I} RP_x(h_i)$$

Bragg R-Factors:

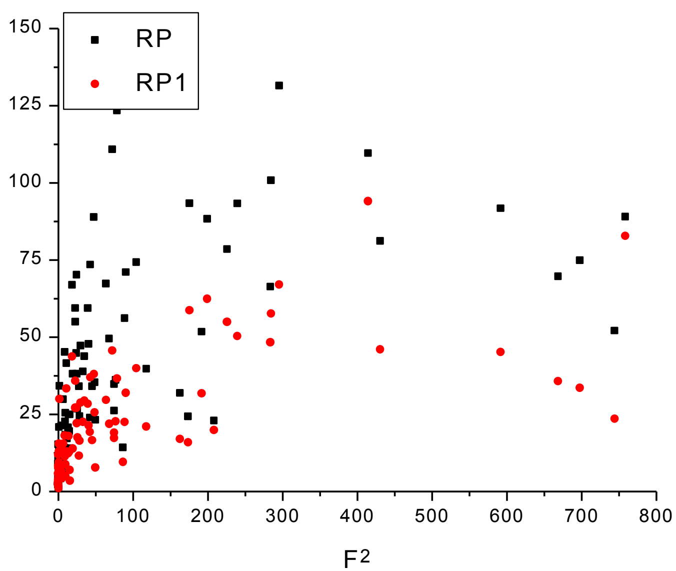
$$RB_x(h_i) = \frac{\sum_{j=1}^{J}\left[\tilde{P}_{h_i}^{o}(y_j) - \tilde{P}_{h_i}^{c}(y_j)\right]^2}{\sum_{j=1}^{J}\tilde{P}_{h_i}^{o\,2}(y_j)}\,\theta\left(x, \tilde{P}_{h_i}^{o}(y_j)\right)$$

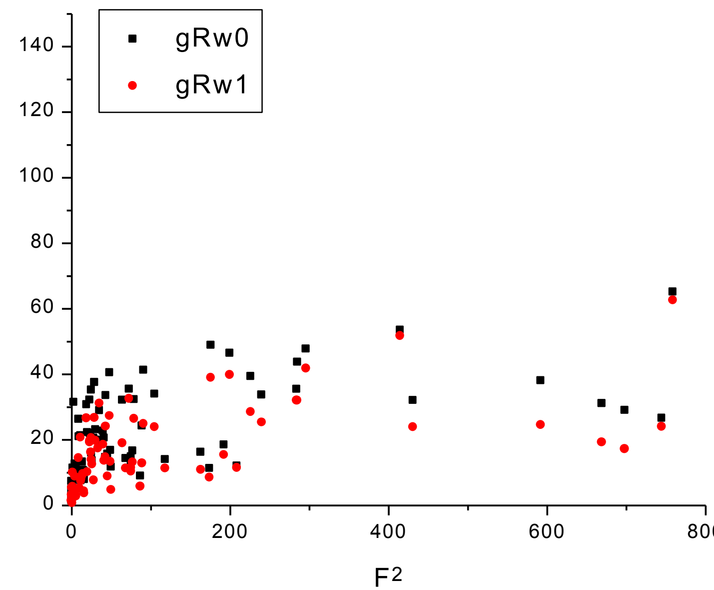
Weighted Rw-Factors:

$$Rw_x(h_i) = \frac{\sum_{j=1}^{J}\left[w_{ij}^{o} I_{h_i}^{o}(y_j) - w_{ij}^{c} I_{h_i}^{c}(y_j)\right]^2}{\sum_{j=1}^{J} w_{ij}^{o} I_{h_i}^{z\,2}(y_j)}\,\theta\left(x, \tilde{P}_{h_i}^{o}(y_j)\right)$$

$$w_{ij} = \frac{1}{\sqrt{I_{h_i}^{o}(y_j)}}$$

RPs vary much with texture strength than Rws





Estimators of Texture Strength

Texture Index:

$$F^2 = \frac{1}{8\pi^2} \sum_i f(g_i) \Delta g_i$$

Entropy:

$$S = \frac{-1}{8\pi^2} \sum_i f(g_i) \ln[f(g_i)] \Delta g_i$$

Measurements / Orientation Space Coverage

Say 20 measured (5° x 5°) complete pole figures:

= 20 x 1398 = 27960 experimental points

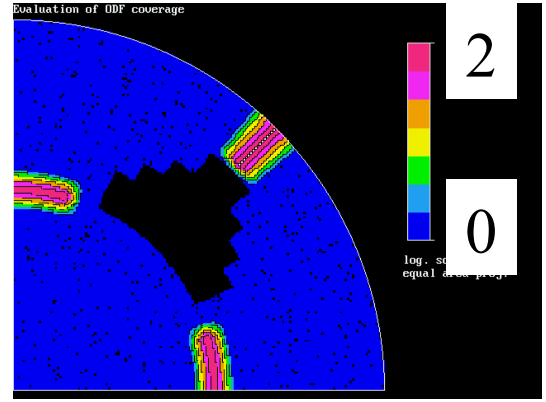
ODF (5° x 5° x 5°, triclinic): 98496 points to refine

strongly underdetermined system !

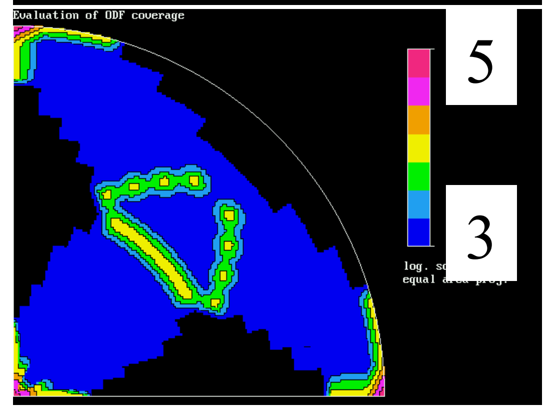
Evaluation of the OD coverage

Cubic Crystal Structure:

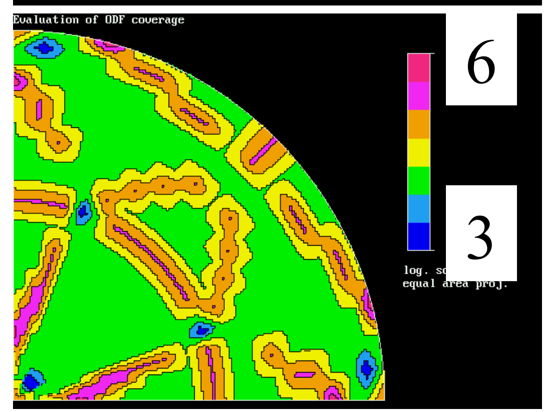
{100} pole figure, measured up to c = 45°:



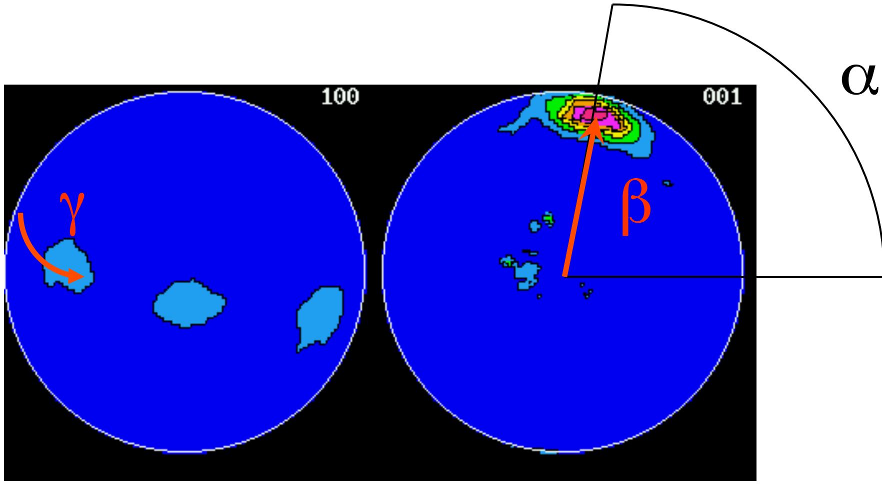
{100} + {110}, measured up to c = 45°:



{100} + {110} + {111}, up to c = 45°:

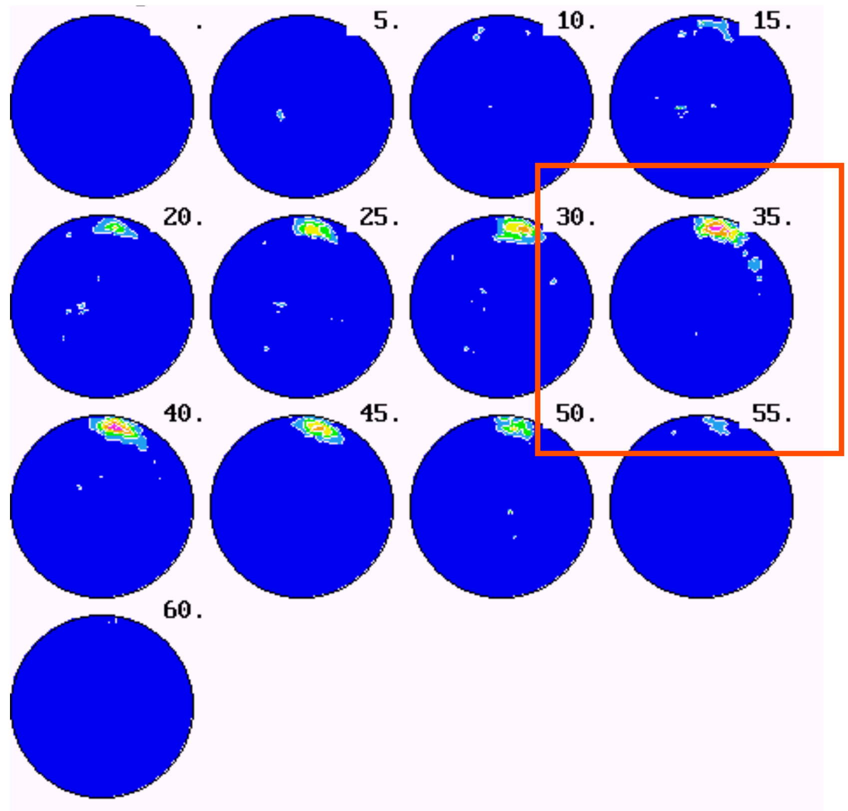


Deal with components in the ODF space



Pole figures

ODF γ-sections



Component:
(Hexagonal system)
g = {85,80,35}