Using Texture for Structure Solution

Christian Baerlocher and Lynne B. McCusker
Laboratory of Crystallography, ETH, Zurich
Using Texture for Structure Solution

Solving the overlap problem experimentally
Using Texture for Structure Solution

Solving the overlap problem experimentally

Changing environment
Using Texture for Structure Solution

Solving the overlap problem experimentally

Changing environment
  Exploiting Anisotropic Thermal Expansion
Using Texture for Structure Solution

Solving the overlap problem experimentally

Changing environment
  Exploiting Anisotropic Thermal Expansion
  Crystallization conditions for proteins (pH, salt)
Using Texture for Structure Solution

Solving the overlap problem experimentally

Changing environment
   Exploiting Anisotropic Thermal Expansion
   Crystallization conditions for proteins (pH, salt)
   Pressure
Using Texture for Structure Solution

Solving the overlap problem experimentally

Changing environment
  Exploiting Anisotropic Thermal Expansion
  Crystallization conditions for proteins (pH, salt)
  Pressure

Exploiting preferred orientation
Using Texture for Structure Solution

Solving the overlap problem experimentally

Changing environment
   Exploiting Anisotropic Thermal Expansion
   Crystallization conditions for proteins (pH, salt)
   Pressure

Exploiting preferred orientation

recover 3-dimensionality
Using Texture for Structure Solution

Introduction
Using Texture for Structure Solution

Introduction

How to measure texture
Using Texture for Structure Solution

Introduction

How to measure texture
How to describe texture
Using Texture for Structure Solution

Introduction
  How to measure texture
  How to describe texture

Reflection method
Using Texture for Structure Solution

Introduction
- How to measure texture
- How to describe texture

Reflection method
- Example: Zeolite UTD-1F
Using Texture for Structure Solution

Introduction
   How to measure texture
   How to describe texture

Reflection method
   Example: Zeolite UTD-1F

Transmission method
Using Texture for Structure Solution

Introduction
  How to measure texture
  How to describe texture

Reflection method
  Example: Zeolite UTD-1F

Transmission method
  using an area detector
Using Texture for Structure Solution

Introduction

How to measure texture
How to describe texture

Reflection method

Example: Zeolite UTD-1F

Transmission method

using an area detector
using a linear detector
Using Texture for Structure Solution

Introduction
   How to measure texture
   How to describe texture

Reflection method
   Example: Zeolite UTD-1F

Transmission method
   using an area detector
   using a linear detector

Other possibilities and Conclusion
Using Texture for Structure Solution

X-rays

1 μm³
Using Texture for Structure Solution

X-rays
Using Texture for Structure Solution

X-rays

Diagram showing the effect of X-rays on a material, leading to a structured solution.
Using Texture for Structure Solution
Using Texture for Structure Solution

Reflection Overlap Problem

X-rays
Using Texture for Structure Solution

Reflection Overlap Problem

X-rays

\[ 2\theta \]
Using Texture for Structure Solution

Reflection Overlap Problem

X-rays
Using Texture for Structure Solution

Reflection Overlap Problem

X-rays
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Reflection Overlap Problem

X-rays
Using Texture for Structure Solution

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X-rays
Using Texture for Structure Solution

X-rays

2θ
Using Texture for Structure Solution

X-rays

2θ
Using Texture for Structure Solution

X-rays

2θ
Reflection mode - experimental setup
Reflection mode - experimental setup
Reflection mode - experimental setup

X-ray source → Sample → Focusing circle → Detector
Reflection mode - experimental setup

X-ray source

Sample

θ

Focusing circle

Detector
Reflection mode - experimental setup

X-ray source → Sample → Focusing circle → Detector

$\theta$
Reflection mode - experimental setup

X-ray source

Sample

Detector

Focusing circle

$\theta$

$\phi$ (rotation)
Reflection mode - experimental setup

- X-ray source
- Sample
- Focusing circle
- Detector

θ
φ (rotation)
Reflection mode - experimental setup

- X-ray source
- Sample
- Focusing circle
- Detector

Angles:
- $\chi$ (tilt)
- $\theta$
- $\phi$ (rotation)
Reflection mode - experimental setup

- X-ray source
- Focusing circle
- Detector
- Sample
- \( \theta \) (rotation)
- \( \phi \) (rotation)
- \( \chi \) (tilt)
Reflection mode - experimental setup

Focusing circle

\[ \chi \text{ (tilt)} \]

\[ \theta \]

\[ \phi \text{ (rotation)} \]

Sample
Reflection mode - experimental setup

- Parallel beam
- Focusing circle
- Sample
- Analyzer
- Detector
- \[ \chi \text{ (tilt)} \]
- \[ \theta \]
- \[ \phi \text{ (rotation)} \]
Texture Analysis

measure every 5° in $\phi$ and $\chi$
Texture Analysis

measure every 5° in $\phi$ and $\chi$
measure every 5° in $\phi$ and $\chi$
Texture Analysis

measure every 5° in $\phi$ and $\chi$
Texture Analysis

measure every 5° in $\phi$ and $\chi$

$\phi = 35^\circ$, $\chi = 50^\circ$
measure every 5° in $\phi$ and $\chi$

$\phi = 35^\circ, \chi = 50^\circ$

1152 measurements
(80° tilt)
Texture Analysis

measure every $5^\circ$ in $\phi$ and $\chi$

Each reflection measured at each orientation

$1152$ measurements 
(80° tilt)

$\phi = 35^\circ$, $\chi = 50^\circ$
Texture Analysis
Texture Analysis
Texture Analysis
Texture Analysis
Texture Analysis

60%  

30%
Texture Analysis

60%

30%

a

b
c
Texture Analysis

60%

30%

100
Texture Analysis

60%

30%

100
Texture Analysis

60%  a  30%

b  c

100
Texture Analysis

60% 30%

a b c

100 010
Texture Analysis

60% 30%

a b c

100 010
Texture Analysis

60%  

30%  

a  
b  
c  

100  

010  

001
Texture Analysis

Pole figures are normalized  $\rightarrow$ average value $= 1$
Pole figures are normalized $\rightarrow$ average value = 1
Calculate orientation distribution function (ODF) from these pole figures
Texture Analysis

Pole figures are normalized → average value = 1
Calculate orientation distribution function (ODF) from these pole figures
From the ODF one can calculate the pole figures for any reflection
Effect of Tilt Angle in Reflection Mode

Footprint of the X-ray beam on sample

- $0^\circ \chi$
- $4^\circ 2\theta$
- $16^\circ 2\theta$
- $30^\circ 2\theta$
- $50^\circ 2\theta$
Effect of Tilt Angle in Reflection Mode

Footprint of the X-ray beam on sample

<table>
<thead>
<tr>
<th>4° 2θ</th>
<th>16° 2θ</th>
<th>30° 2θ</th>
<th>50° 2θ</th>
</tr>
</thead>
<tbody>
<tr>
<td>0° χ</td>
<td><img src="image1.png" alt="Footprint" /></td>
<td><img src="image2.png" alt="Footprint" /></td>
<td><img src="image3.png" alt="Footprint" /></td>
</tr>
<tr>
<td>10° χ</td>
<td><img src="image5.png" alt="Footprint" /></td>
<td><img src="image6.png" alt="Footprint" /></td>
<td><img src="image7.png" alt="Footprint" /></td>
</tr>
</tbody>
</table>
Effect of Tilt Angle in Reflection Mode

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<tr>
<th>$4^\circ 2\theta$</th>
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</tr>
</thead>
<tbody>
<tr>
<td>$0^\circ \chi$</td>
<td><img src="image" alt="Footprint" /></td>
<td><img src="image" alt="Footprint" /></td>
<td><img src="image" alt="Footprint" /></td>
</tr>
<tr>
<td>$10^\circ \chi$</td>
<td><img src="image" alt="Footprint" /></td>
<td><img src="image" alt="Footprint" /></td>
<td><img src="image" alt="Footprint" /></td>
</tr>
<tr>
<td>$30^\circ \chi$</td>
<td><img src="image" alt="Footprint" /></td>
<td><img src="image" alt="Footprint" /></td>
<td><img src="image" alt="Footprint" /></td>
</tr>
</tbody>
</table>
Effect of Tilt Angle in Reflection Mode

Footprint of the X-ray beam on sample

<table>
<thead>
<tr>
<th>Tilt Angle (°)</th>
<th>4° 2θ</th>
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<th>50° 2θ</th>
</tr>
</thead>
<tbody>
<tr>
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<td><img src="image1" alt="Footprint" /></td>
<td><img src="image2" alt="Footprint" /></td>
<td><img src="image3" alt="Footprint" /></td>
<td><img src="image4" alt="Footprint" /></td>
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<td><img src="image6" alt="Footprint" /></td>
<td><img src="image7" alt="Footprint" /></td>
<td><img src="image8" alt="Footprint" /></td>
</tr>
<tr>
<td>30° χ</td>
<td><img src="image9" alt="Footprint" /></td>
<td><img src="image10" alt="Footprint" /></td>
<td><img src="image11" alt="Footprint" /></td>
<td><img src="image12" alt="Footprint" /></td>
</tr>
<tr>
<td>50° χ</td>
<td><img src="image13" alt="Footprint" /></td>
<td><img src="image14" alt="Footprint" /></td>
<td><img src="image15" alt="Footprint" /></td>
<td><img src="image16" alt="Footprint" /></td>
</tr>
</tbody>
</table>
Effect of Tilt Angle in Reflection Mode

Footprint of the X-ray beam on sample

<table>
<thead>
<tr>
<th>θ (°)</th>
<th>4° 2θ</th>
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</thead>
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<td><img src="image" alt="30° footprint" /></td>
<td><img src="image" alt="50° footprint" /></td>
</tr>
<tr>
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<td><img src="image" alt="0° footprint" /></td>
<td><img src="image" alt="16° footprint" /></td>
<td><img src="image" alt="30° footprint" /></td>
<td><img src="image" alt="50° footprint" /></td>
</tr>
<tr>
<td>80° χ</td>
<td><img src="image" alt="0° footprint" /></td>
<td><img src="image" alt="16° footprint" /></td>
<td><img src="image" alt="30° footprint" /></td>
<td><img src="image" alt="50° footprint" /></td>
</tr>
</tbody>
</table>
Tilt Angle Correction in Reflection Mode
Effect of Tilt Angle Correction in Reflection Mode

Pole figure for the 102 Reflection of ZSM-5

no tilt correction
Effect of Tilt Angle Correction in Reflection Mode

Pole figure for the 102 Reflection of ZSM-5

no tilt correction     after tilt correction
Does it work?
Does it work?

High-silica zeolite UTD-1F
Does it work?
High-silica zeolite UTD-1F

Unit Cell

<table>
<thead>
<tr>
<th>Space Group</th>
<th>P2$_1$/c</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>14.9701 Å</td>
</tr>
<tr>
<td>b</td>
<td>8.4761 Å</td>
</tr>
<tr>
<td>c</td>
<td>30.0278 Å</td>
</tr>
<tr>
<td>$\beta$</td>
<td>102.65°</td>
</tr>
</tbody>
</table>

Data Collection (reflection mode)

<table>
<thead>
<tr>
<th>Pole figures (for ODF)</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Full powder patterns for intensity extraction</td>
<td>5</td>
</tr>
</tbody>
</table>
Does it work?

High-silica zeolite UTD-1F
Does it work?
High-silica zeolite UTD-1F

16 Si, 32 O, 1 Co and 20 C
Does it work?
High-silica zeolite UTD-1F

16 Si, 32 O, 1 Co and 20 C
High-silica zeolite UTD-1F
High-silica zeolite UTD-1F

Structure Determination

direct methods
High-silica zeolite UTD-1F

Structure Determination

direct methods
all 16 Si and 17 of the 32 O found in the top E-map
High-silica zeolite UTD-1F

Structure Determination

direct methods
all 16 Si and 17 of the 32 O found in the top E-map
15 O and Co(Cp*)$_2^+$ found in difference Fourier map
High-silica zeolite UTD-1F

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Structure Refinement (Rietveld method)
High-silica zeolite UTD-1F

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direct methods
all 16 Si and 17 of the 32 O found in the top E-map
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Structure Refinement (Rietveld method)

non-centrosymmetric  
Pc
High-silica zeolite UTD-1F

Structure Determination

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all 16 Si and 17 of the 32 O found in the top E-map
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Structure Refinement (Rietveld method)

non-centrosymmetric  \text{Pc}
atoms in asymmetric unit  32Si, 64O, 1Co, 20C
High-silica zeolite UTD-1F

Structure Determination

direct methods
all 16 Si and 17 of the 32 O found in the top E-map
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non-centrosymmetric Pc
atoms in asymmetric unit 32Si, 64O, 1Co, 20C
positional parameters 349
High-silica zeolite UTD-1F

Structure Determination

direct methods
all 16 Si and 17 of the 32 O found in the top E-map
15 O and Co(Cp*)$_2^+$ found in difference Fourier map

Structure Refinement (Rietveld method)

non-centrosymmetric  
Pc
atoms in asymmetric unit  
32Si, 64O, 1Co, 20C
positional parameters  
349
$R_{wp}$  
0.134
$R_F$  
0.041
Reflection mode - problems
Reflection mode - problems

Sample
relatively large (ca 20 mm diameter disk, 0.5 mm thick)
homogeneous texture required
Reflection mode - problems

Sample
relatively large (ca 20 mm diameter disk, 0.5 mm thick)
homogeneous texture required

Data analysis
severe corrections for sample tilt required
Reflection mode - problems

Sample
relatively large (ca 20 mm diameter disk, 0.5 mm thick)
homogeneous texture required

Data analysis
severe corrections for sample tilt required

Synchrotron beamtime
 calibration of setup using untextured sample
1152 low angle diffraction patterns to determine texture
5-10 complete diffraction patterns at different sample orientations
Reflection mode - problems

Sample
relatively large (ca 20 mm diameter disk, 0.5 mm thick)
homogeneous texture required

Data analysis
severe corrections for sample tilt required

Synchrotron beamtime
calibration of setup using untextured sample
1152 low angle diffraction patterns to determine texture
5-10 complete diffraction patterns at different sample orientations

ca. 3 days per sample
Transmission mode - experimental setup

Area detector
Transmission mode - experimental setup

Area detector

Sample
Transmission mode - experimental setup

Area detector

X-ray Beam

Sample

Area Detector
Transmission mode - experimental setup

Area detector

X-ray Beam

Sample

Area Detector

Friday, June 10, 2011
Transmission mode - experimental setup

Area detector

Only one rotation required
5° steps
Transmission mode with area detector

Data analysis
Transmission mode with area detector

Data analysis
Transmission mode with area detector

Data analysis

$\delta = 0^\circ$
Transmission mode with area detector

Data analysis

$\delta = 0^\circ$

72 sectors
Transmission mode with area detector

Data analysis

$\psi = 30^\circ$
Transmission mode with area detector

Data analysis

\( \delta = 0^\circ \)

\( \psi = 30^\circ \)

\( \psi = 30^\circ, \delta = 0^\circ \)
Transmission mode with area detector

Data analysis

\[ \delta = 0^\circ \]

\[ \psi = 30^\circ, \delta = 0^\circ \]

\[ \delta = 90^\circ \]

\[ \psi = 30^\circ, \delta = 90^\circ \]
Transmission mode with area detector

Data analysis

extract 1296 unique patterns with good statistics
Preparing a textured sample
Preparing a textured sample

mix sample in a dissolved polymer (polystyrene)
Preparing a textured sample

mix sample in a dissolved polymer (polystyrene)
evaporate solvent till mixture becomes viscous
Preparing a textured sample

mix sample in a dissolved polymer (polystyrene)
evaporate solvent till mixture becomes viscous
put in center of groove in die and press with top part
Preparing a textured sample

mix sample in a dissolved polymer (polystyrene)
evaporate solvent till mixture becomes viscous
put in center of groove in die and press with top part
open and remove film from die and fold
Preparing a textured sample

- Mix sample in a dissolved polymer (polystyrene).
- Evaporate solvent till mixture becomes viscous.
- Put in center of groove in die and press with top part.
- Open and remove film from die and fold.
Preparing a textured sample

mix sample in a dissolved polymer (polystyrene)
evaporate solvent till mixture becomes viscous
put in center of groove in die and press with top part
open and remove film from die and fold
repeat procedure several times
Transmission mode - experimental setup

Area detector
Transmission mode - experimental setup

Area detector

Pros
Sample very small, easy to prepare
Full data collection in 6 hours with MAR image plate
No tilt correction required
Good counting statistics
Transmission mode - experimental setup

Area detector

Pros
Sample very small, easy to prepare
Full data collection in 6 hours with MAR image plate
No tilt correction required
Good counting statistics

Cons
broader peaks
restricted 2θ range
Transmission mode - experimental setup

Area detector

Pros
Sample very small, easy to prepare
Full data collection in 6 hours with MAR image plate
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Cons
broader peaks
restricted 2θ range

Put detector further away
Resolution limited by pixel size
reduces 2θ range
Transmission mode - experimental setup

1D detector

SLS MS beam line

Mythen detector
120° 2θ range
Eularian cradle
Transmission mode - experimental setup using the Mythen linear Si-strip detector at the SLS
Transmission mode - experimental setup
using the Mythen linear Si-strip detector at the SLS
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Transmission mode - experimental setup

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Transmission mode - experimental setup using the Mythen linear Si-strip detector at the SLS
Texture Analysis

every 5° in $\phi$ and $\chi$

1296 measurements
Texture Analysis

optimized coverage

MAUD software

302 measurements
Texture Analysis

shorter data collection time

optimized coverage

MAUD software

302 measurements
Transmission mode

Advantages of the SLS Setup

\[ \text{Intensity [cts]} \]

\[ \begin{align*}
\text{2 theta [deg.]} & \quad -60 & \quad -40 & \quad -20 & \quad 0 & \quad 20 & \quad 40 & \quad 60 \\
0 & \quad 1 \times 10^5 & \quad 2 \times 10^5 & \quad 3 \times 10^5
\end{align*} \]

\[ \text{phi 65° / chi 50°} \]
Transmission mode

Advantages of the SLS Setup

Can be used to check if a sample has preferred orientation
Transmission mode

Advantages of the SLS Setup
Transmission mode

Advantages of the SLS Setup

1° 2θ

30° 2θ

missing cone
Transmission mode

Advantages of the SLS Setup (Mythen detector)

• High resolution
• Large angular range
• Very fast, 2-10 sec per pattern $\rightarrow$ 300 patterns (10-50 min)
• Good counting statistics
• $120^\circ$ 20 range $\rightarrow$ 2 patterns at the same time
• Local integration by oscillating sample $\pm 2.5^\circ$ in $\delta$ and $\psi$
• Helpful beamline staff
Test Example ZrPO$_4$-pyr

Some powder patterns
Transmission mode

Analysis Procedure
Transmission mode

Analysis Procedure

• Prepare textured sample (using sheer forces in polymer matrix)
Transmission mode

Analysis Procedure

• Prepare textured sample (using sheer forces in polymer matrix)
• Fast measurement of optimized coverage (302 orientations (patterns))
Transmission mode

Analysis Procedure

• Prepare textured sample (using sheer forces in polymer matrix)
• Fast measurement of optimized coverage (302 orientations (patterns))
• Determine Texture (ODF) using non-overlapping low angle reflections
Transmission mode

Analysis Procedure

• Prepare textured sample (using sheer forces in polymer matrix)
• Fast measurement of optimized coverage (302 orientations (patterns))
• Determine Texture (ODF) using non-overlapping low angle reflections (with program MAUD)
Transmission mode

Analysis Procedure

• Prepare textured sample (using sheer forces in polymer matrix)
• Fast measurement of optimized coverage (302 orientations (patterns))
• Determine Texture (ODF) using non-overlapping low angle reflections (with program MAUD)
• Analyze texture to select most useful sample orientations
Transmission mode

Analysis Procedure

- Prepare textured sample (using sheer forces in polymer matrix)
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- Analyze texture to select most useful sample orientations
- De-convolute overlapping reflections using selected patterns
Transmission mode

Analysis Procedure

- Prepare textured sample (using sheer forces in polymer matrix)
- Fast measurement of optimized coverage (302 orientations (patterns))
- Determine Texture (ODF) using non-overlapping low angle reflections (with program MAUD)
- Analyze texture to select most useful sample orientations
- De-convolute overlapping reflections using selected patterns
- Solve structure using direct methods
Test Example ZrPO$_4$-pyr

Polfigures used for the texture determination

measured
Polfigures used for the texture determination

Test Example ZrPO$_4$-pyr

measured

calculated from ODF
Test Example ZrPO$_4$-pyr

Select most useful sample orientations using all calculated pole figures

Overlapped reflections 760 and 940
Test Example ZrPO$_4$-pyr
Select most useful sample orientations using all calculated pole figures
Overlapped reflections 760 and 940
Test Example ZrPO₄-pyr

Select most useful sample orientations using all calculated pole figures

Overlapped reflections 760 and 940
Test Example $\text{ZrPO}_4$-pyr

How many different orientations are needed?
Test Example $\text{ZrPO}_4\text{-pyr}$

How many different orientations are needed?

![Graph showing R values for ZrPO$_4$-pyr test structure with legends for different reflection sets.](image-url)
Test Example $\text{ZrPO}_4\text{-pyr}$

$F(\text{extracted})$ vs. $F(\text{calculated})$

untextured data

equipartitioned
Test Example ZrPO$_4$-pyr

$F$(extracted) vs. $F$(calculated)

untextured data
equipartitioned

texture data
Other benefits from texture data
Other benefits from texture data

Pole figures look like a stereographic plot of a single crystal
Other benefits from texture data

Pole figures look like a stereographic plot of a single crystal
Other benefits from texture data

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Pole figures look like a stereographic plot of a single crystal
Other benefits from texture data

• Symmetry determination

Pole figures look like a stereographic plot of a single crystal
Other benefits from texture data

- Symmetry determination

Sample symmetry: mm2

Pole figures look like a stereographic plot of a single crystal
Other benefits from texture data

- Symmetry determination

sample symmetry: mm2

Crystal symmetry: triclinic

Pole figures look like a stereographic plot of a single crystal
Other benefits from texture data

• Symmetry determination
• Indexing

sample symmetry: mm2
crystal symmetry: triclinic

Pole figures look like a stereographic plot of a single crystal
Other benefits from texture data

Indexing
Other benefits from texture data

Indexing

Maxima in pole figures give direction of lattice planes $\rightarrow$ Normal of corresponding crystal face
Other benefits from texture data

Indexing

Maxima in pole figures give direction of lattice planes → Normal of corresponding crystal face
Other benefits from texture data

Indexing

Maxima in pole figures give direction of lattice planes → Normal of corresponding crystal face
Other benefits from texture data

Indexing

Maxima in pole figures give direction of lattice planes $\rightarrow$ Normal of corresponding crystal face
d-values of reflections give length of reciprocal lattice vector $\rightarrow$ reciprocal lattice
Other benefits from texture data

Indexing

Maxima in pole figures give direction of lattice planes → Normal of corresponding crystal face
d-values of reflections give length of reciprocal lattice vector → reciprocal lattice
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Conclusions
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It is now possible to do a texture measurement almost as routinely as a normal powder data collection, i.e. given a textured sample, good texture data can be collected in 10min.
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Such data can be used to overcome the overlap problem to a large extent to yield more single-crystal-like data.
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It is now possible to do a texture measurement almost as routinely as a normal powder data collection, i.e. given a textured sample, good texture data can be collected in 10min.

Such data can be used to overcome the overlap problem to a large extent to yield more single-crystal-like data.

Pole figures can help in determining the space group and indexing the powder pattern.
Conclusions

It is now possible to do a texture measurement almost as routinely as a normal powder data collection, i.e. given a textured sample, good texture data can be collected in 10min.

Such data can be used to overcome the overlap problem to a large extent to yield more single-crystal-like data.

Pole figures can help in determining the space group and indexing the powder pattern.

Therefore, a texture measurement is a viable alternative, if a more conventional approach to structure solution fails.
Conclusions

It is now possible to do a texture measurement almost as routinely as a normal powder data collection, i.e. given a textured sample, good texture data can be collected in 10min.

Such data can be used to overcome the overlap problem to a large extent to yield more single-crystal-like data.

Pole figures can help in determining the space group and indexing the powder pattern.

Therefore, a texture measurement is a viable alternative, if a more conventional approach to structure solution fails.

Don’t be afraid of texture. Use it!
We have the tools to deal with it and you can get additional information from it.
Acknowledgments
Acknowledgments

Thomas Wessels
Sinisa Prokic
Lars Massüger
Jürgen Grässlin
Acknowledgments

Thomas Wessels
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Lars Massüger
Jürgen Grässlin

SNBL staff
Phil Pattison
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Thomas Wessels
Sinisa Prokic
Lars Massüger
Jürgen Grässlin

SNBL staff
Phil Pattison

SLS staff
Anna Bergamaschi
Fabia Gozzo
Bernd Schmidt
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Thomas Wessels
Sinisa Prokic
Lars Massüger
Jürgen Grässlin

Luca Lutterotti (MAUD)

SNBL staff
Phil Pattison

SLS staff
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Fabia Gozzo
Bernd Schmidt
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Lars Massüger
Jürgen Grässlin

Luca Lutterotti (MAUD)

SNBL staff
Phil Pattison

SLS staff
Anna Bergamaschi
Fabia Gozzo
Bernd Schmidt

Lynne McCusker