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:

\[
\text{RP}_x (h_i) = \frac{\sum_{j=1}^{J} |\tilde{P}_{h_i}^o (y_j) - \tilde{P}_{h_i}^c (y_j)|}{\sum_{j=1}^{J} \tilde{P}_{h_i}^o (y_j)} \theta(x, \tilde{P}_{h_i}^o (y_j))
\]

Averaged:

\[
\overline{\text{RP}}_x = \frac{1}{I} \sum_{i=1}^{I} \text{RP}_x (h_i)
\]

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

\[
x = \varepsilon, 1, 10 \ldots
\]
Bragg R-Factors:

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

Weighted Rw-Factors:

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

\[
w_{ij} = \frac{1}{\sqrt{I_{h_i}^o(y_j)}}
\]
RPs vary much with texture strength than Rws

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**Diagram 1:**
- X-axis: \( F_2 \)
- Y-axis: RP
- Data points represent RP and RP1

**Diagram 2:**
- X-axis: \( F_2 \)
- Y-axis: gRw0 and gRw1
- Data points for gRw0 and gRw1
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 \((5^\circ \times 5^\circ)\) complete pole figures:

\[= 20 \times 1398 = 27960\] experimental points

ODF \((5^\circ \times 5^\circ \times 5^\circ, \text{triclinic})\): 98496 points to refine

strongly underdetermined system!
Evaluation of the OD coverage

Cubic Crystal Structure:

\{100\} pole figure, measured up to \(c = 45^\circ\):

\{100\} + \{110\}, measured up to \(c = 45^\circ\):

\{100\} + \{110\} + \{111\}, up to \(c = 45^\circ\):
Deal with components in the ODF space

Pole figures

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