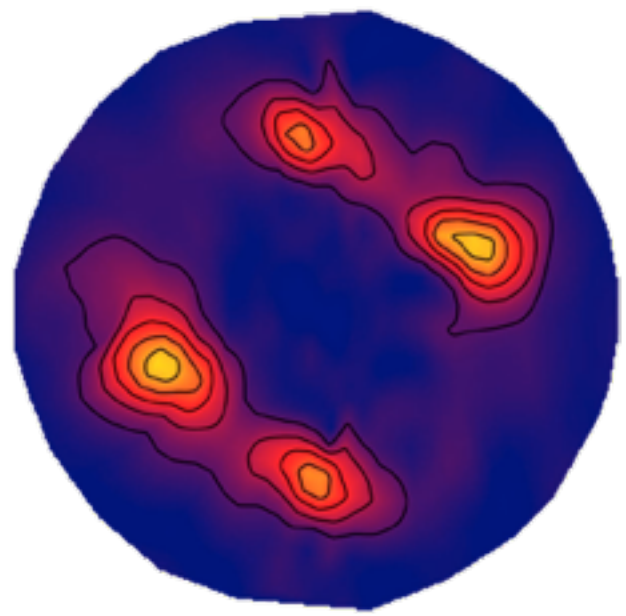
Using Texture for Structure Solution



ChristianBaerlocher 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)

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Exploiting preferred orientation

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Solving the overlap problem experimentally

Changing environment

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- Crystallization conditions for proteins (pH, salt)
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Exploiting preferred orientation

recover 3-dimensionality

Using Texture for Structure Solution

Introduction

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How to measure texture

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Introduction

- How to measure texture
- How to describe texture

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Reflection method

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- Example: Zeolite UTD-1F

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Transmission method

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- using an area detector

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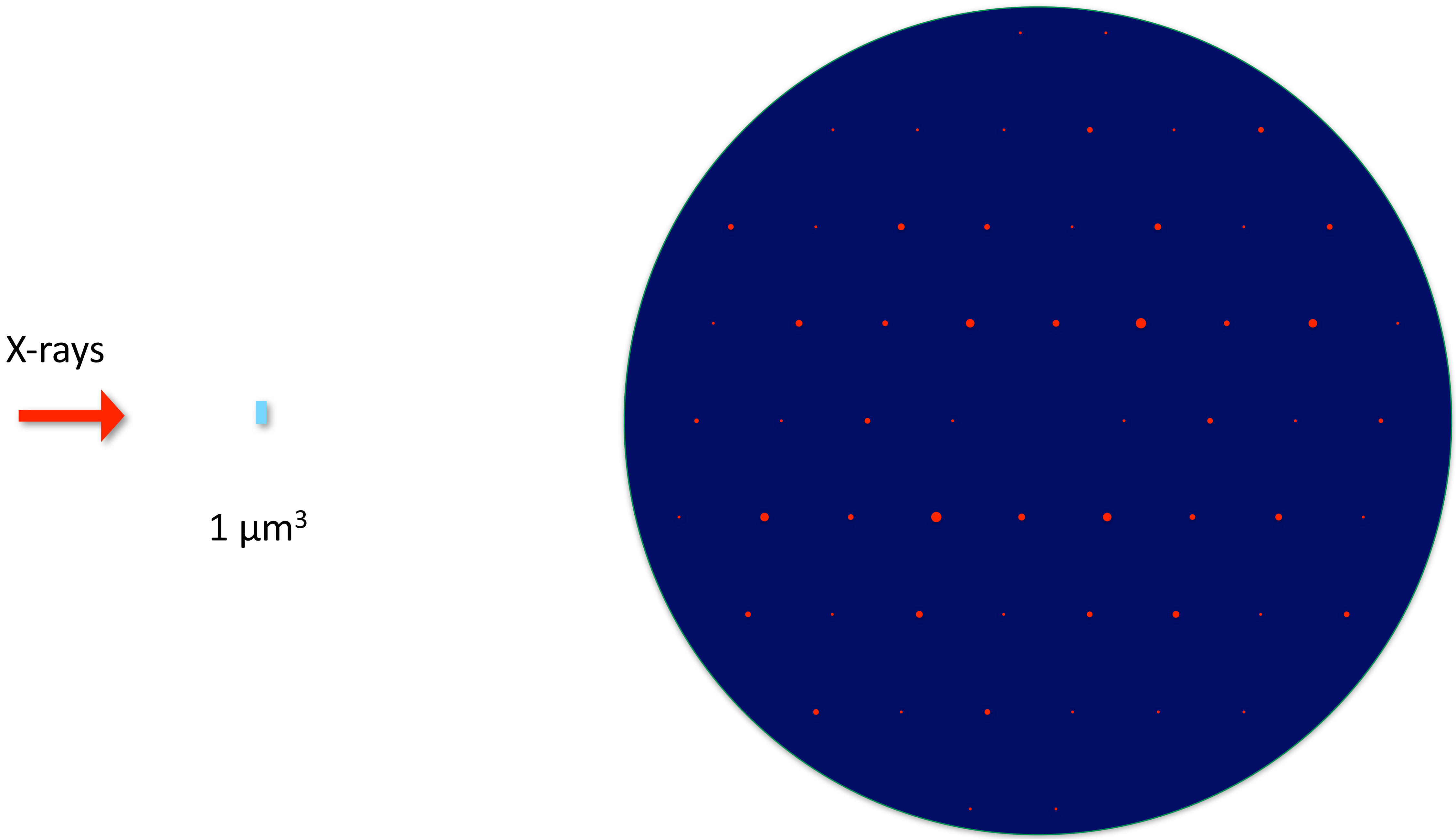
Other possibilities and Conclusion

Using Texture for Structure Solution



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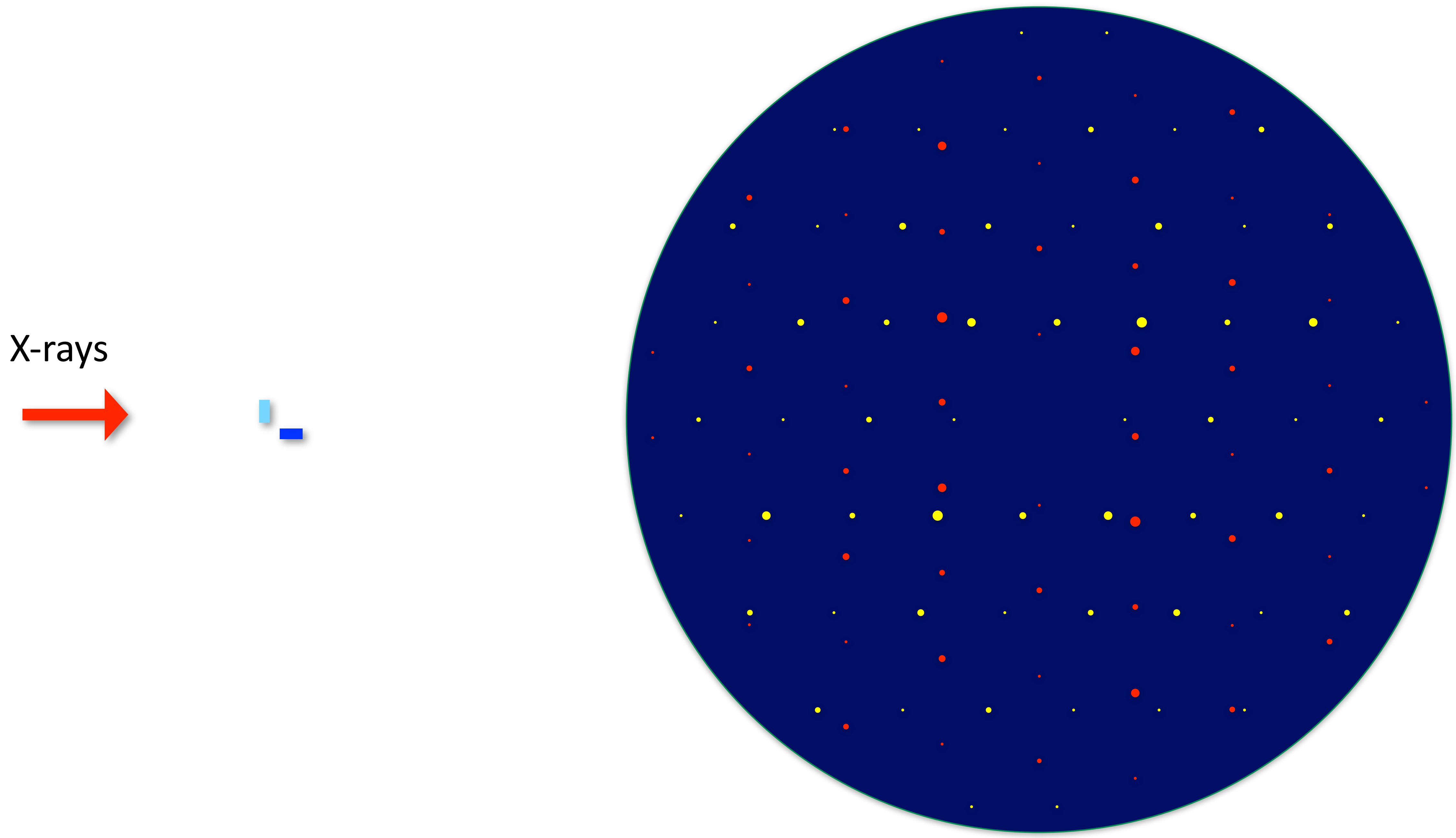

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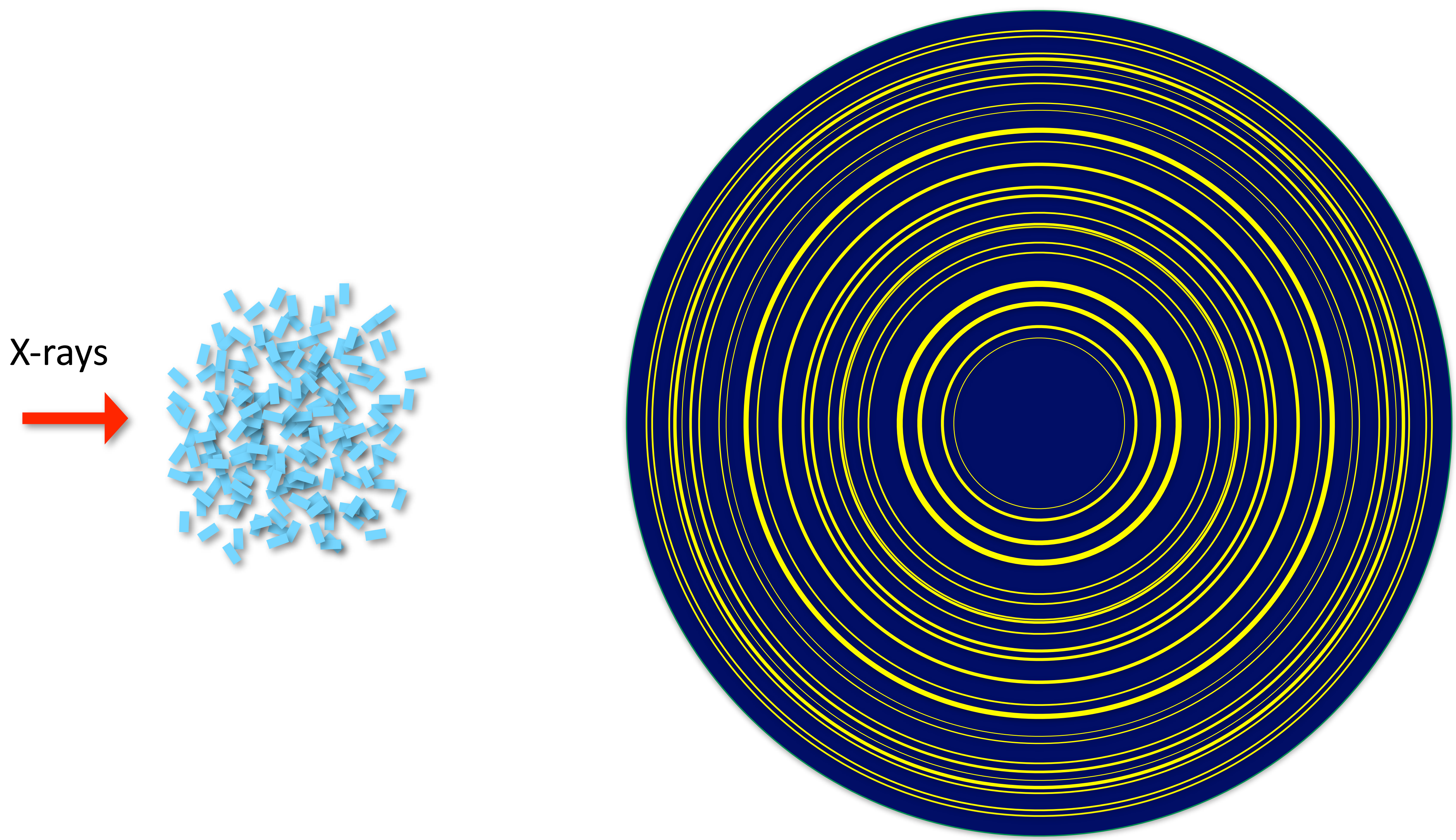

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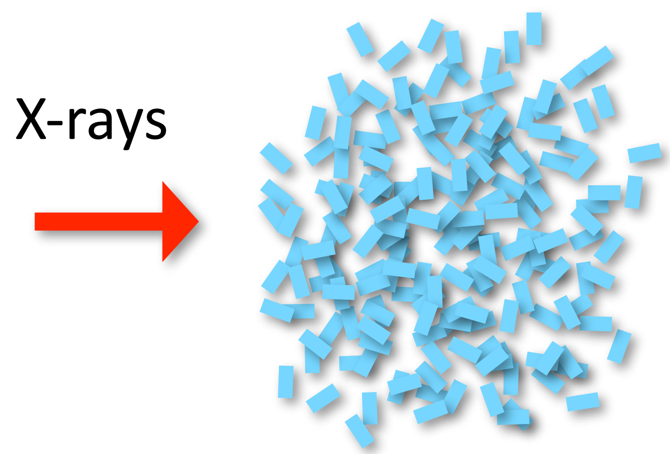
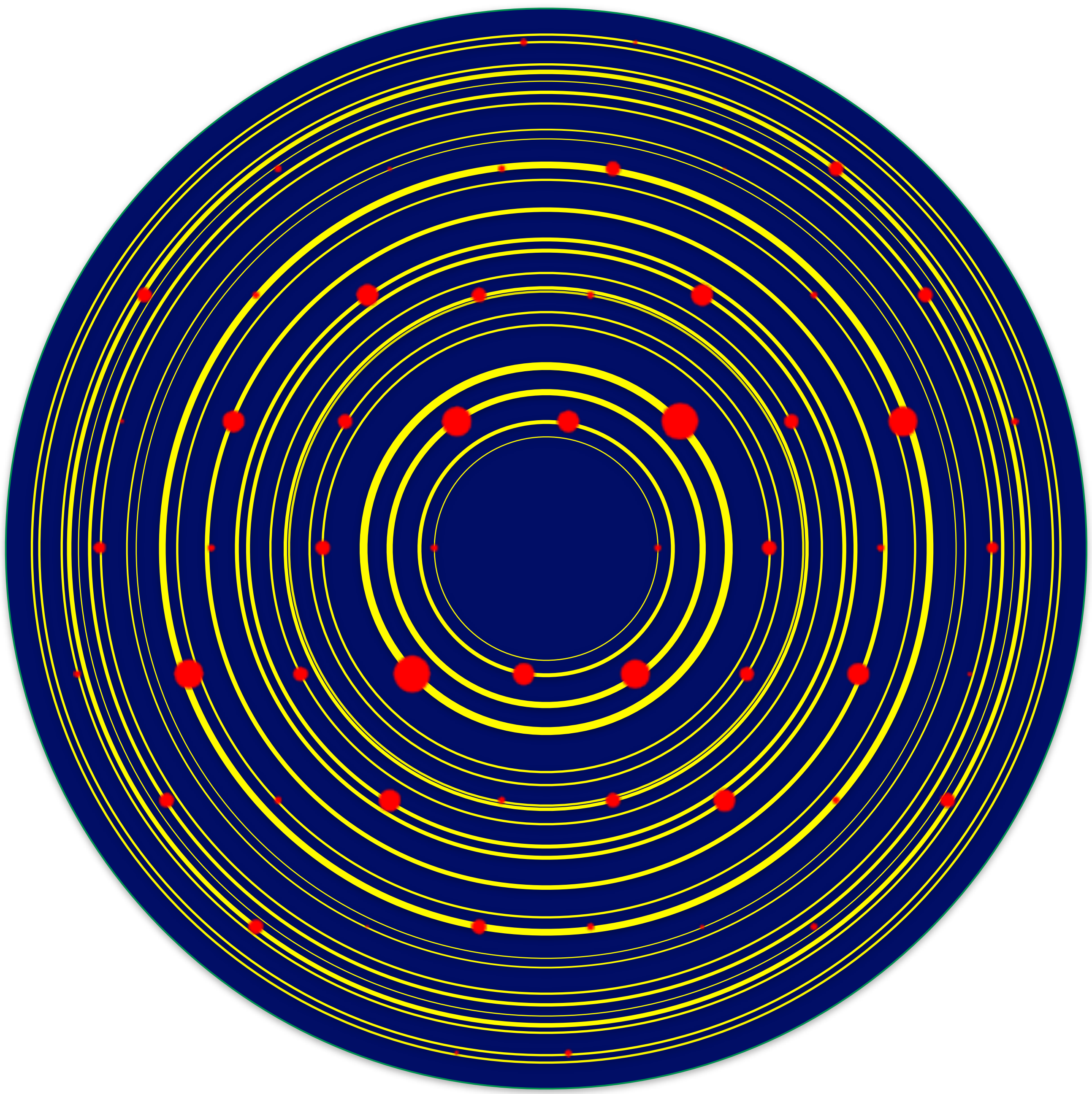
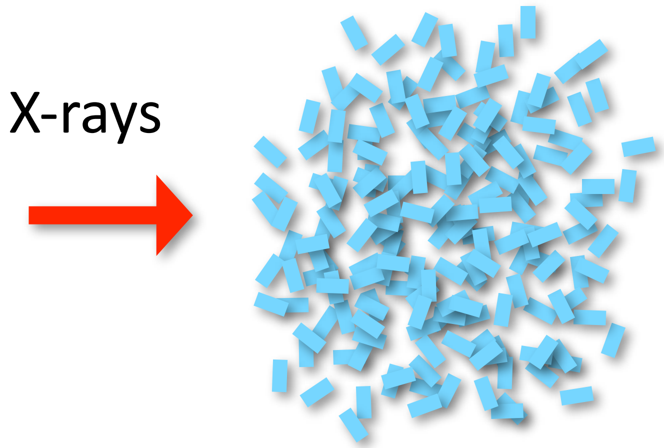
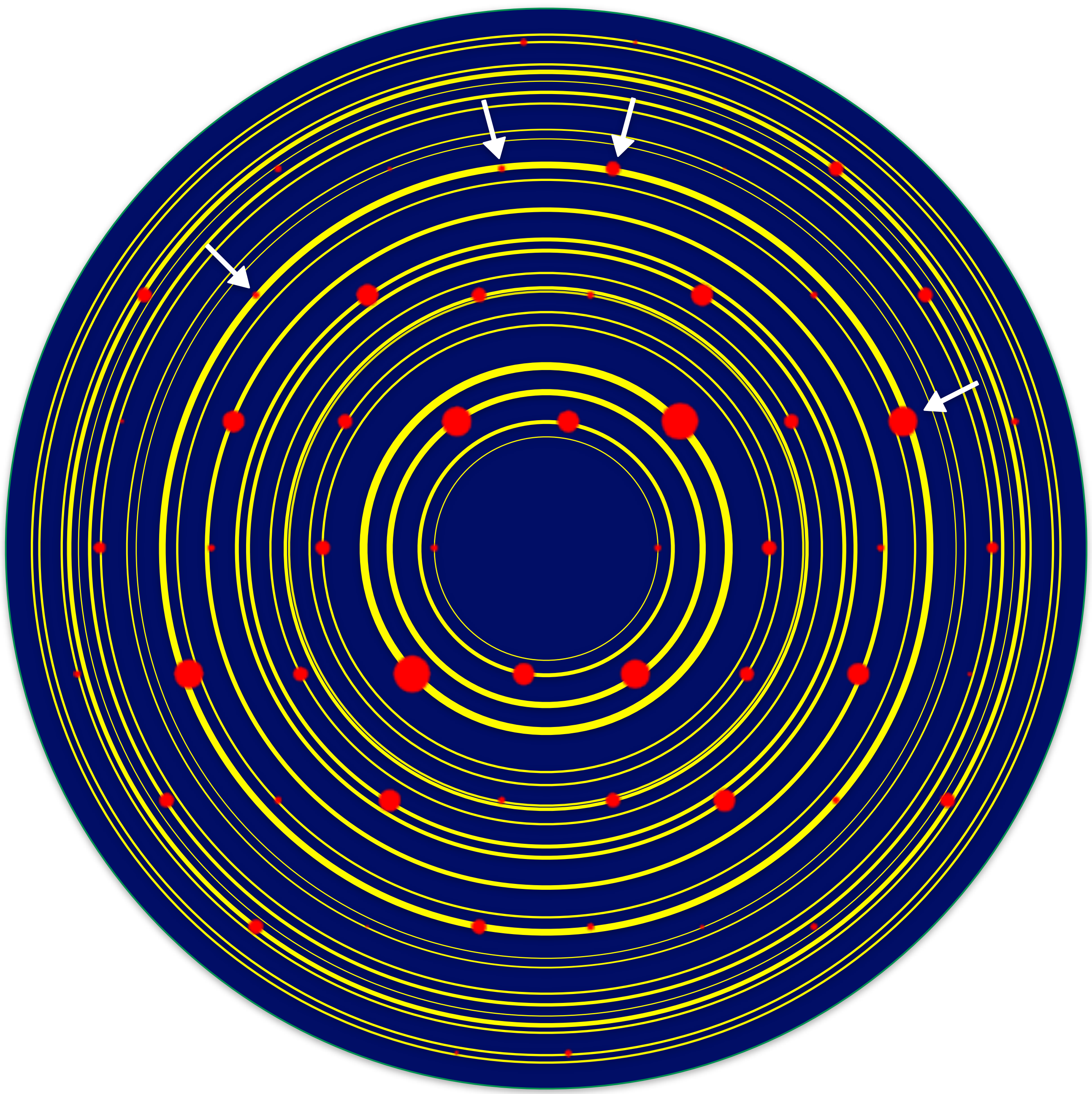




Using Texture for Structure Solution

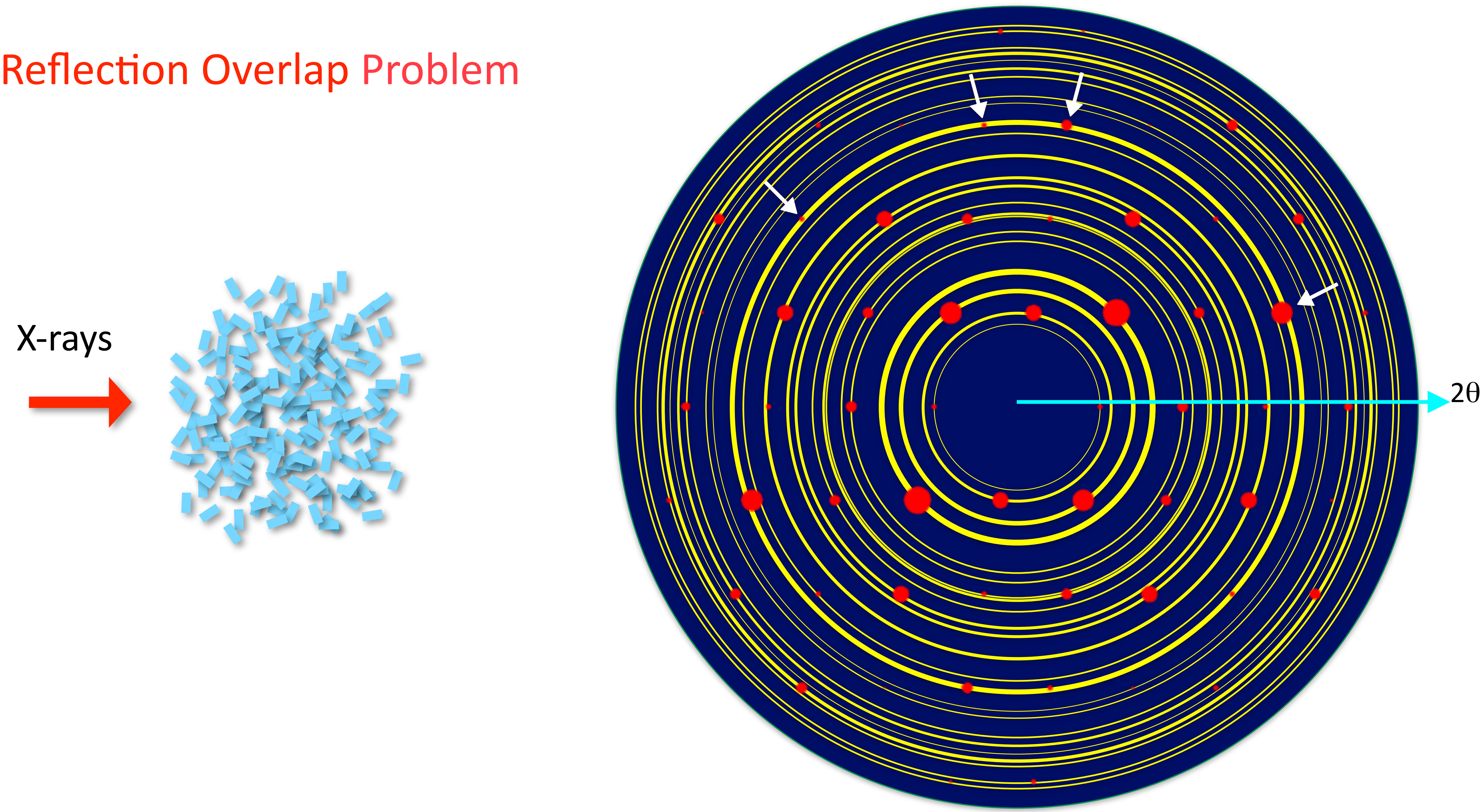
Reflection Overlap Problem





Using Texture for Structure Solution

Reflection Overlap Problem



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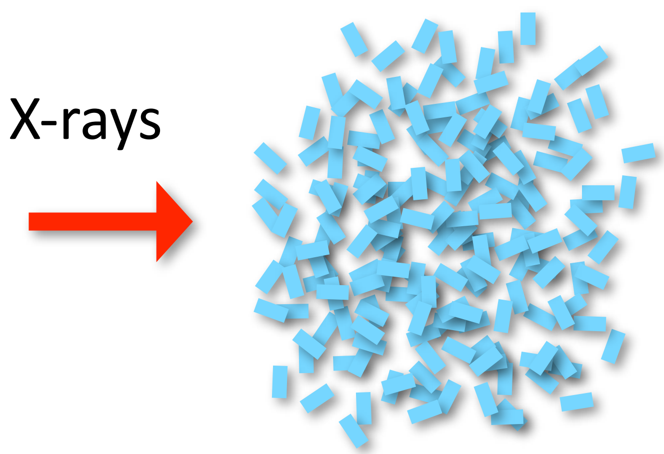
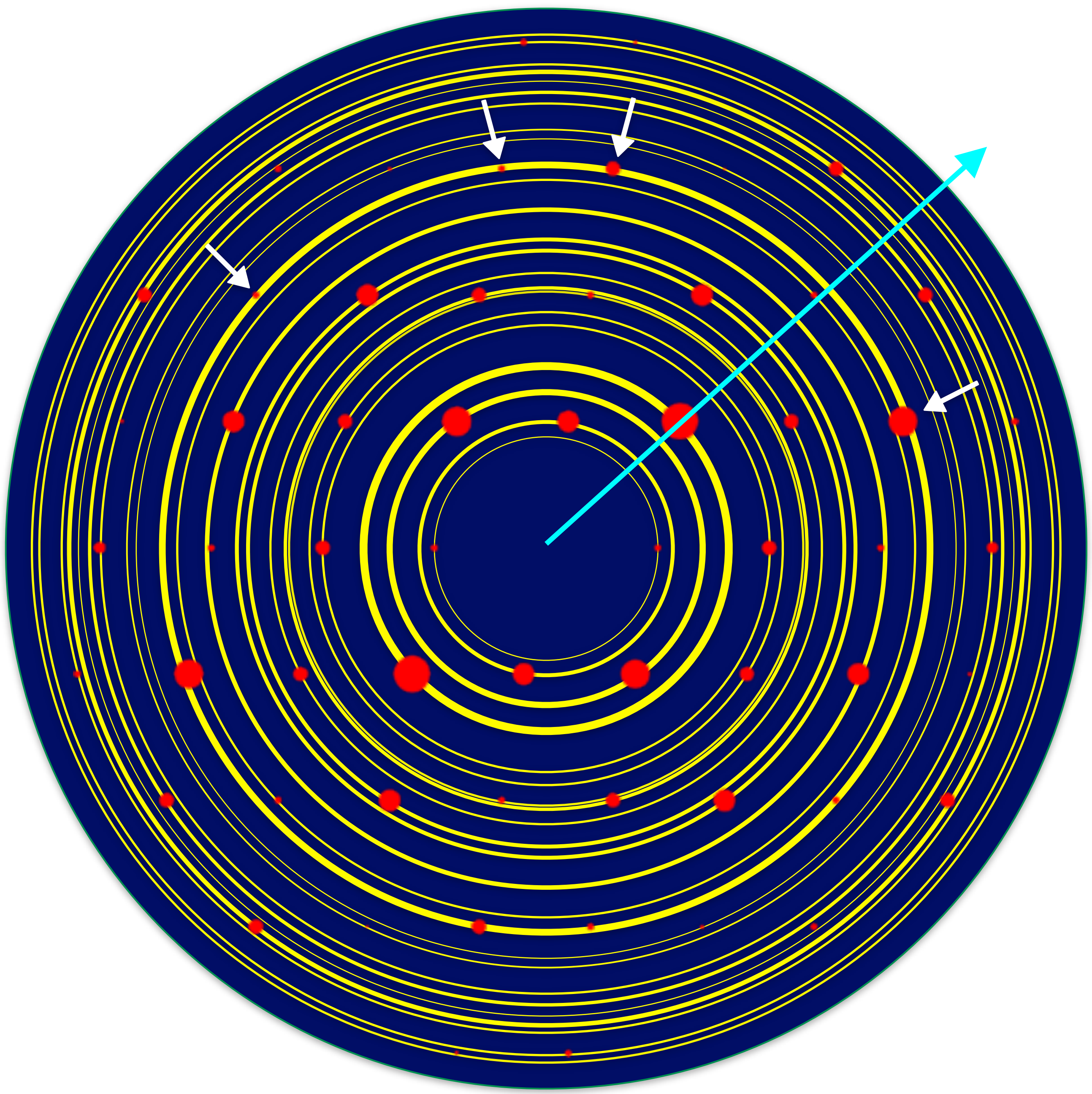
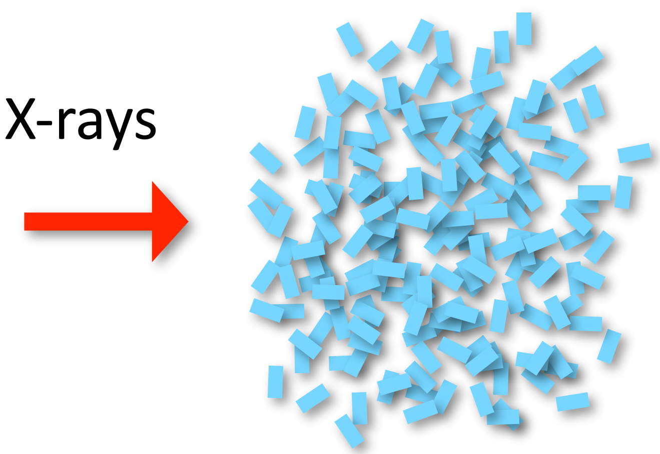


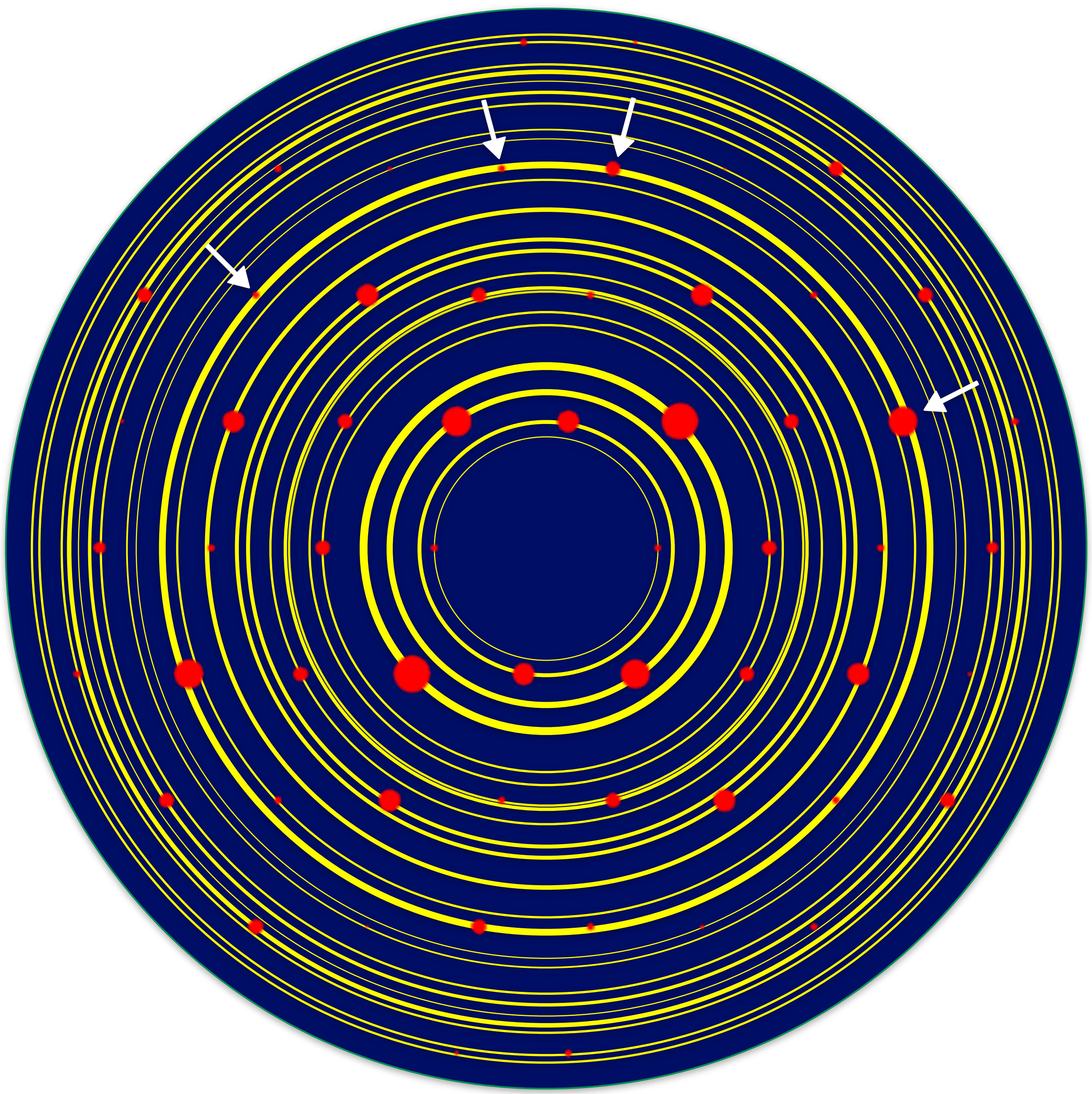


Using Texture for Structure Solution

Reflection Overlap Problem

X-rays





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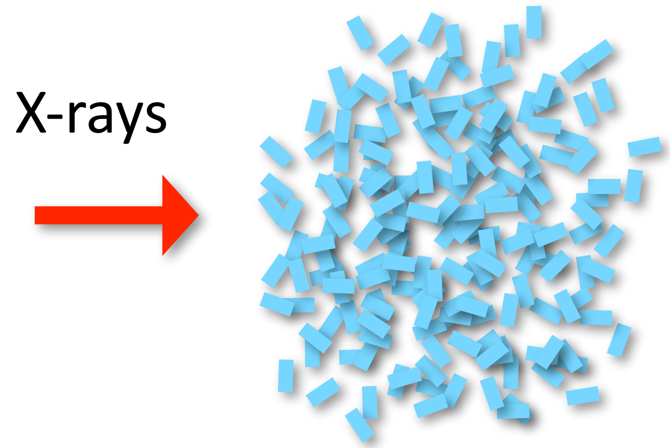

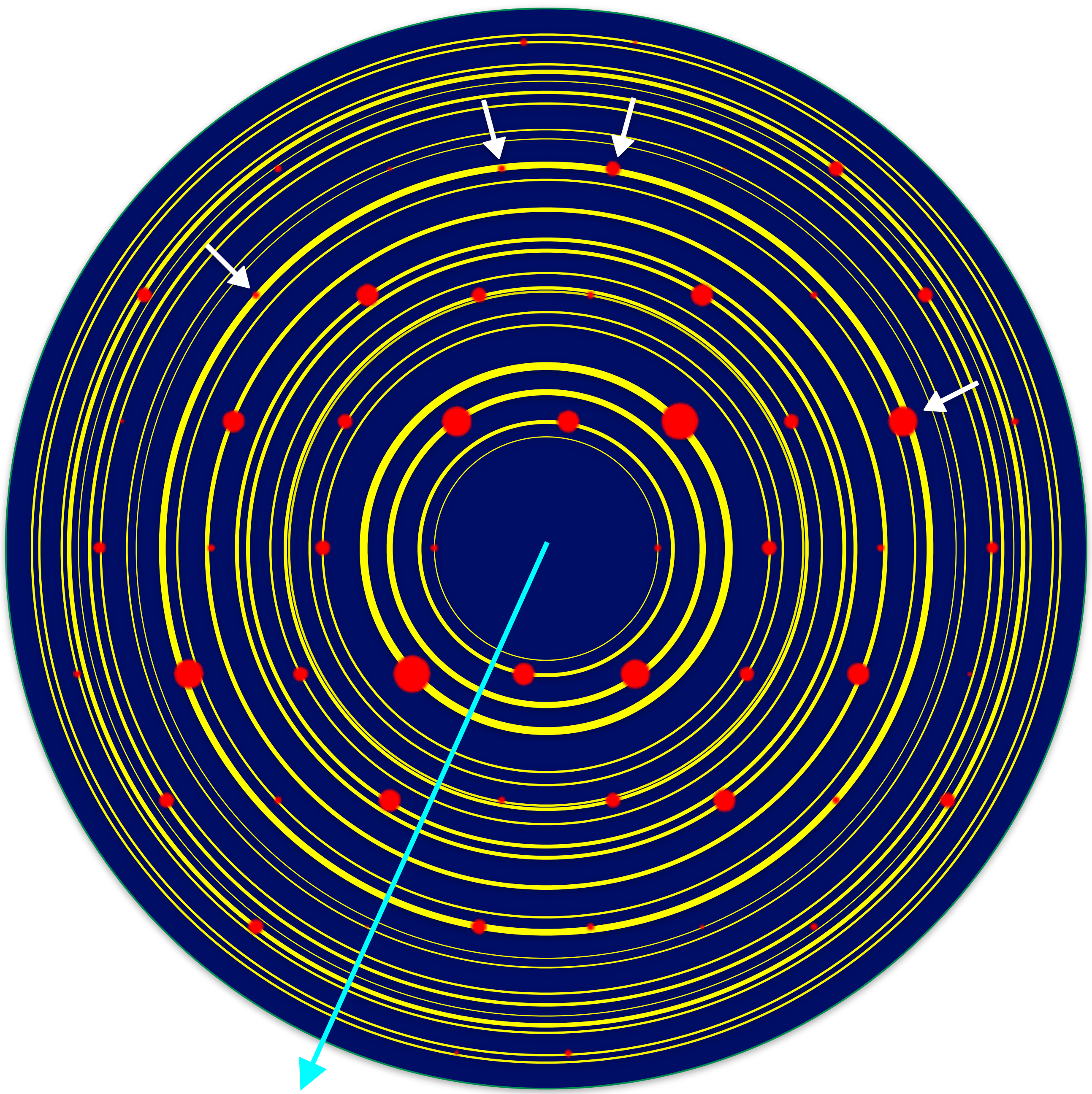

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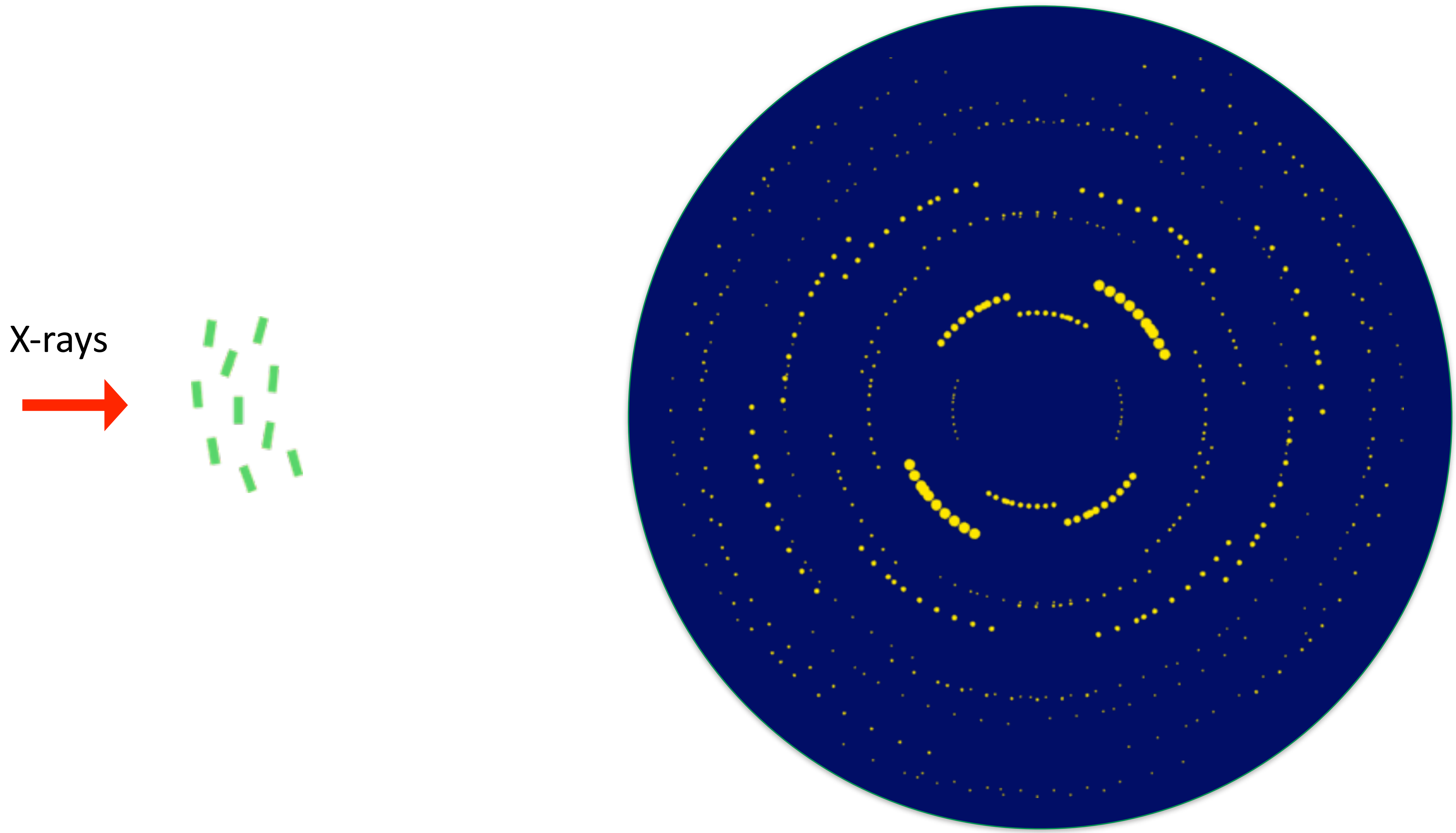

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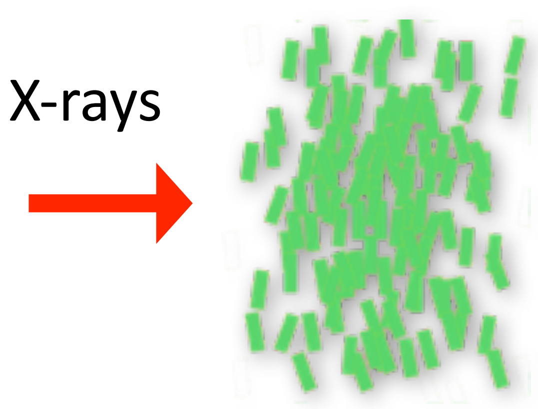

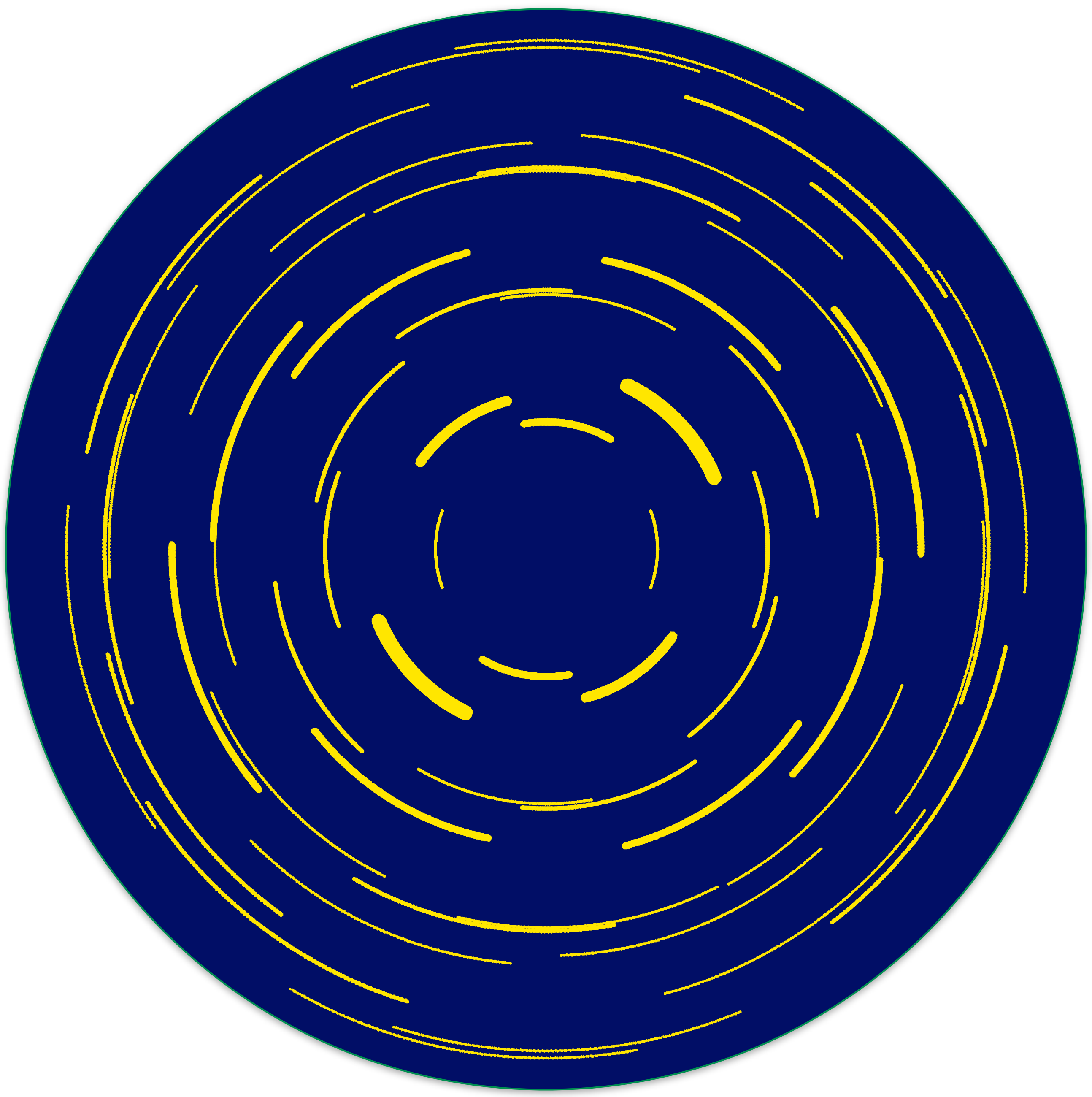

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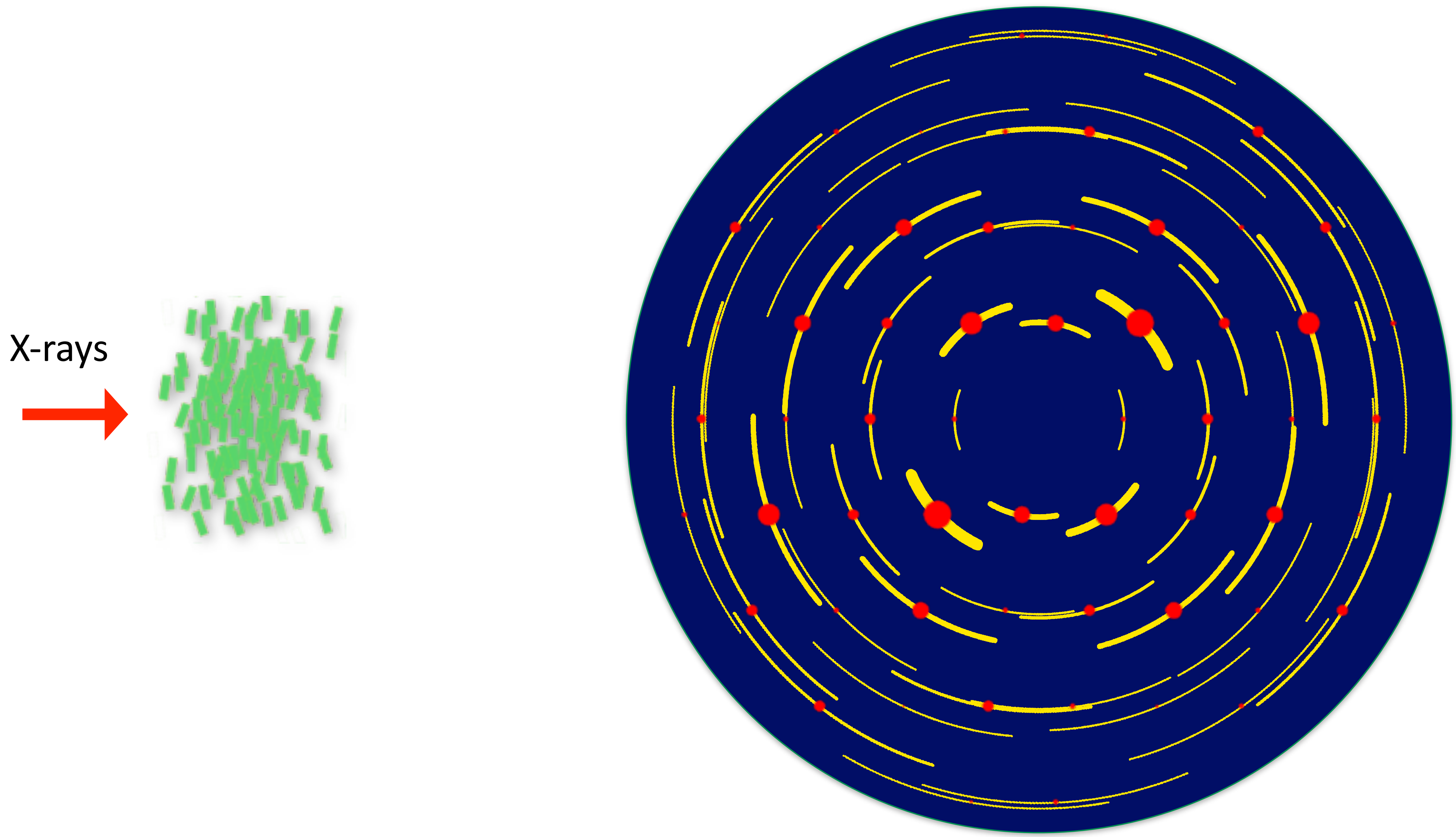

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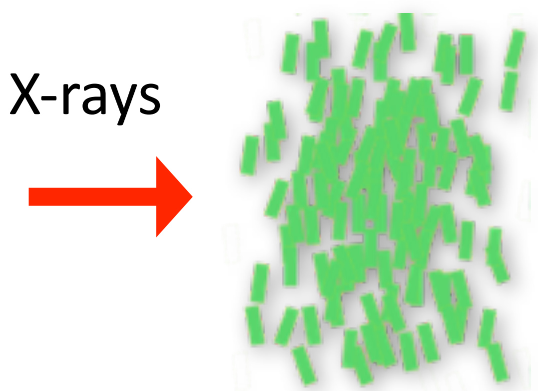

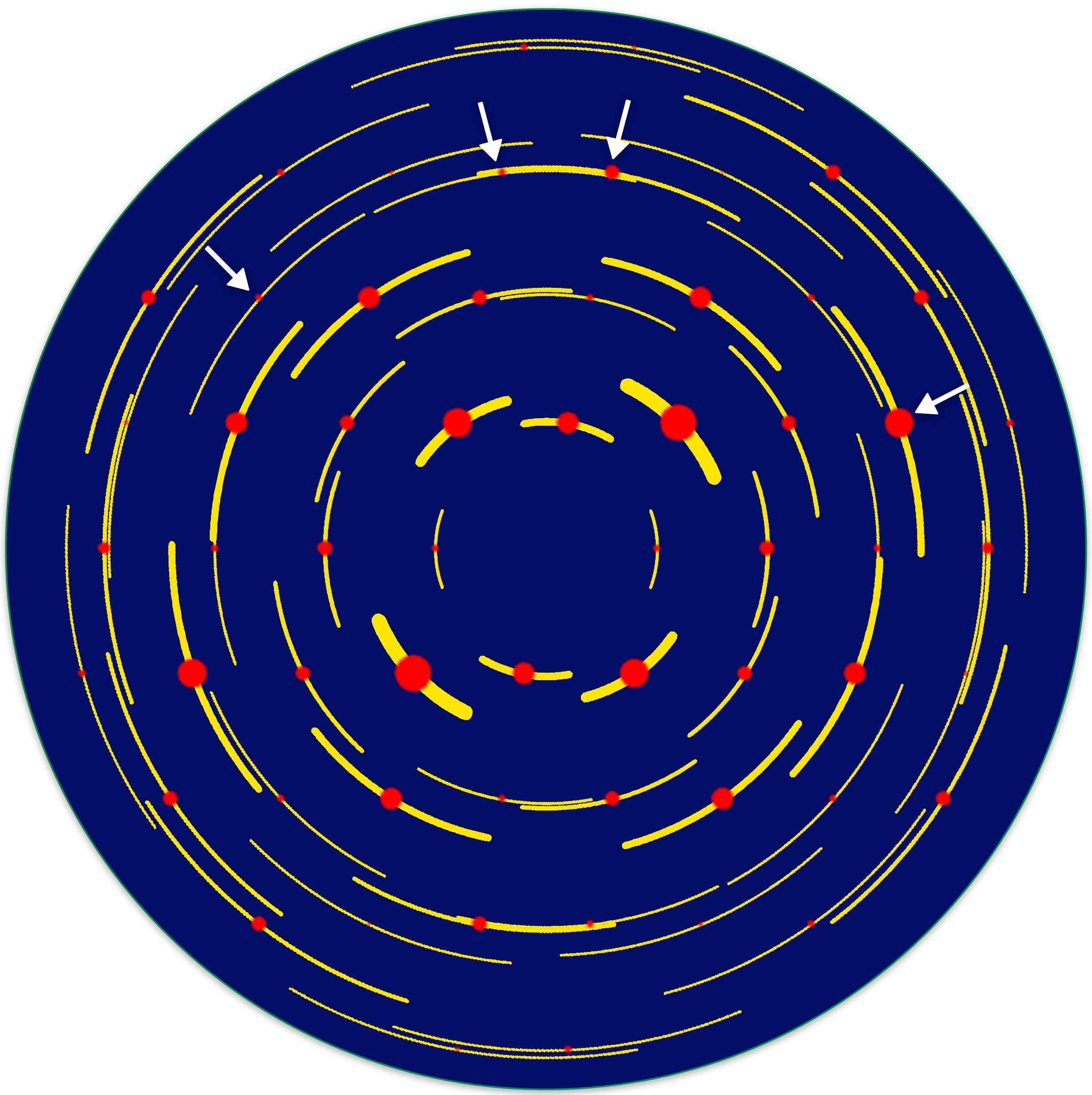

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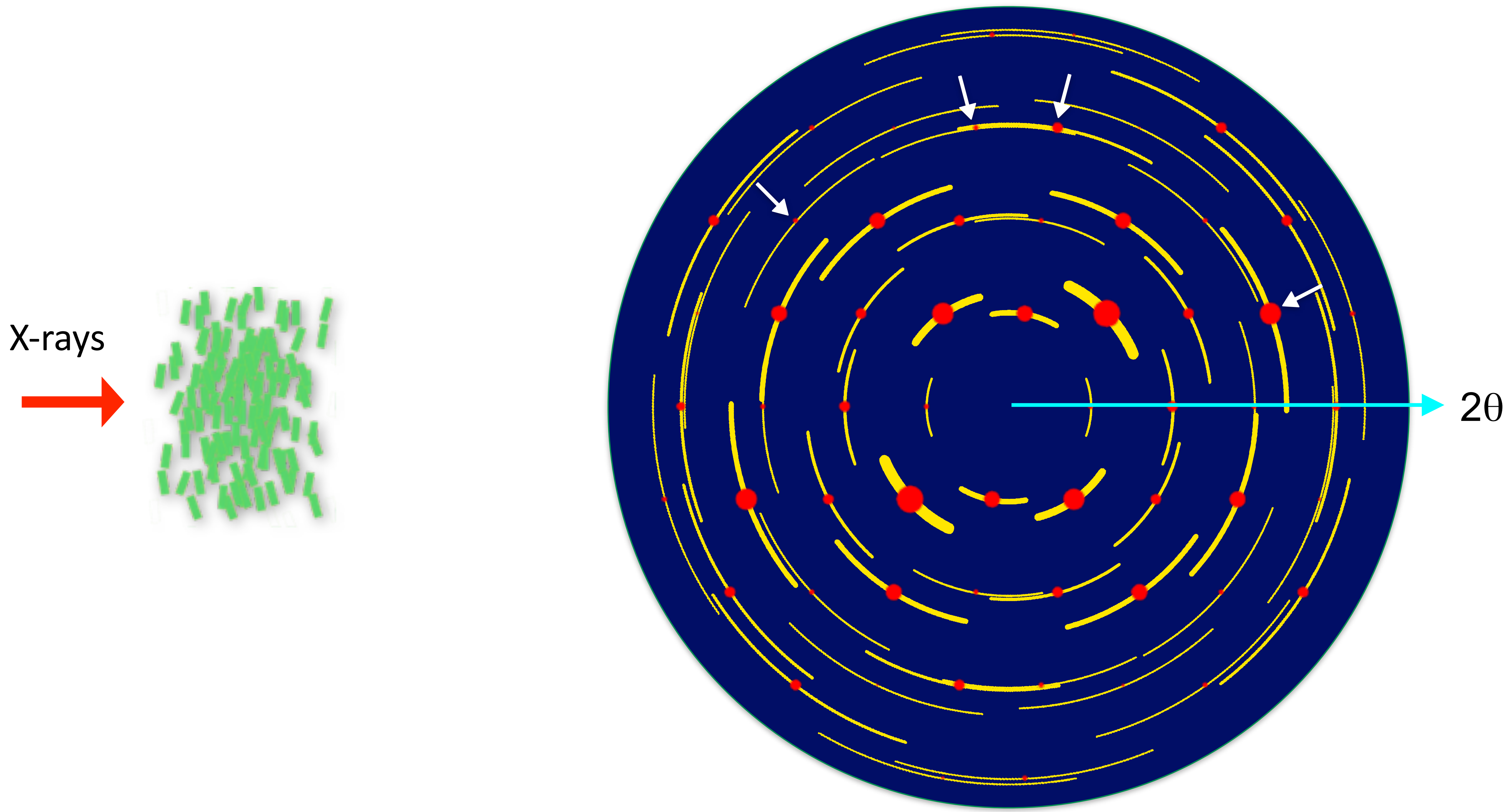

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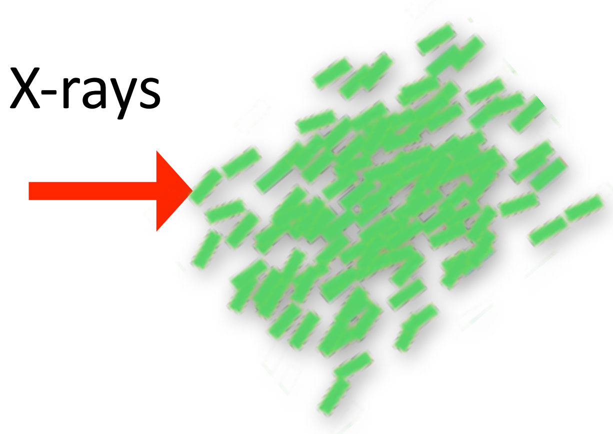

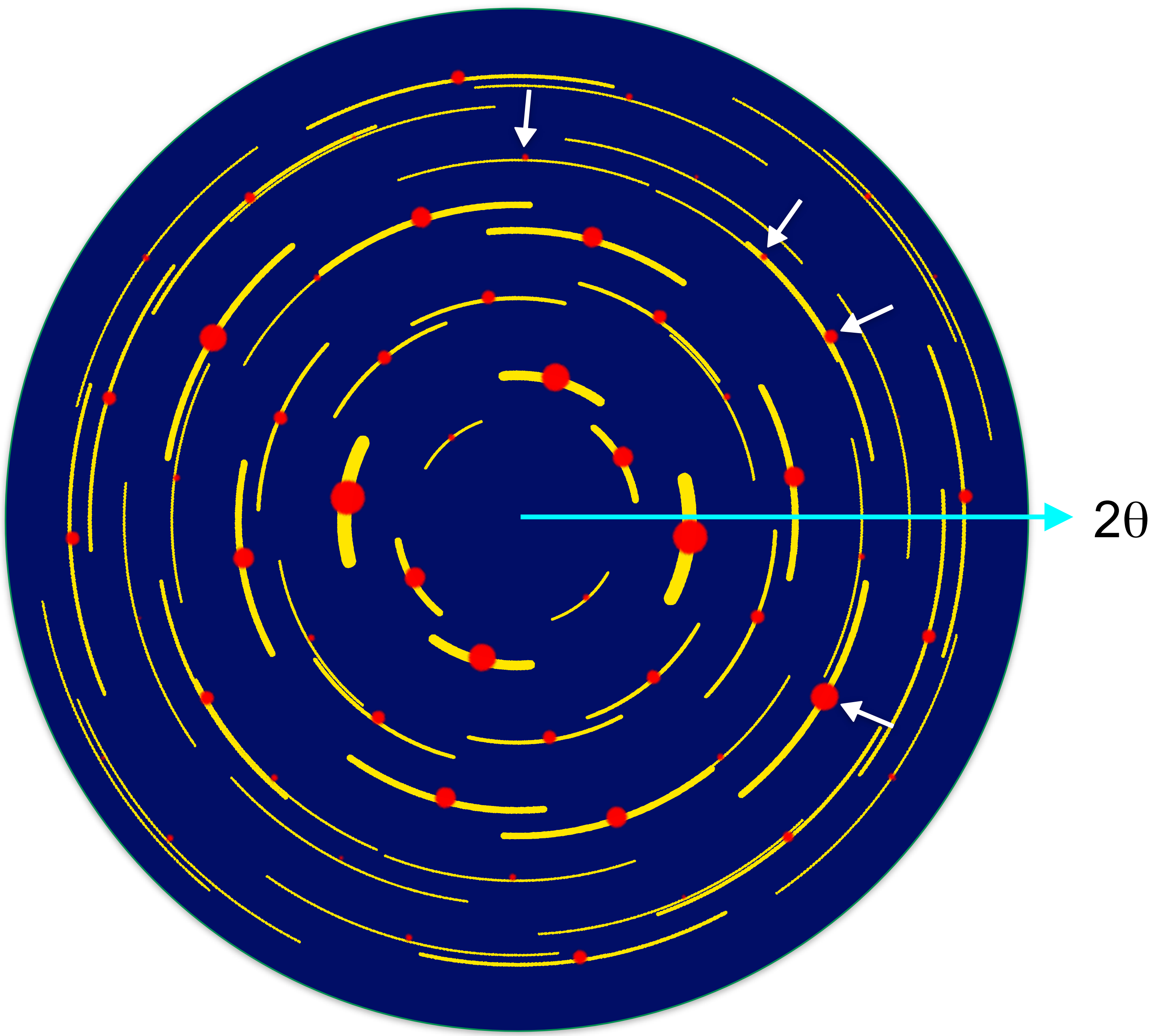

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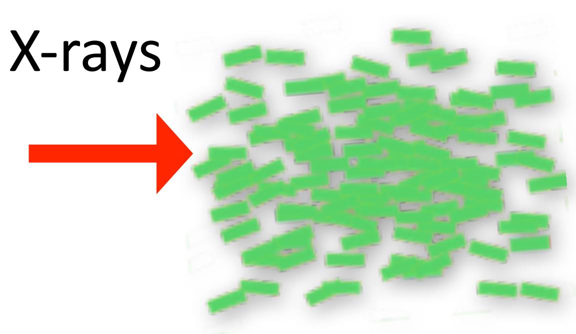
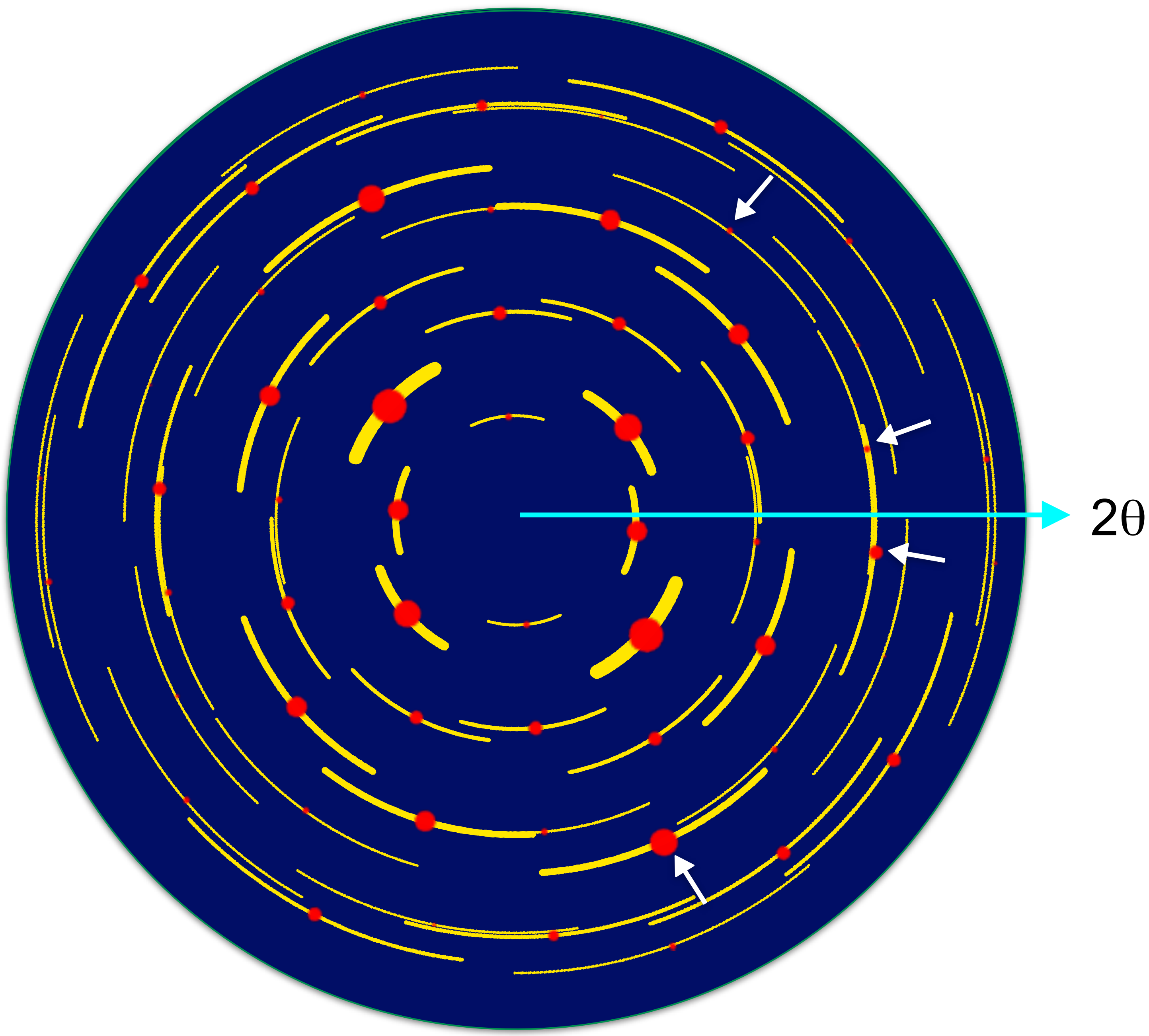
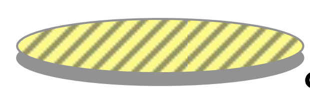
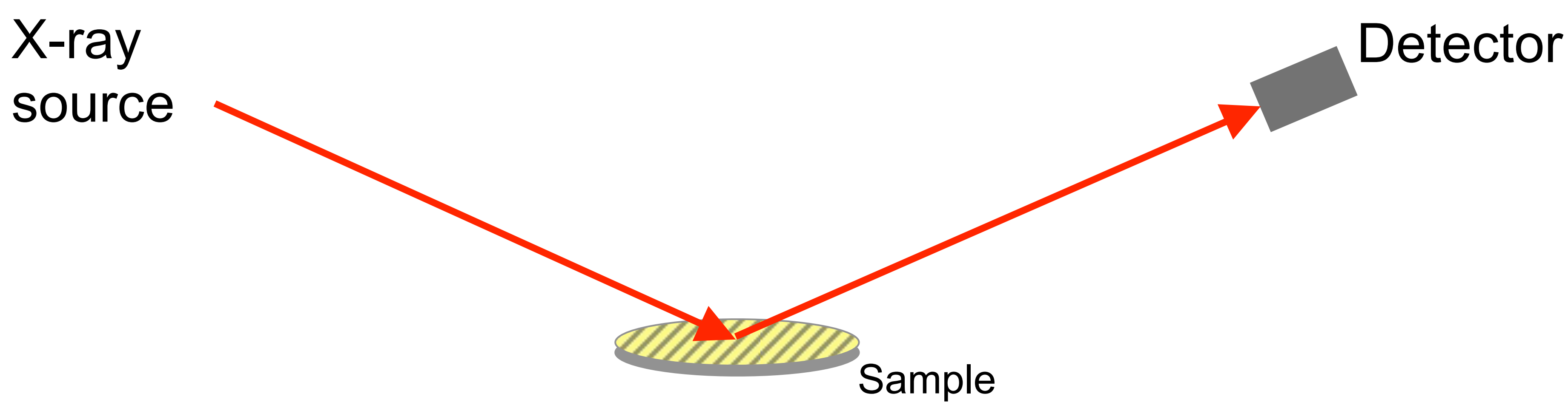




Reflection mode - experimental setup



Reflection mode - experimental setup



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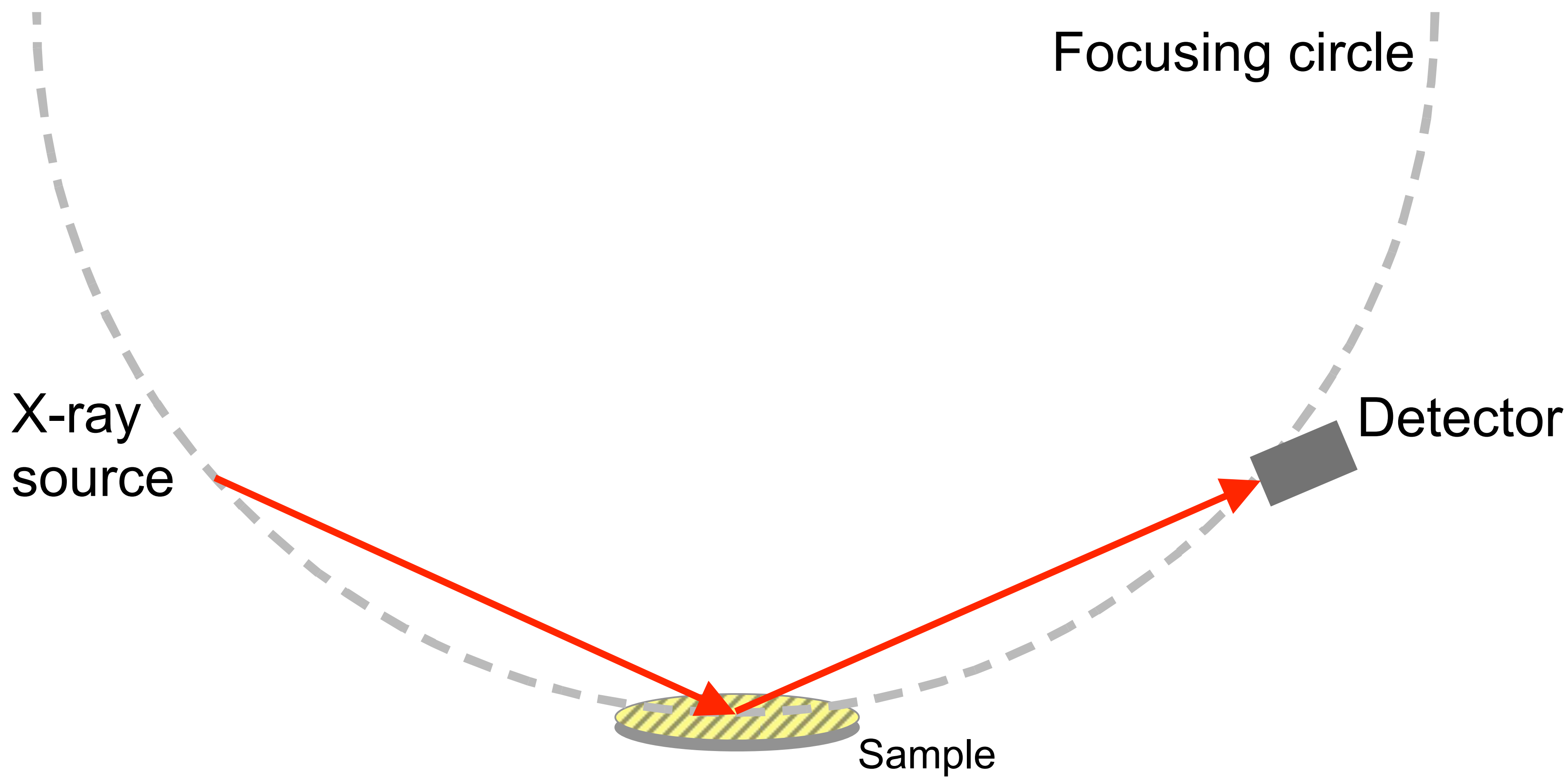

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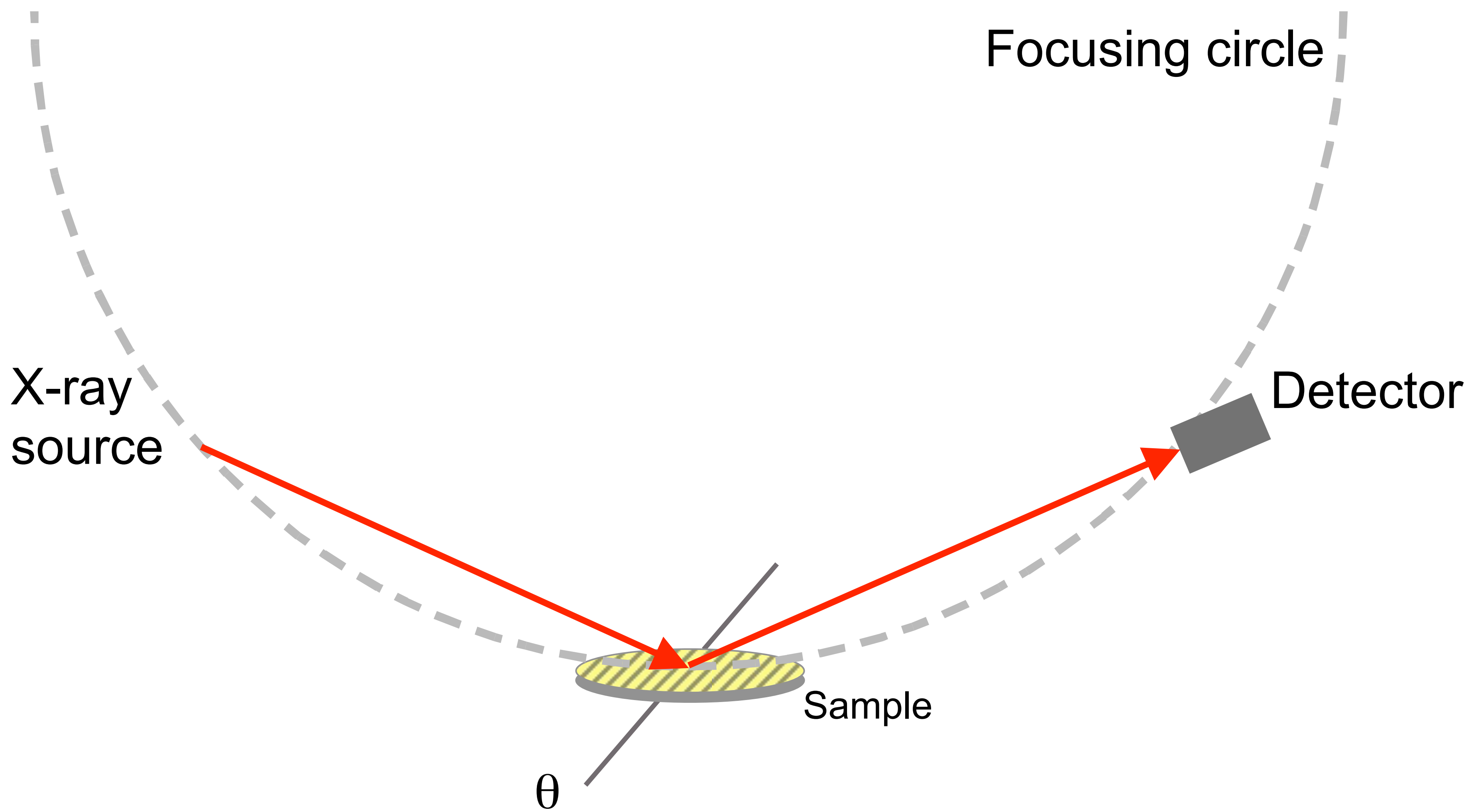

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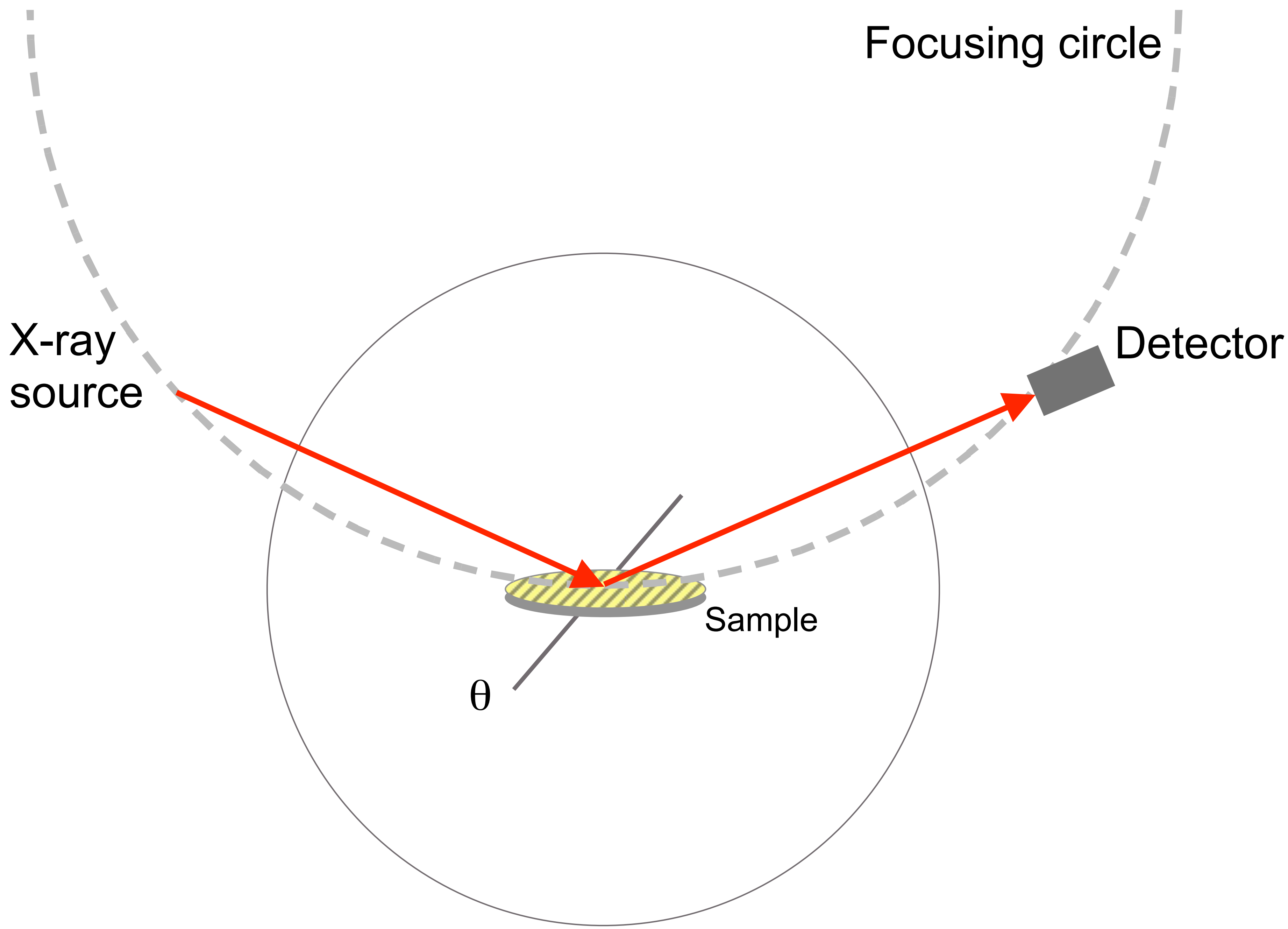

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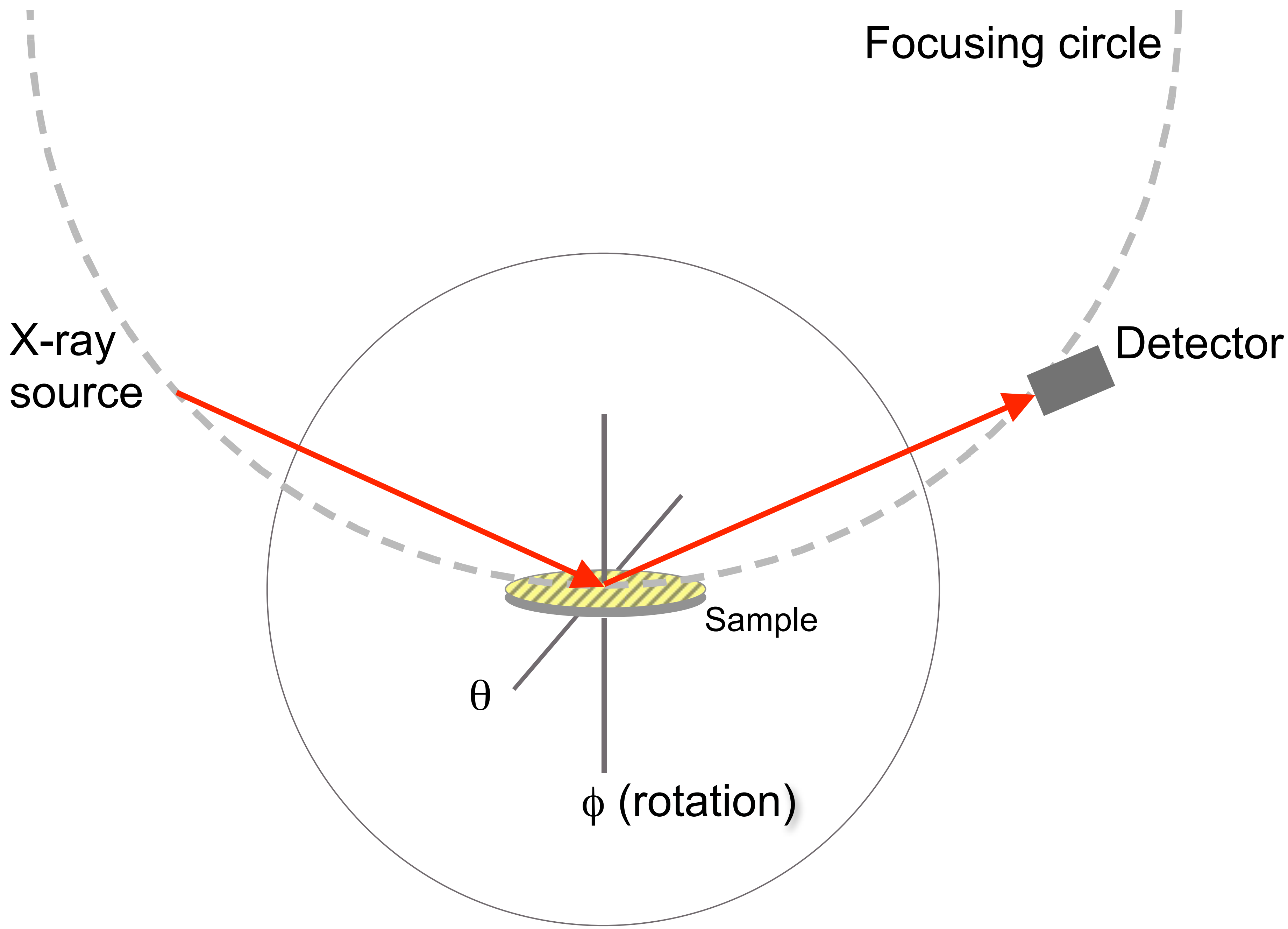

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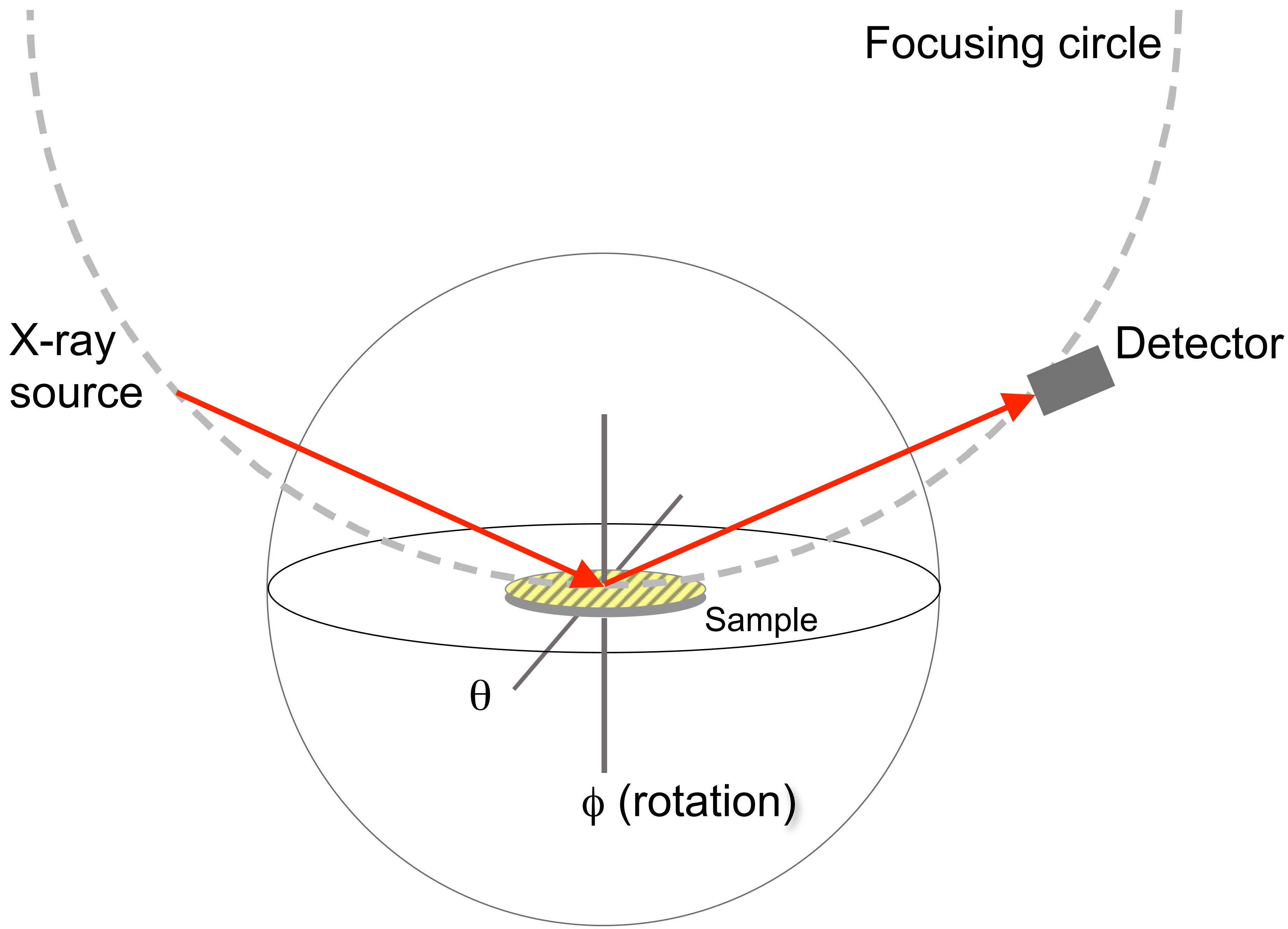

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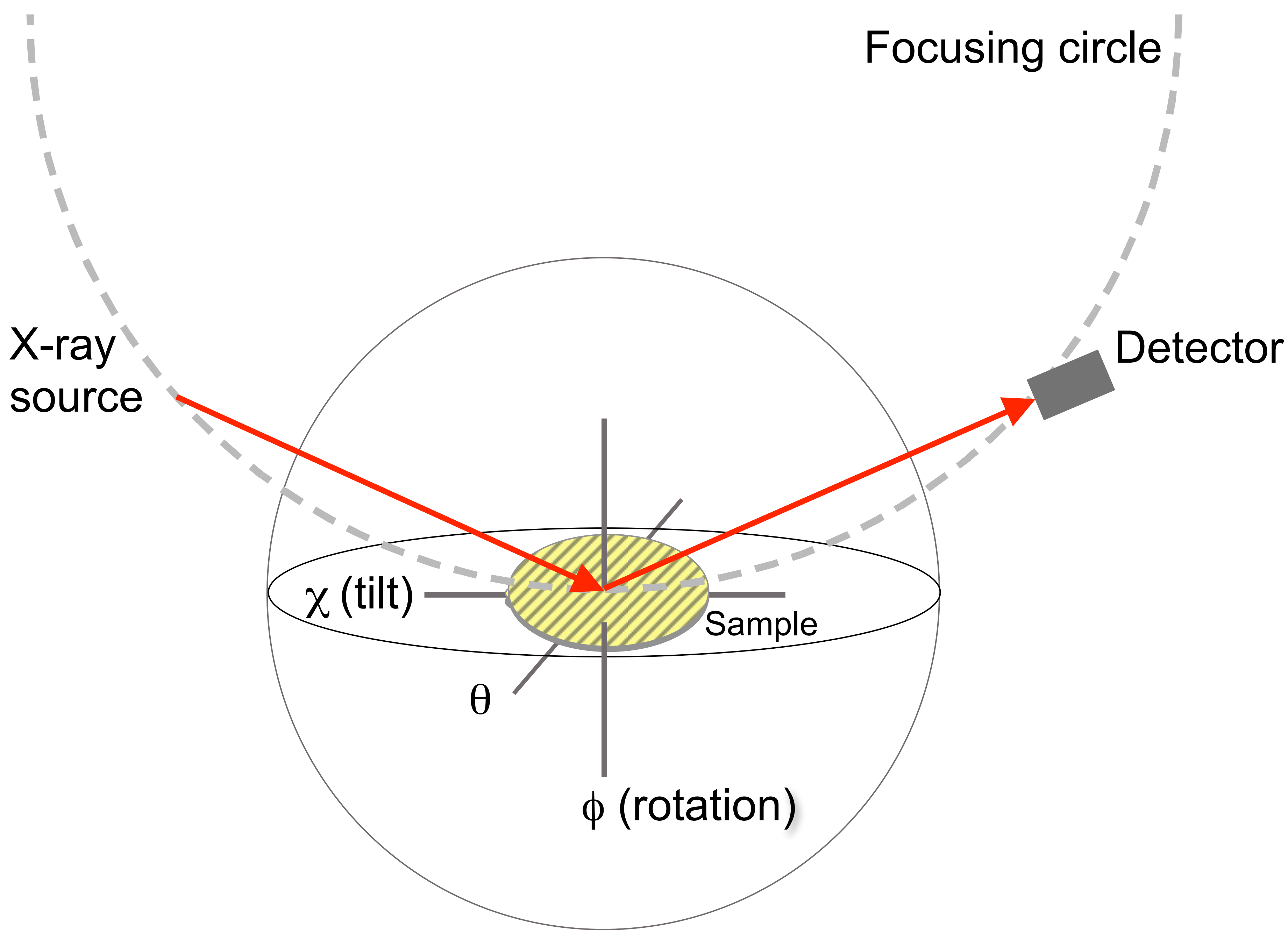

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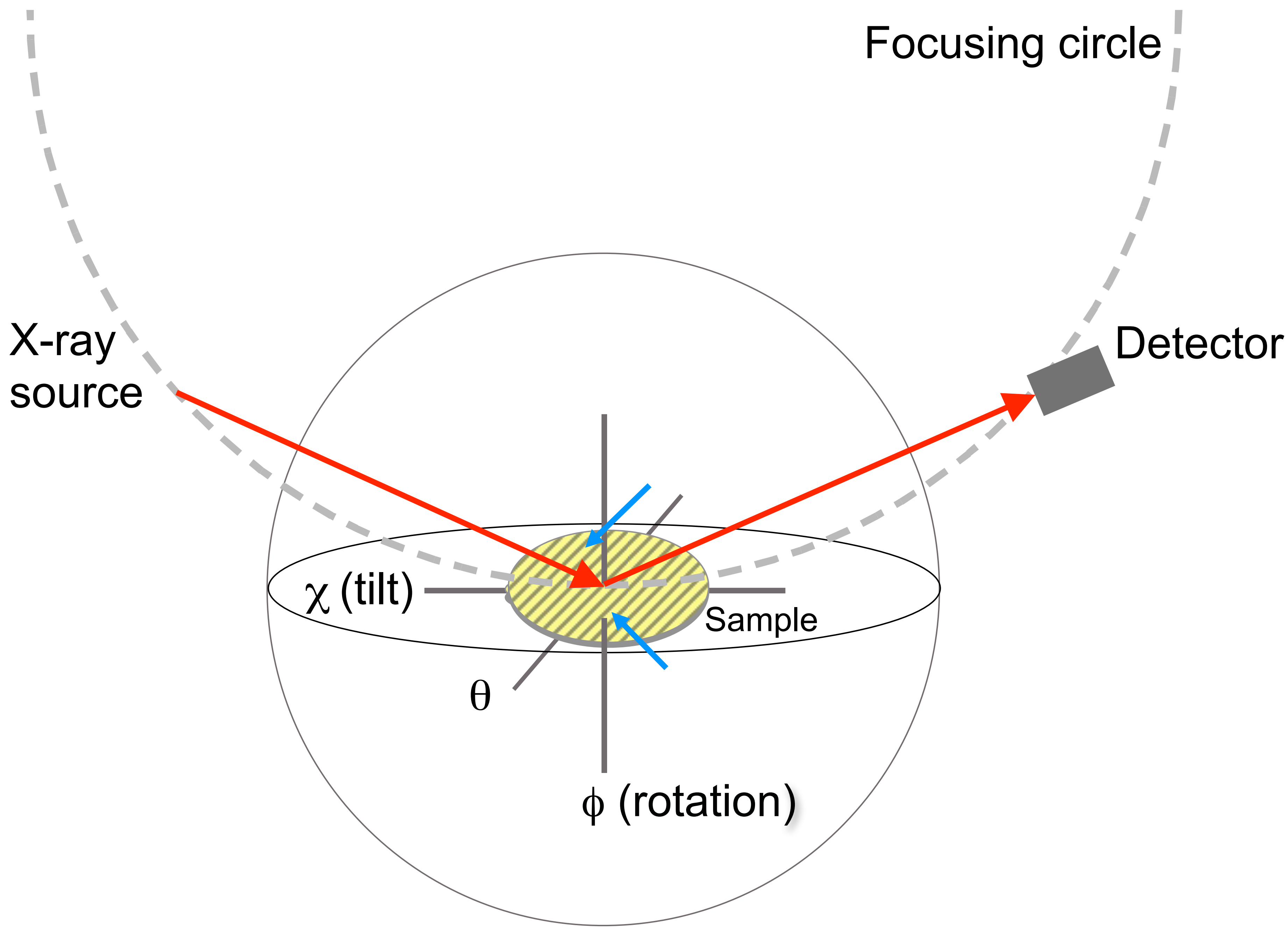

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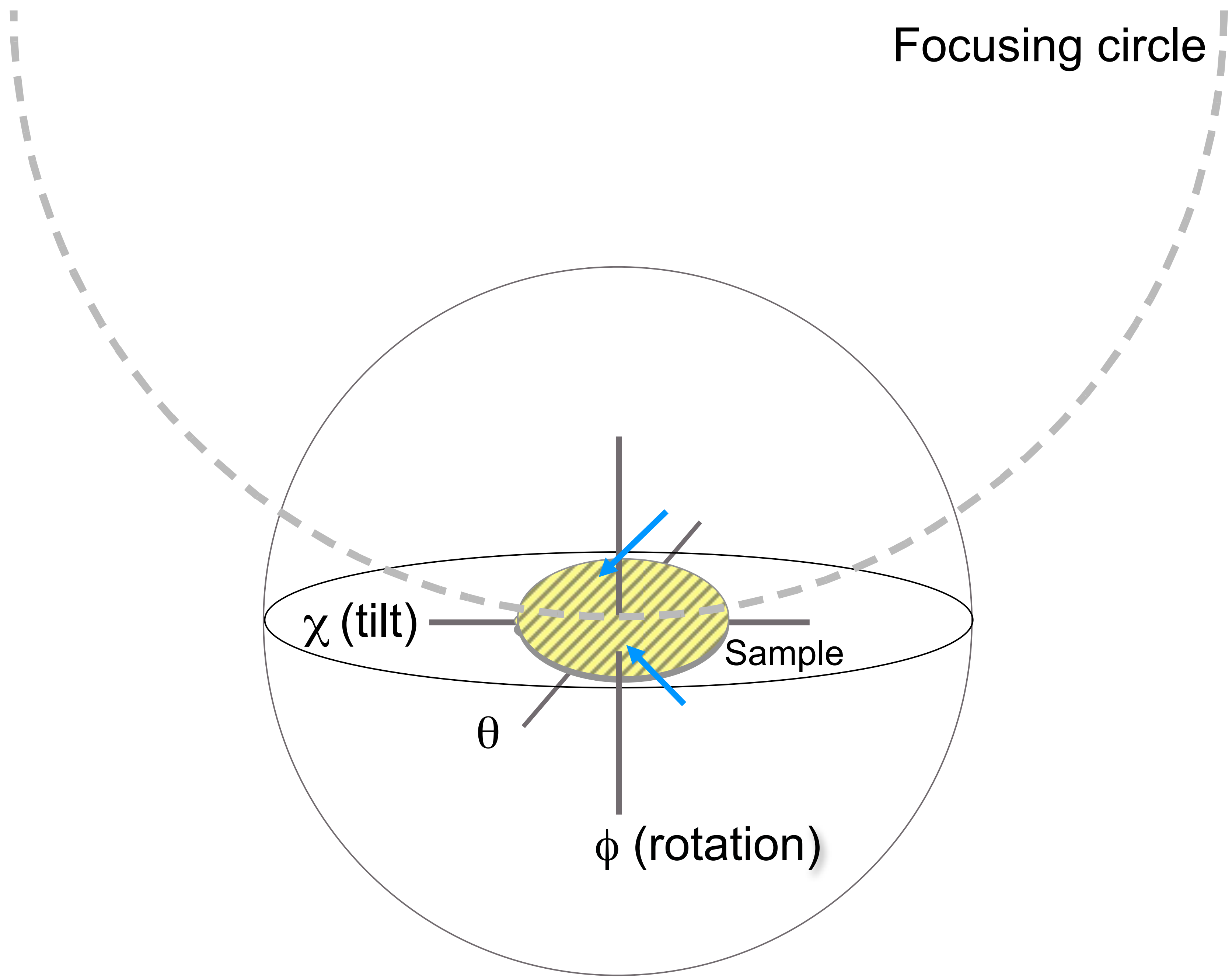

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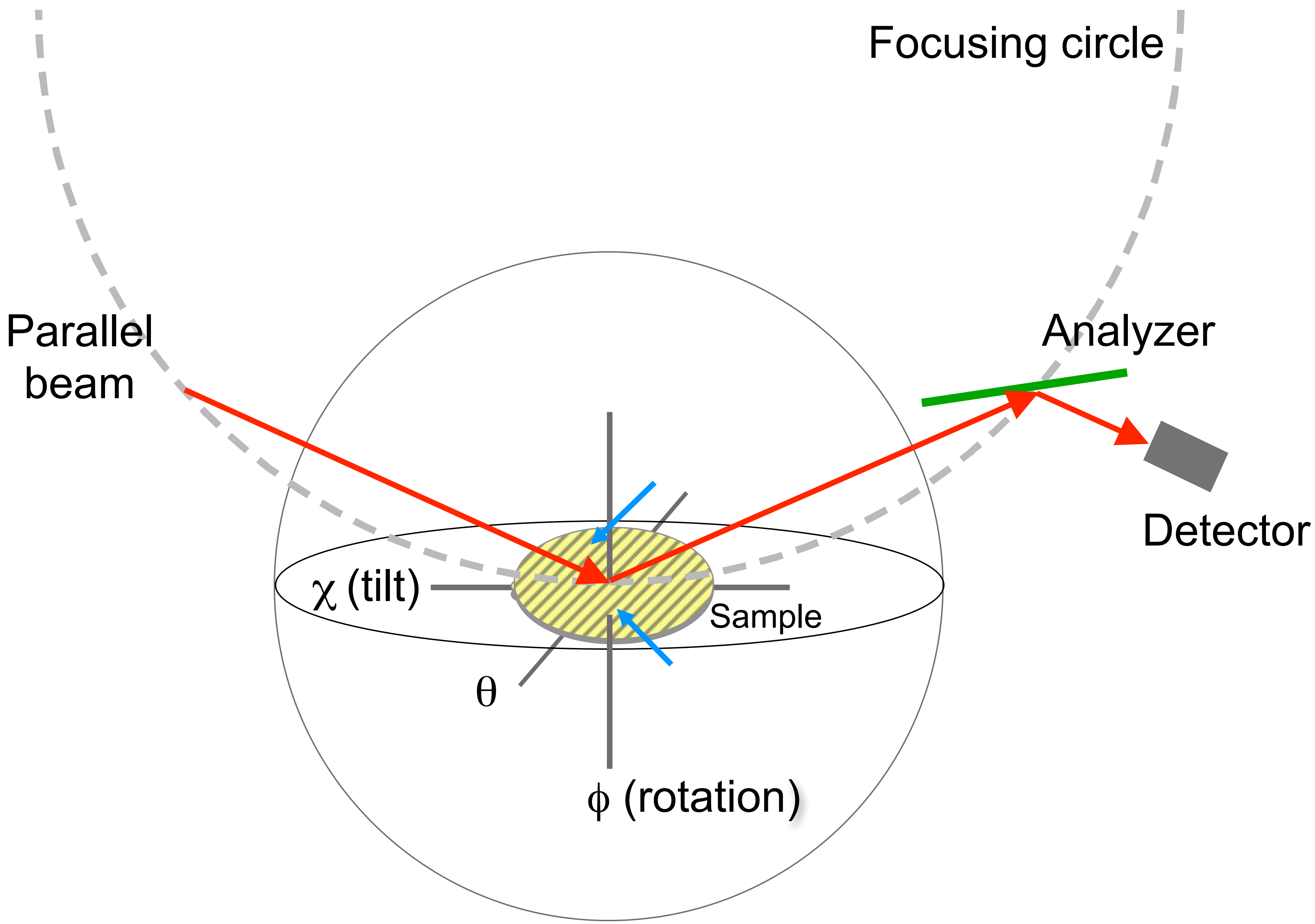

Texture Analysis

measure every 5° in ϕ and χ

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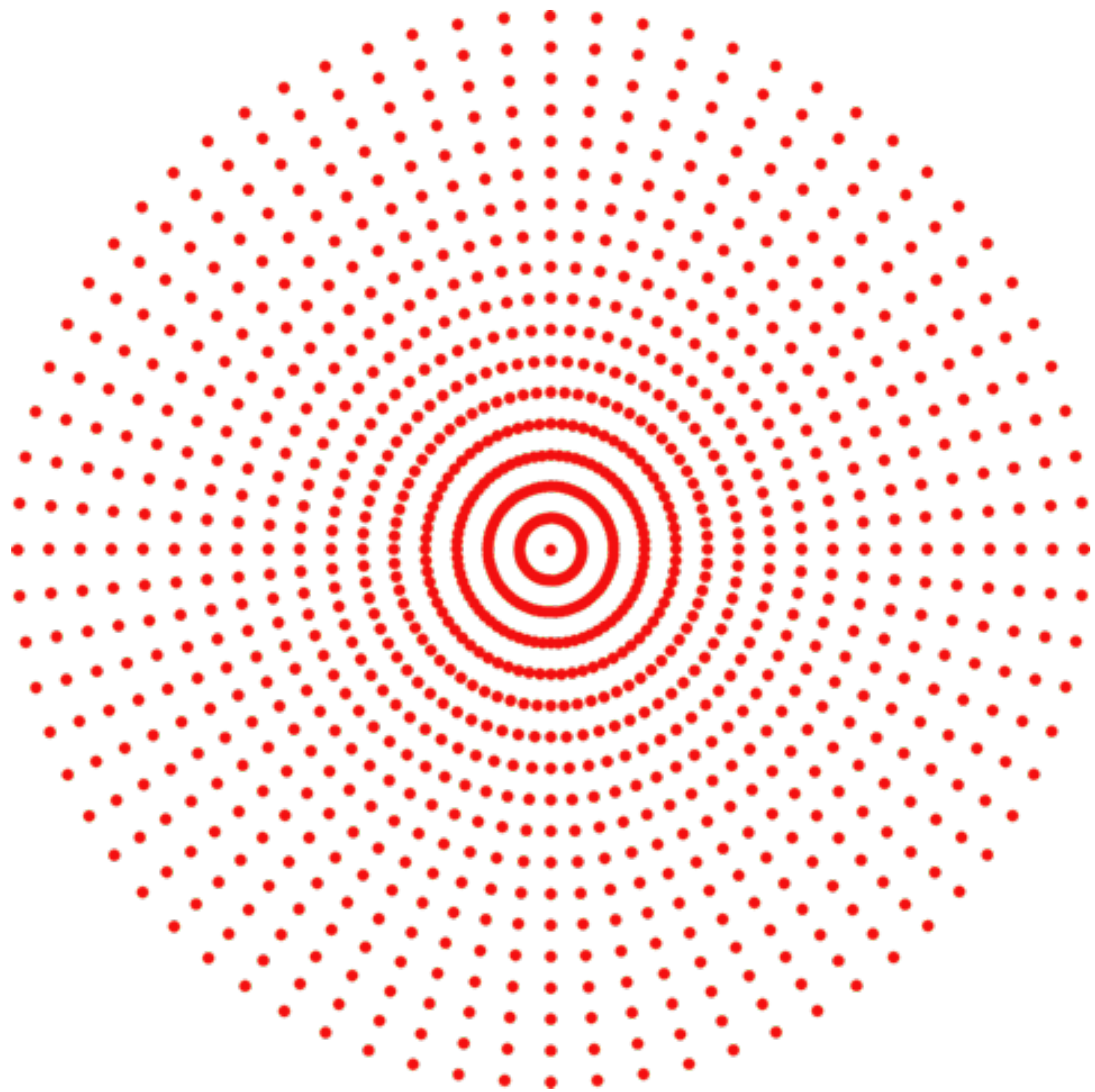

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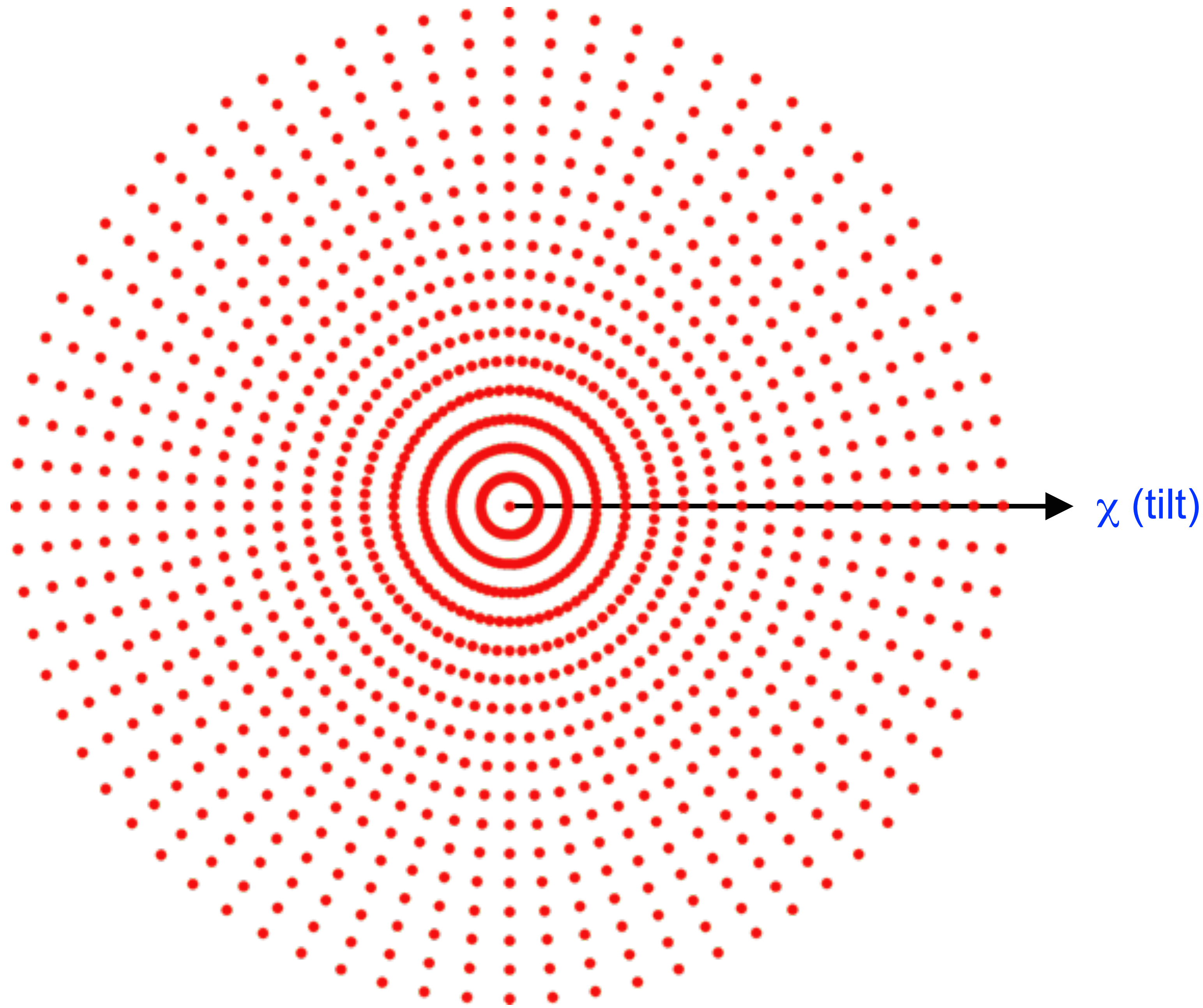

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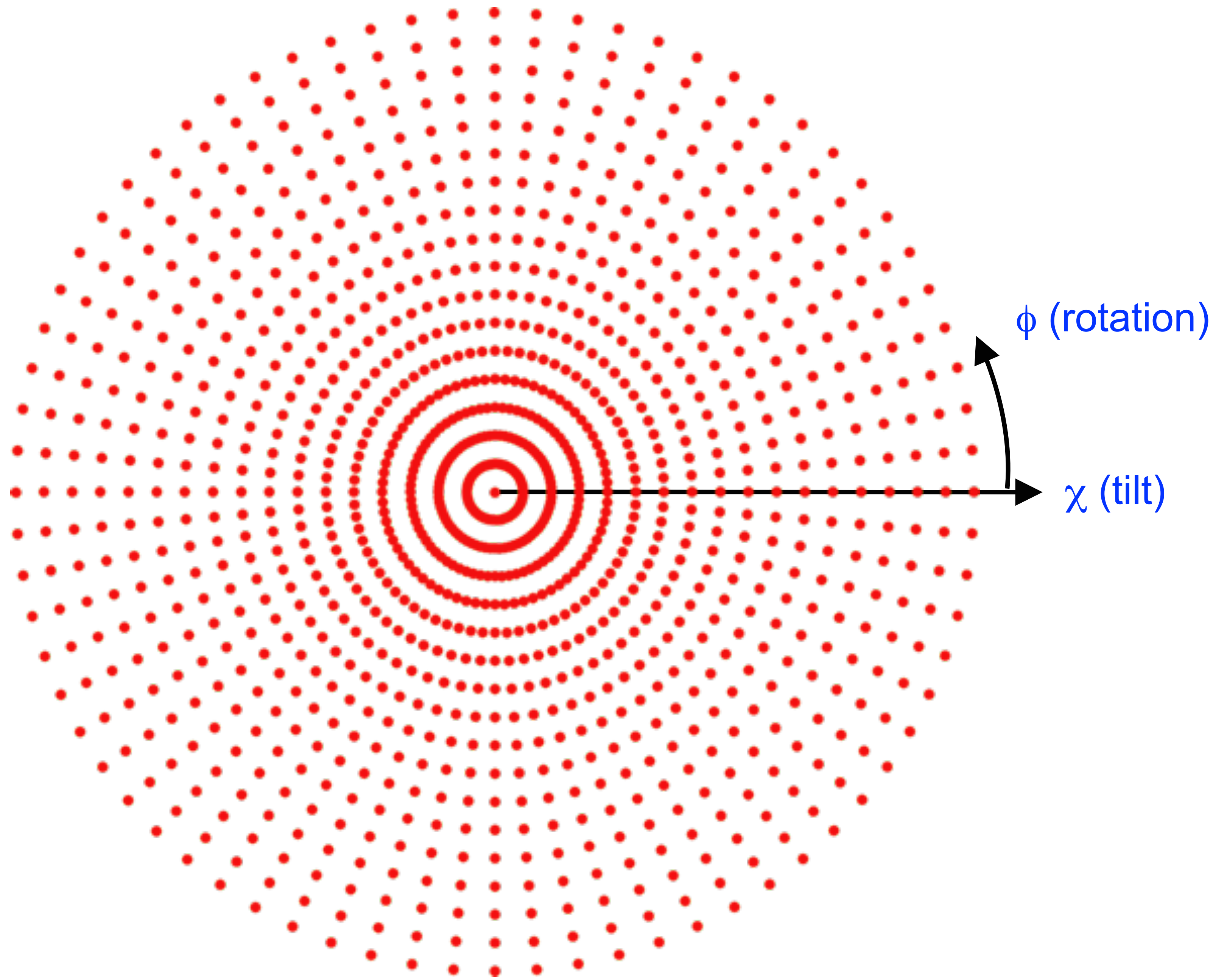

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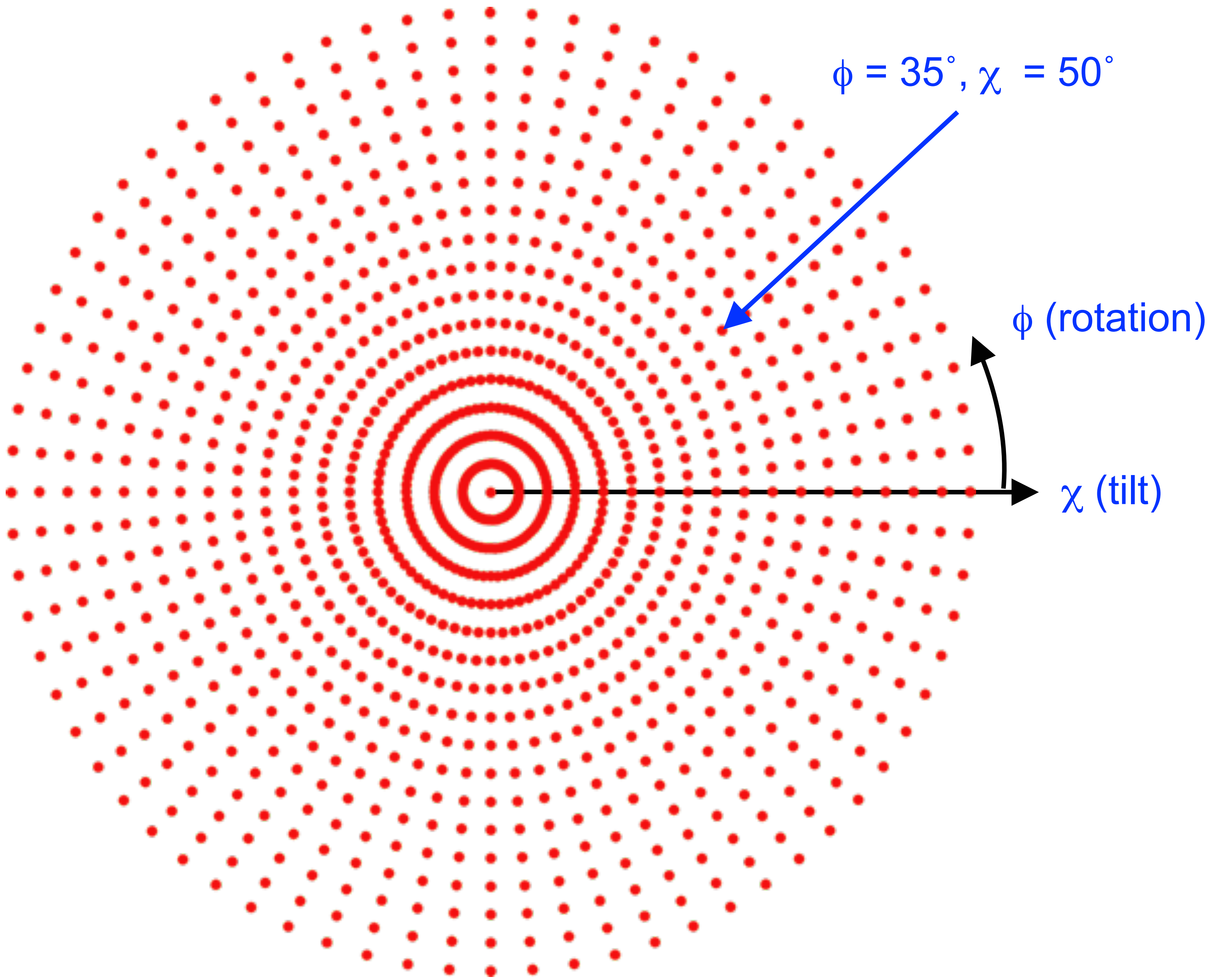

Texture Analysis

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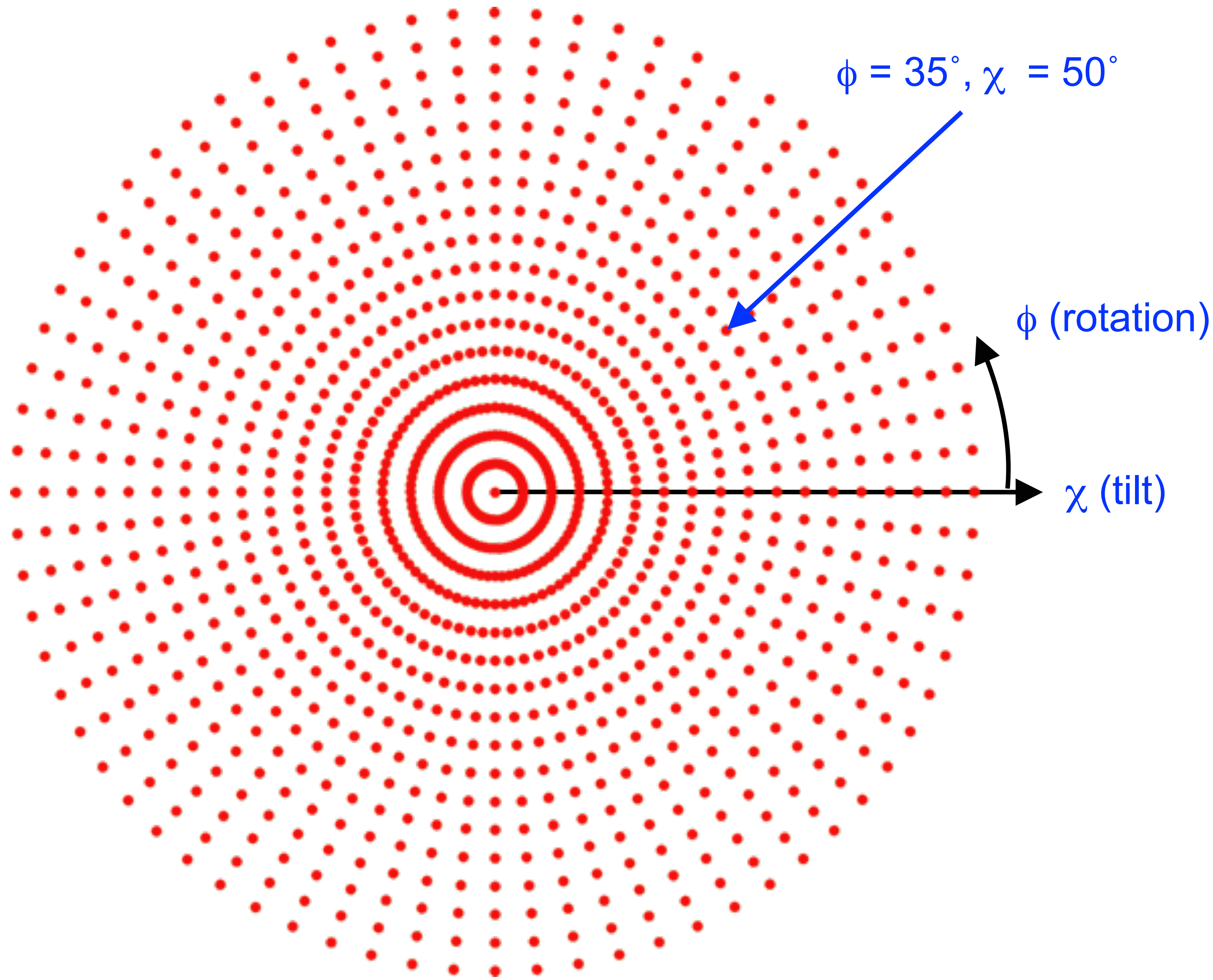
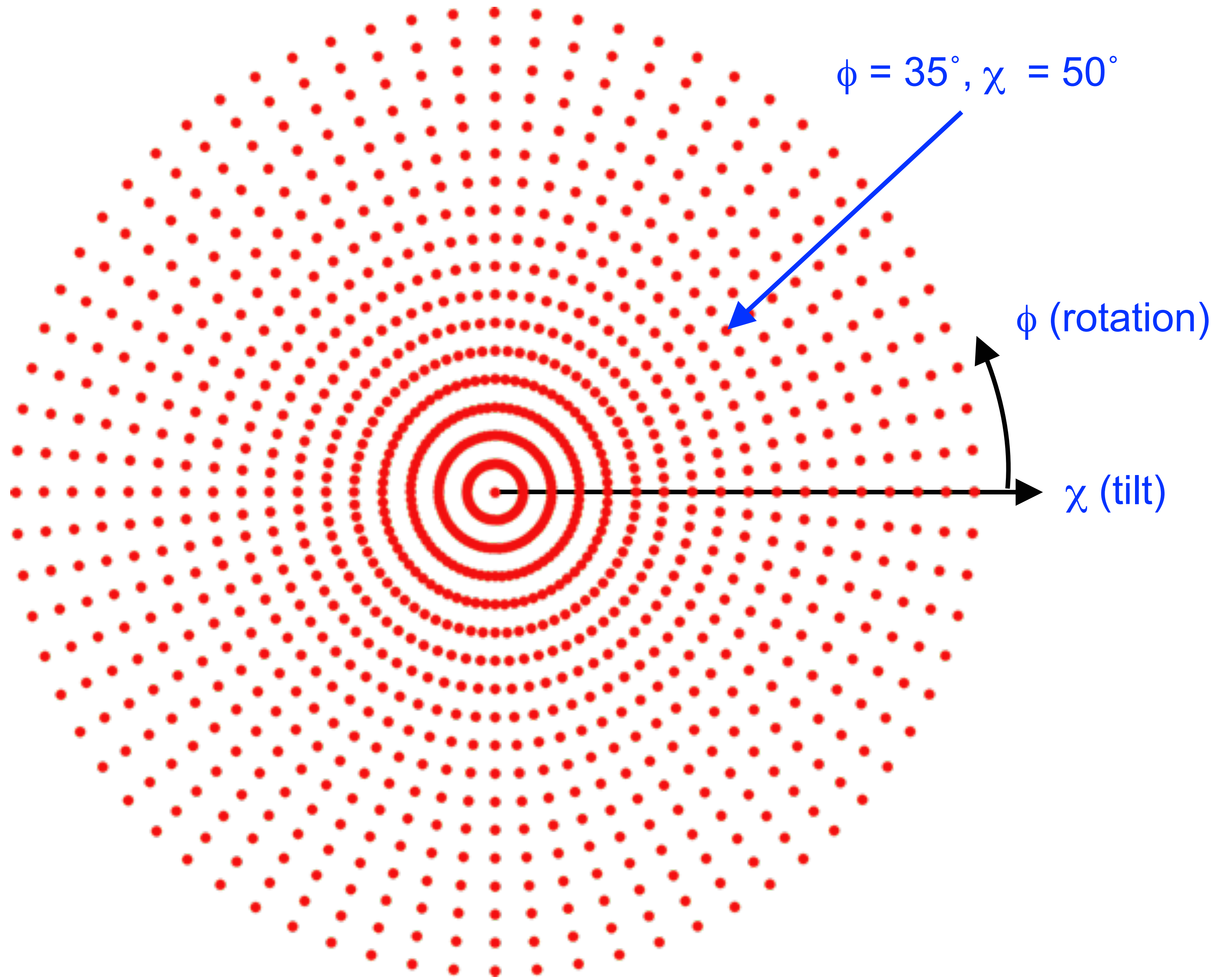


1152 measurements
(80° tilt)

Texture Analysis

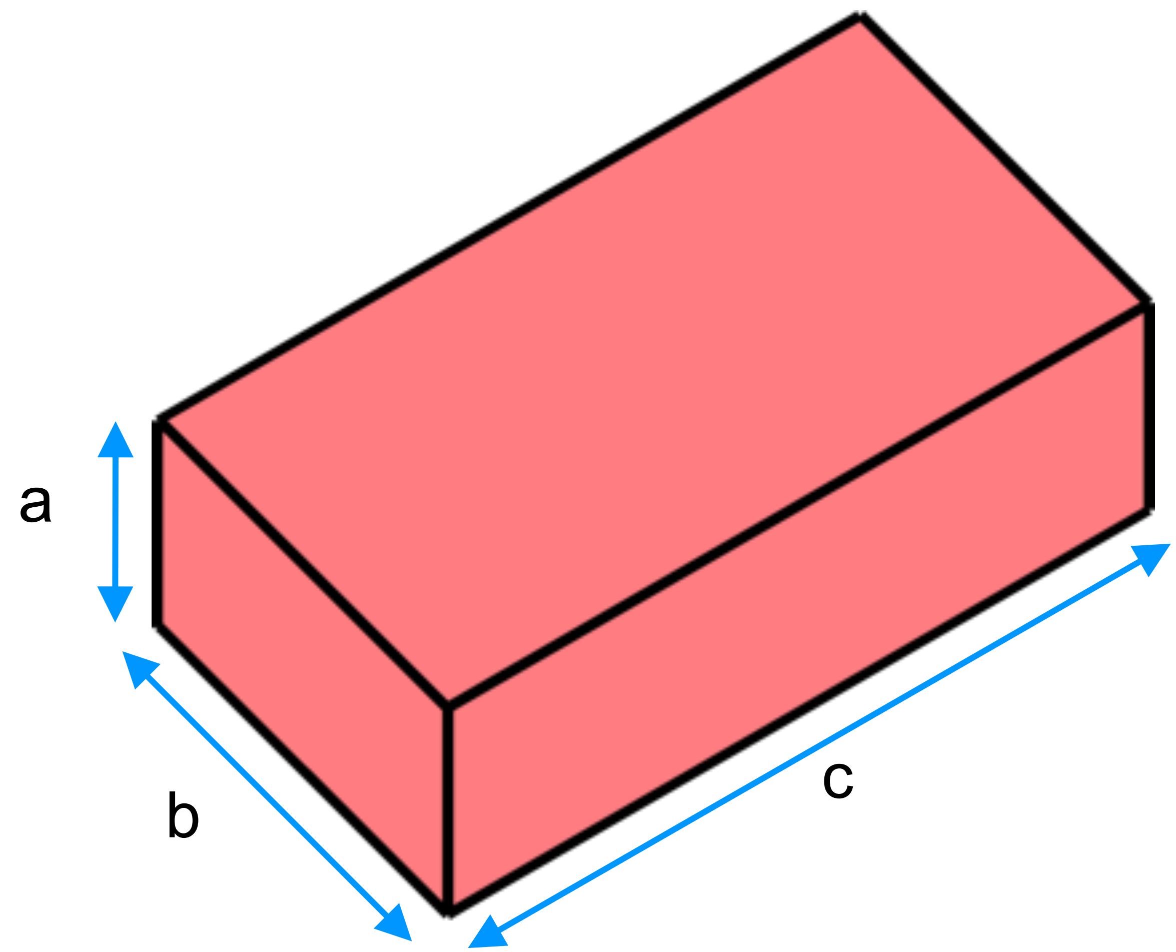
measure every 5° in ϕ and χ



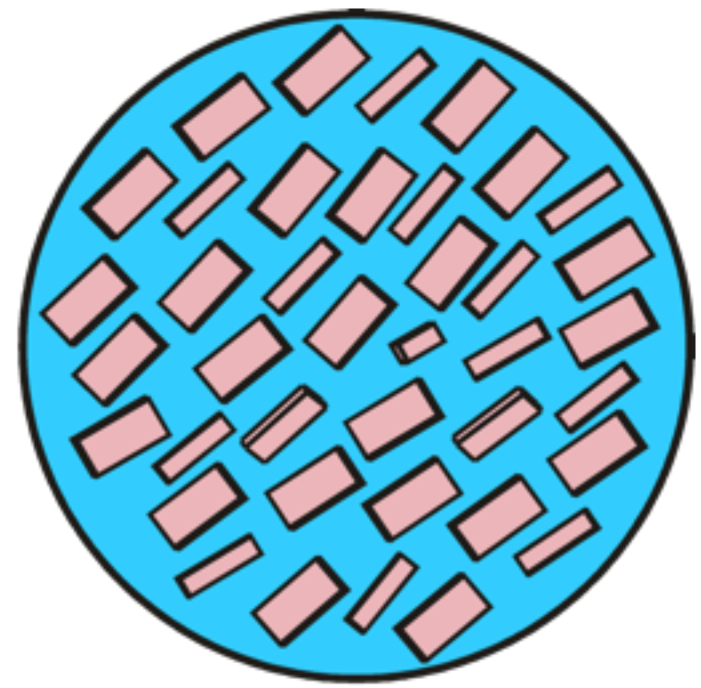
1152 measurements
(80° tilt)

Each reflection measured at each orientation

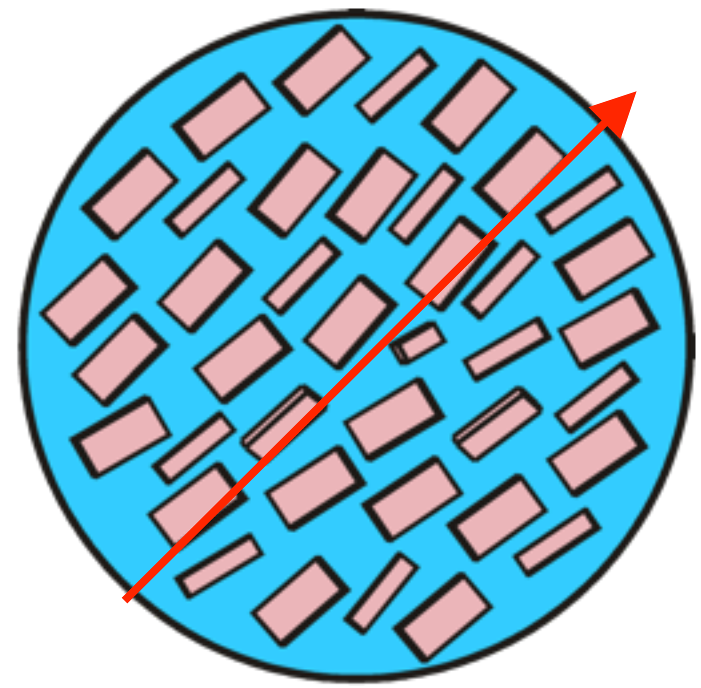
Texture Analysis



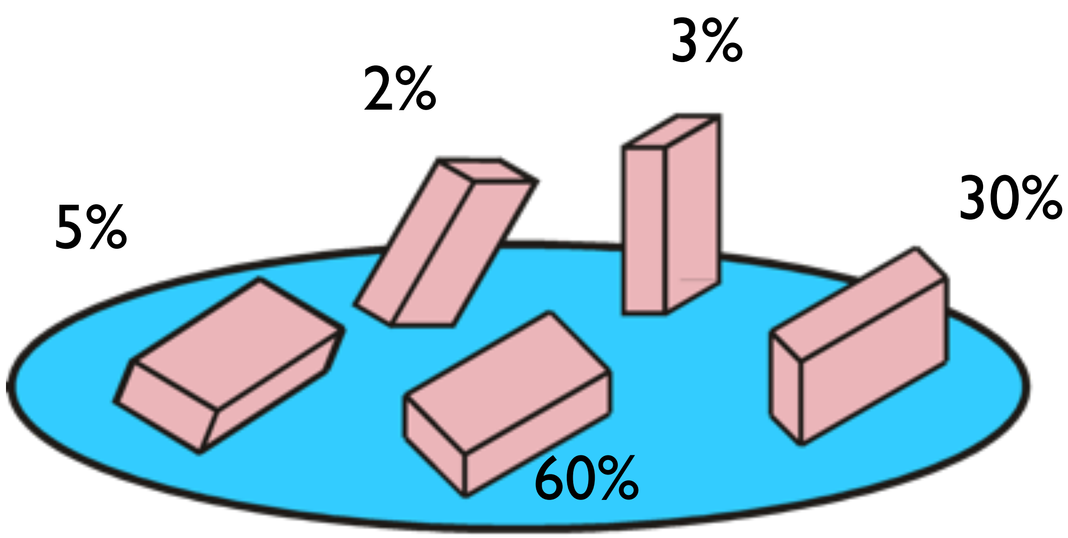
Texture Analysis

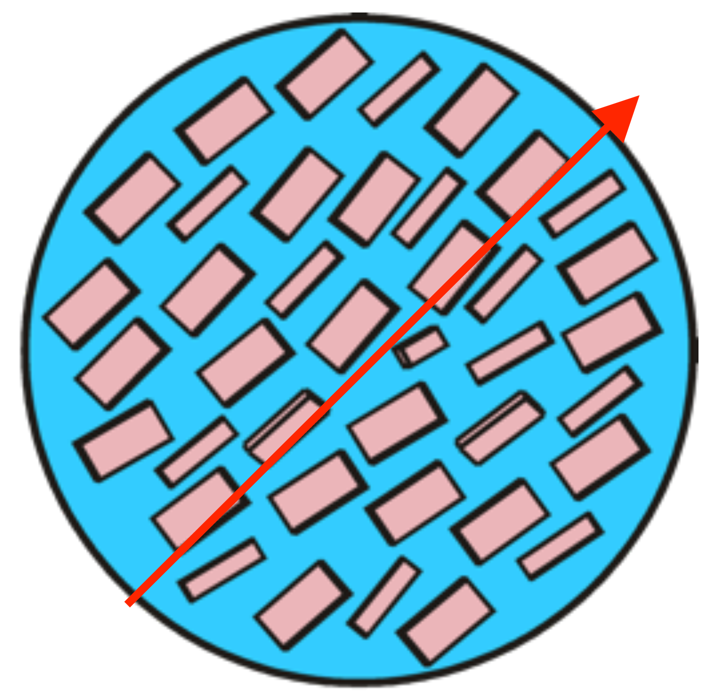


Texture Analysis



Texture Analysis





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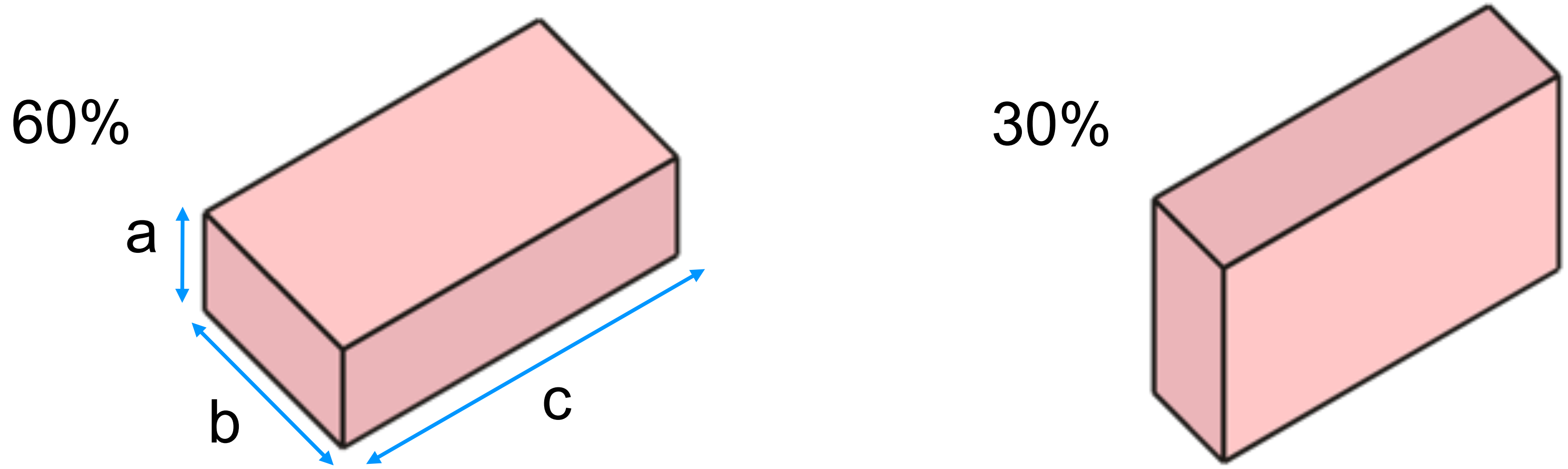

Texture Analysis

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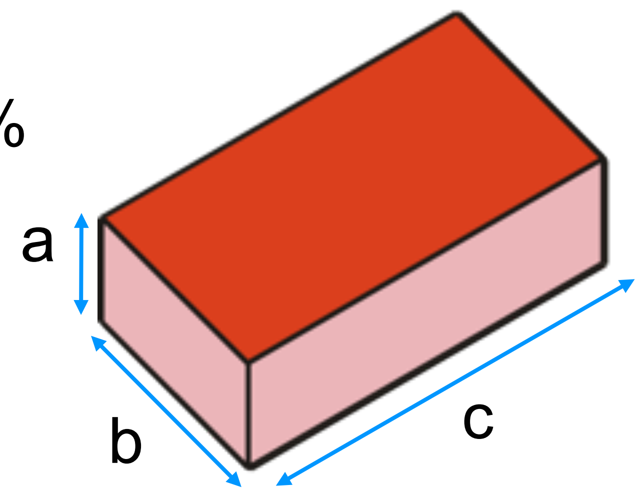

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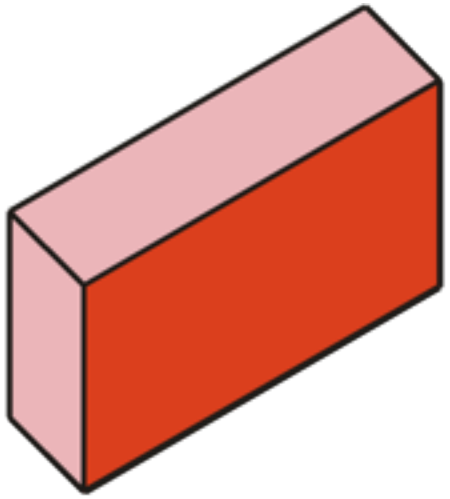
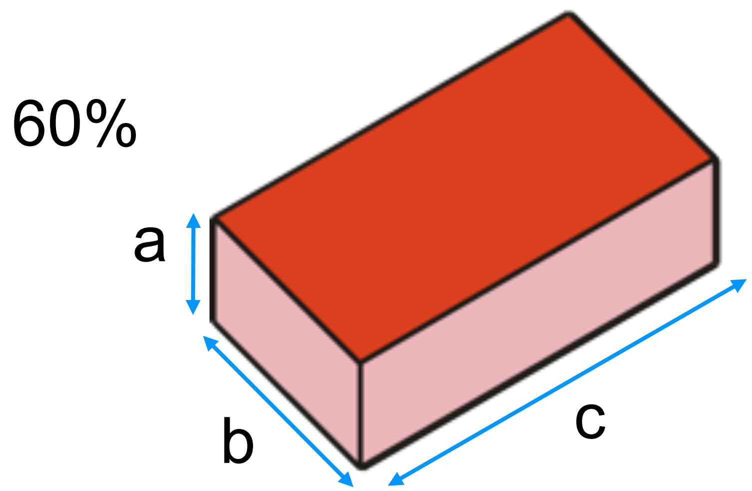
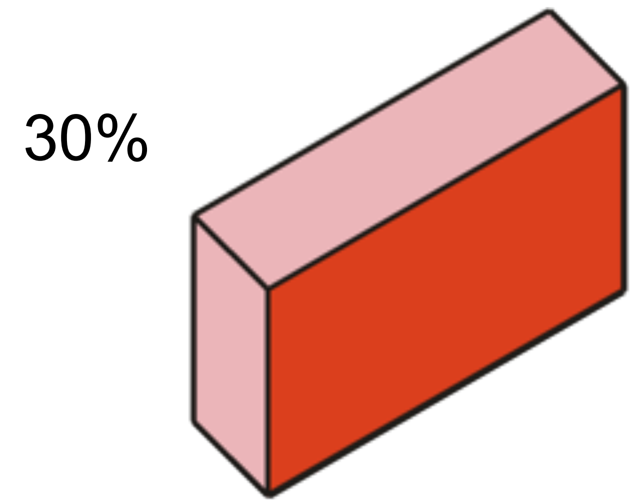
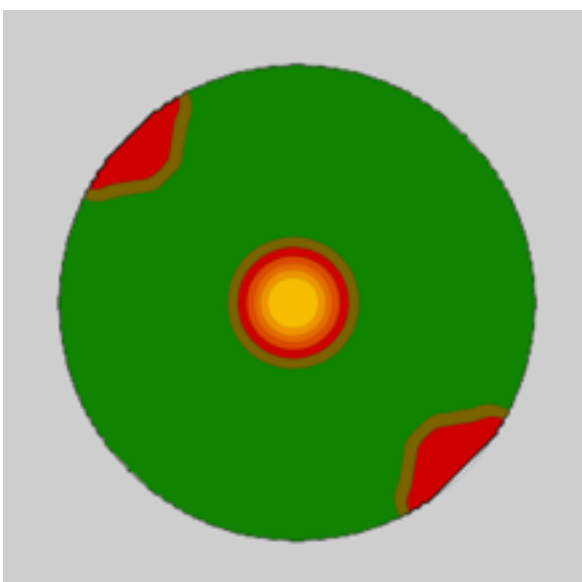


Texture Analysis







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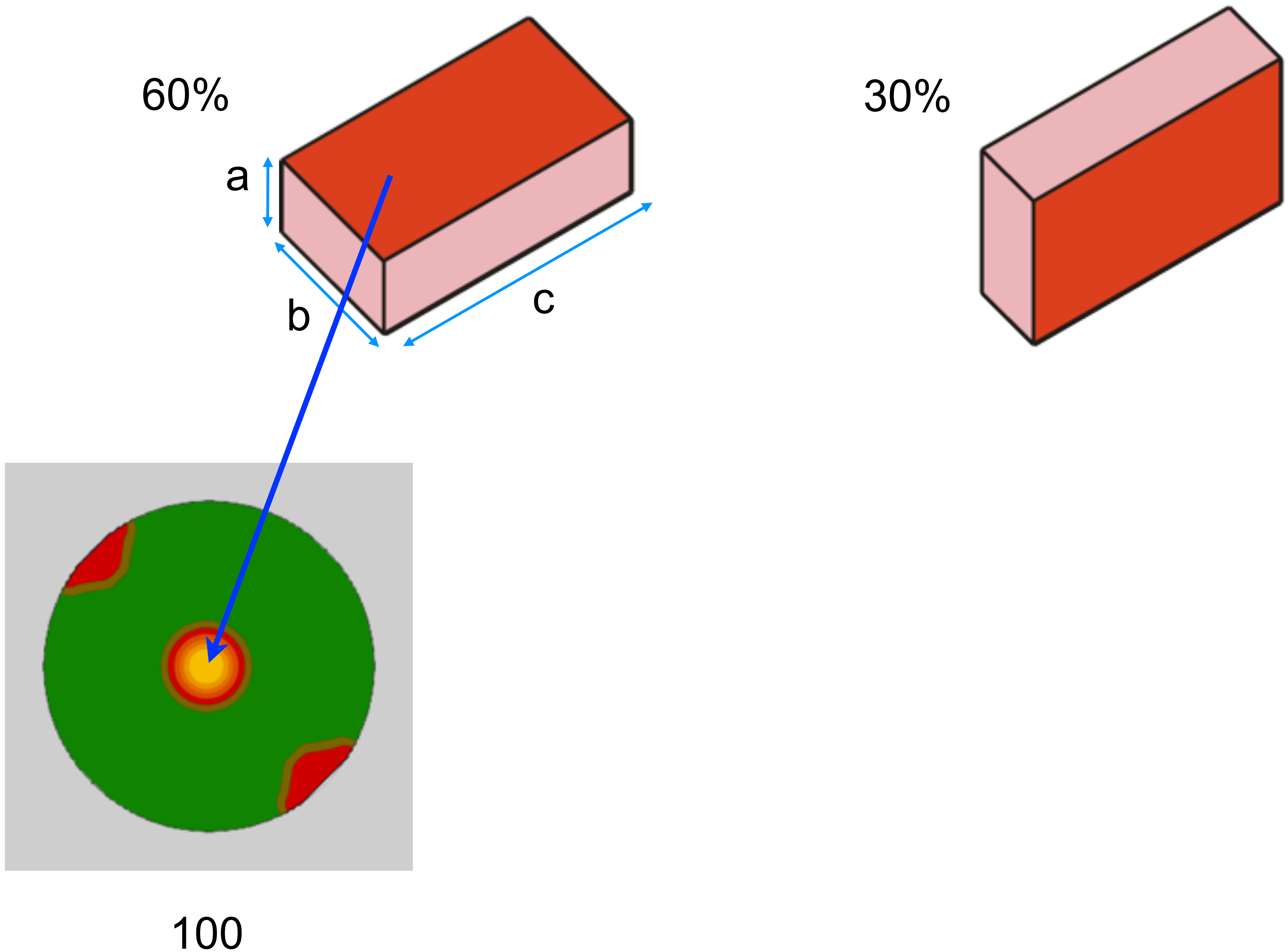
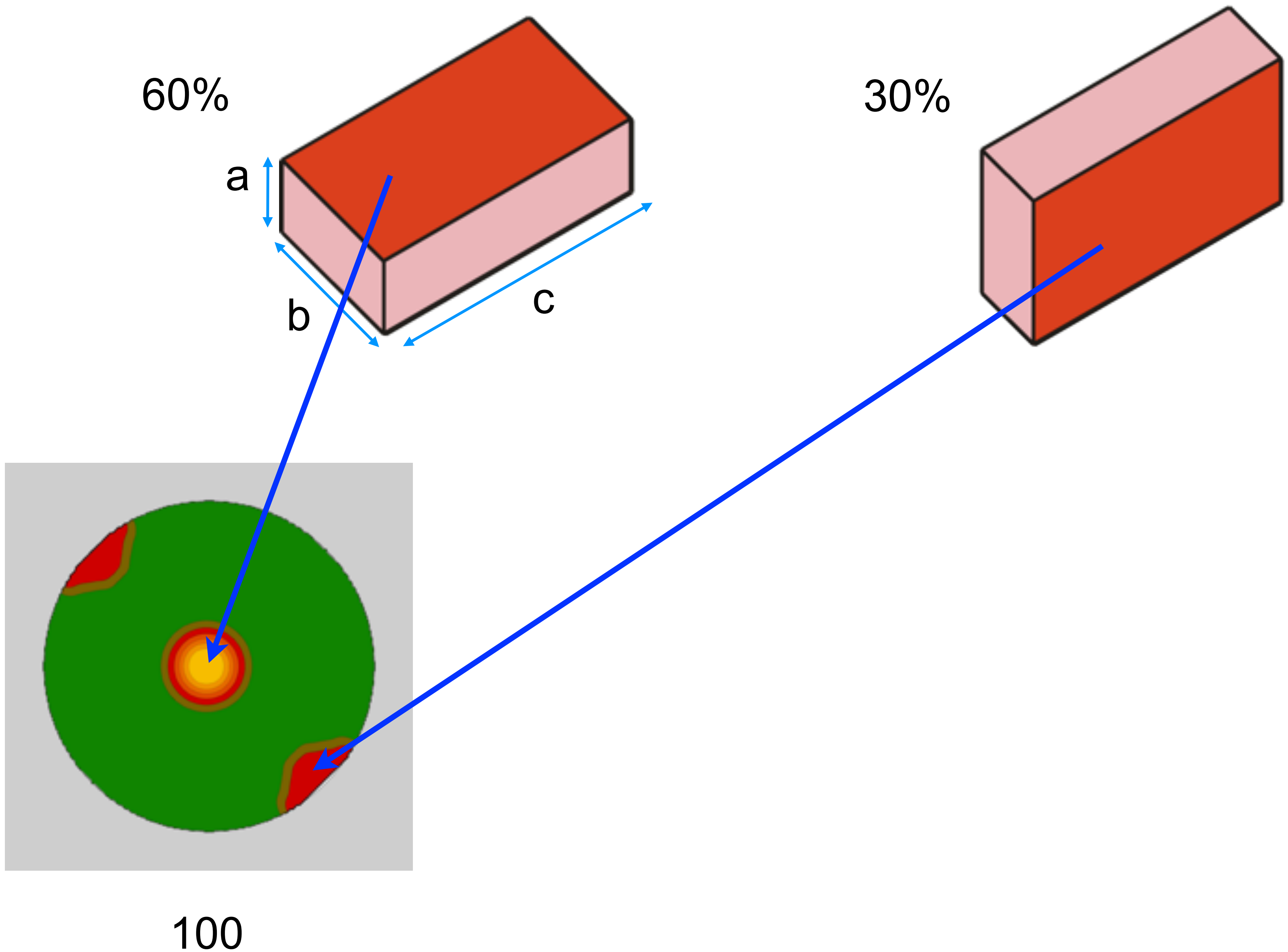
Texture Analysis



Texture Analysis



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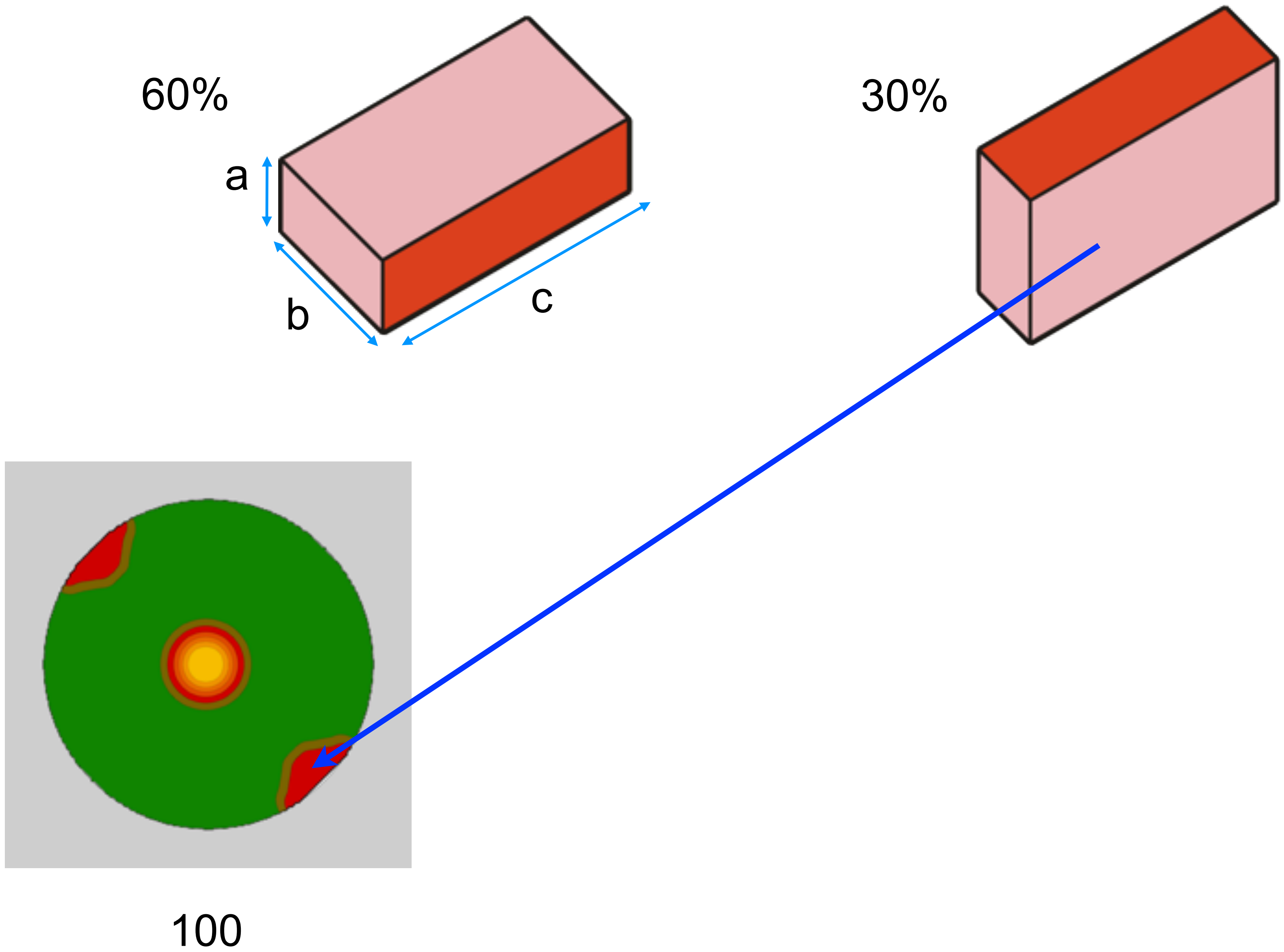

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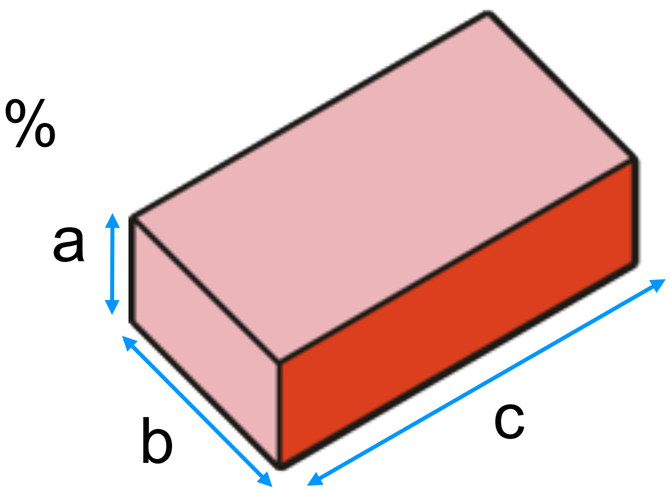

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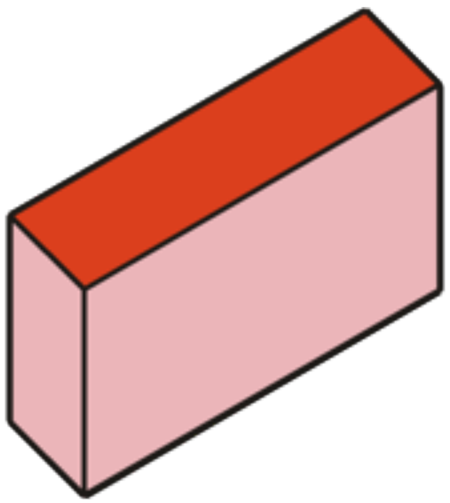

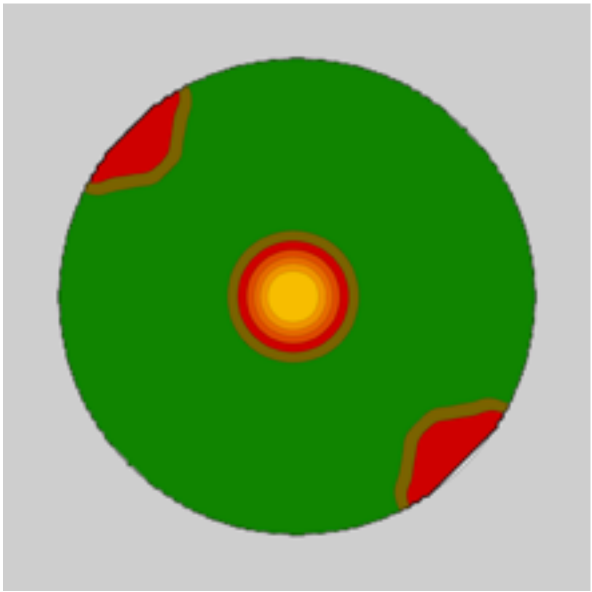

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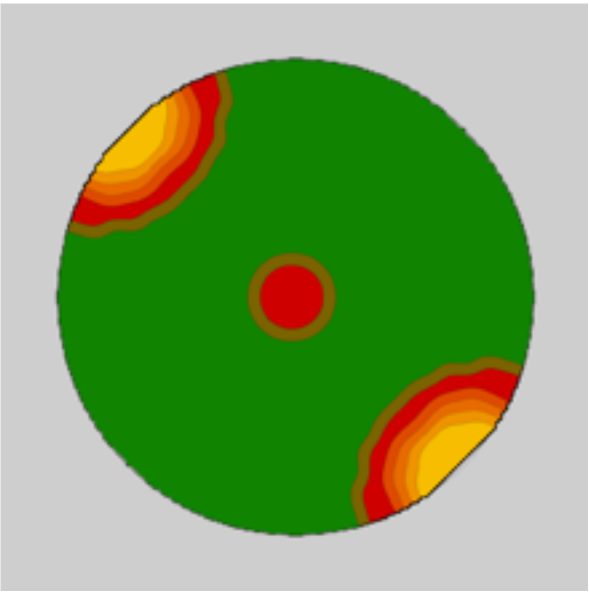
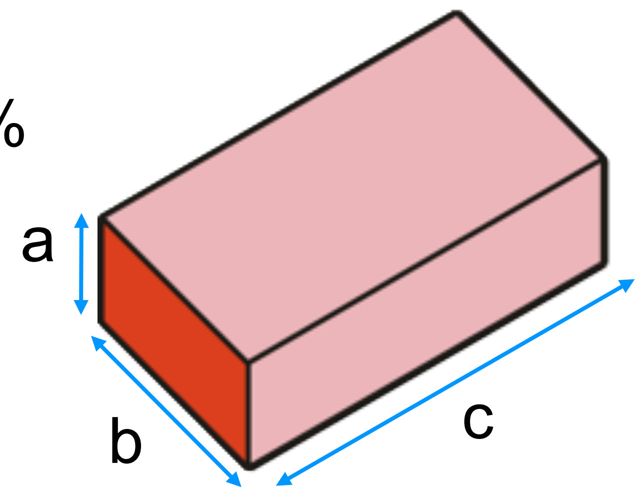


010

Texture Analysis

60%



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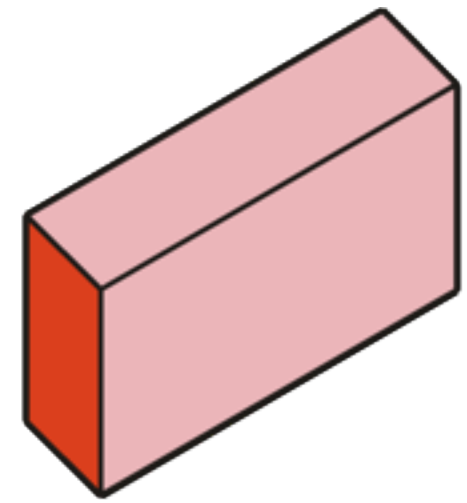

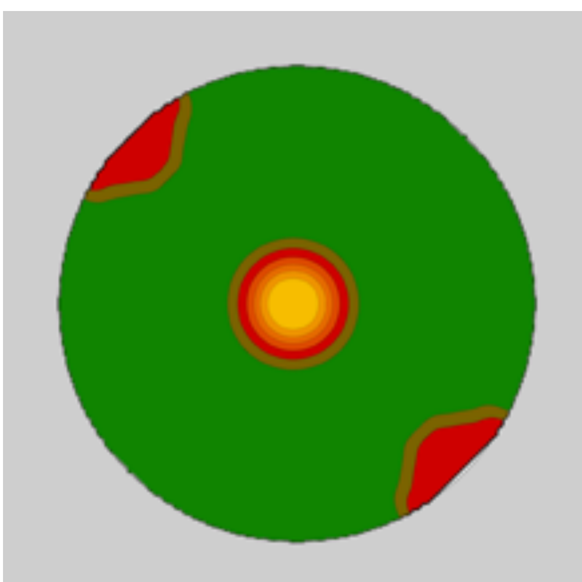

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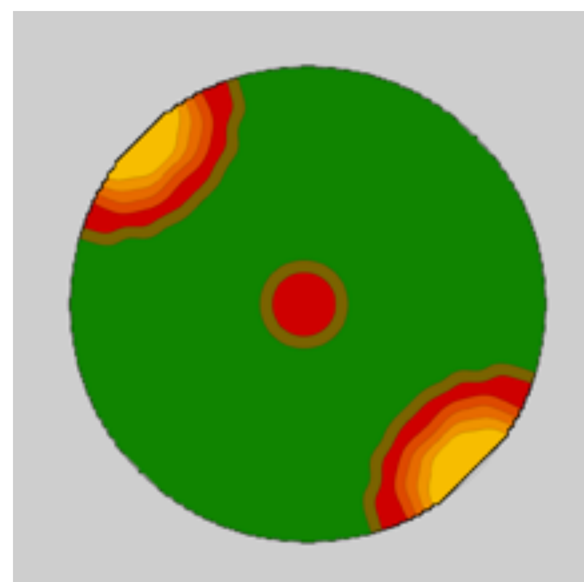

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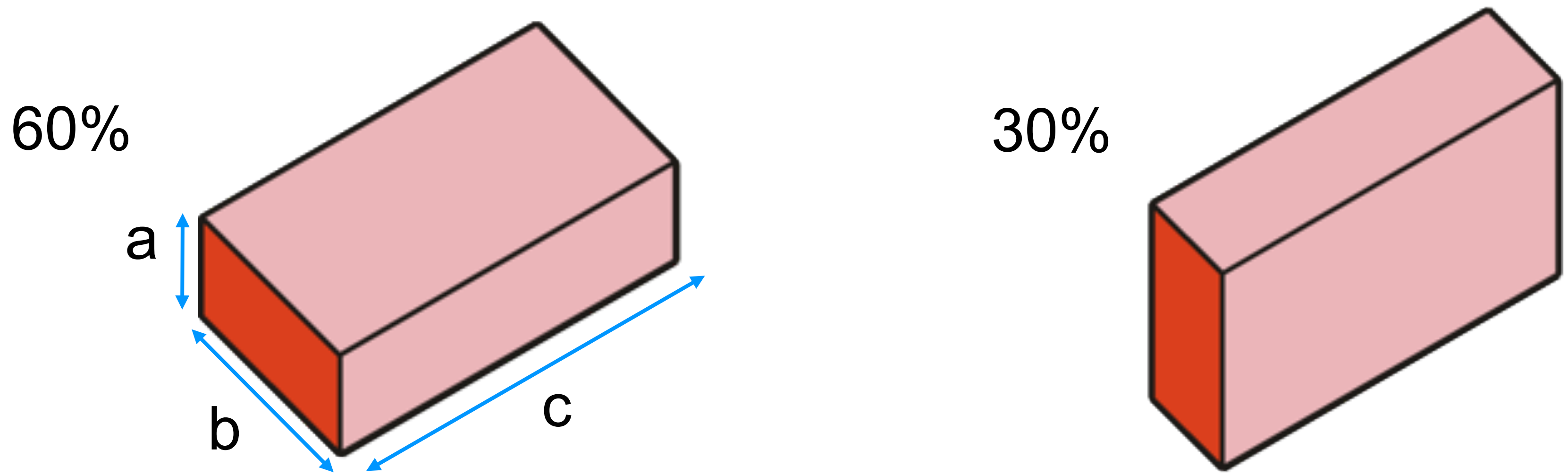
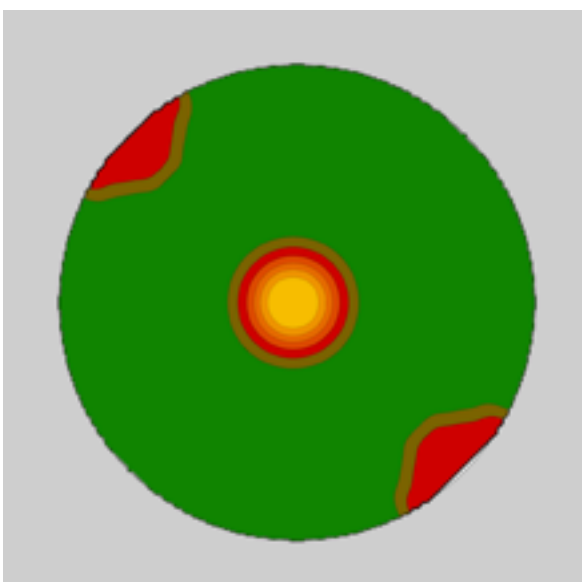
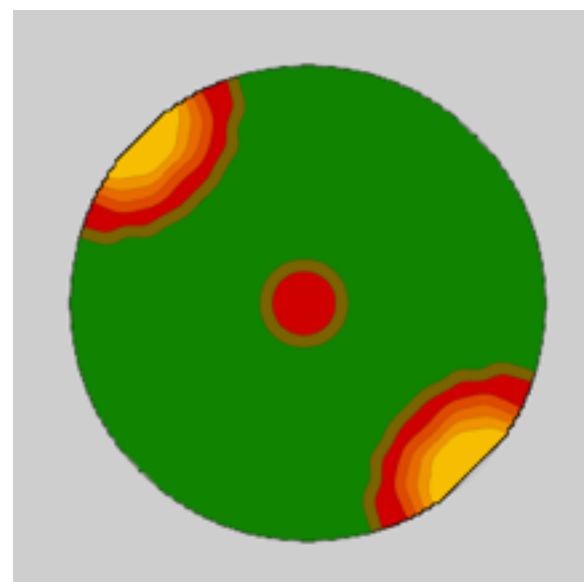
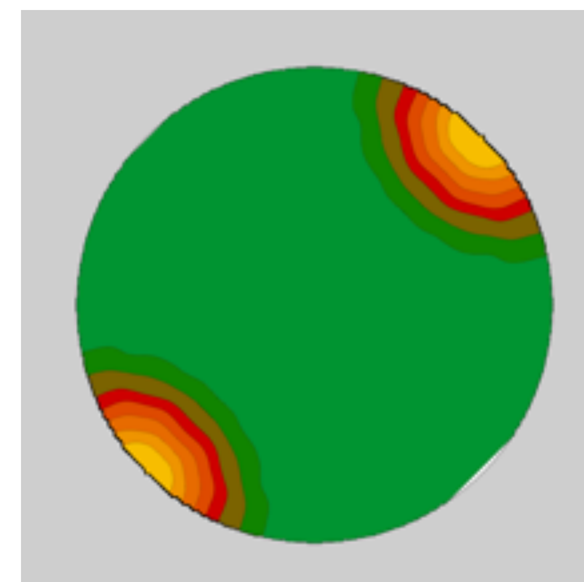




100

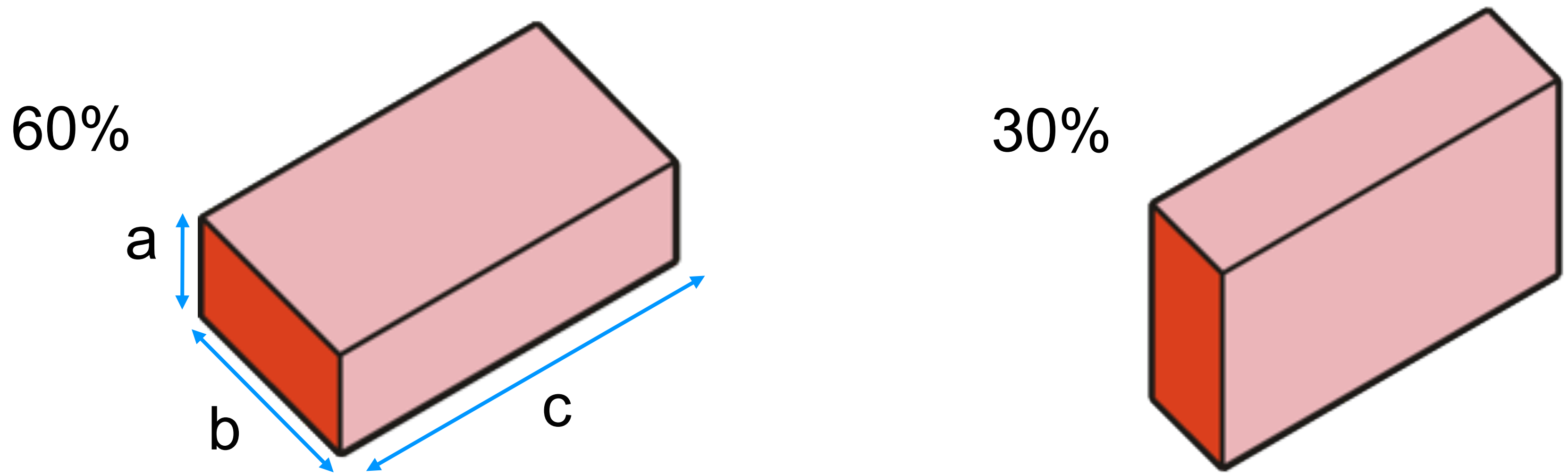


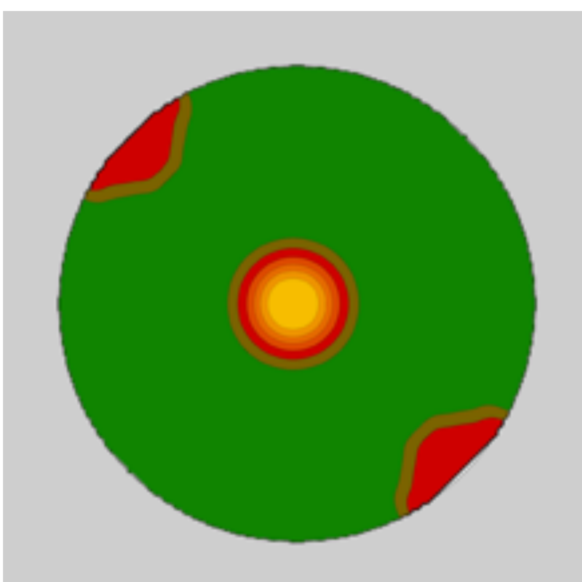
010



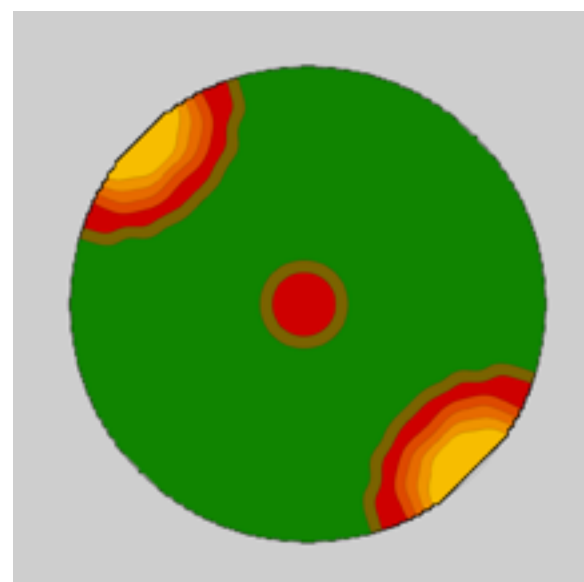
001

Texture Analysis

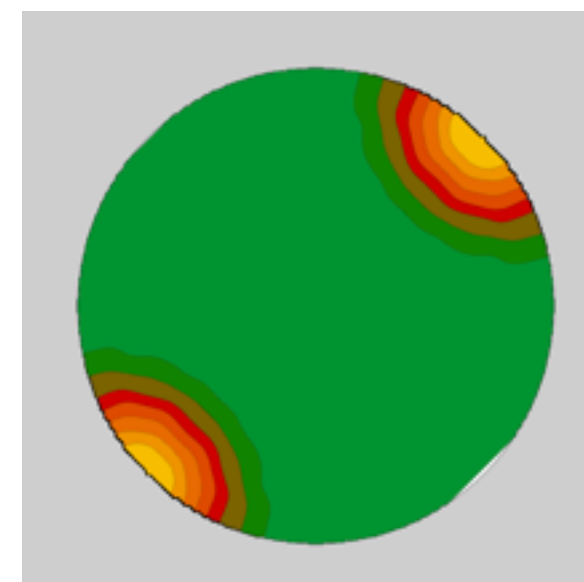




100



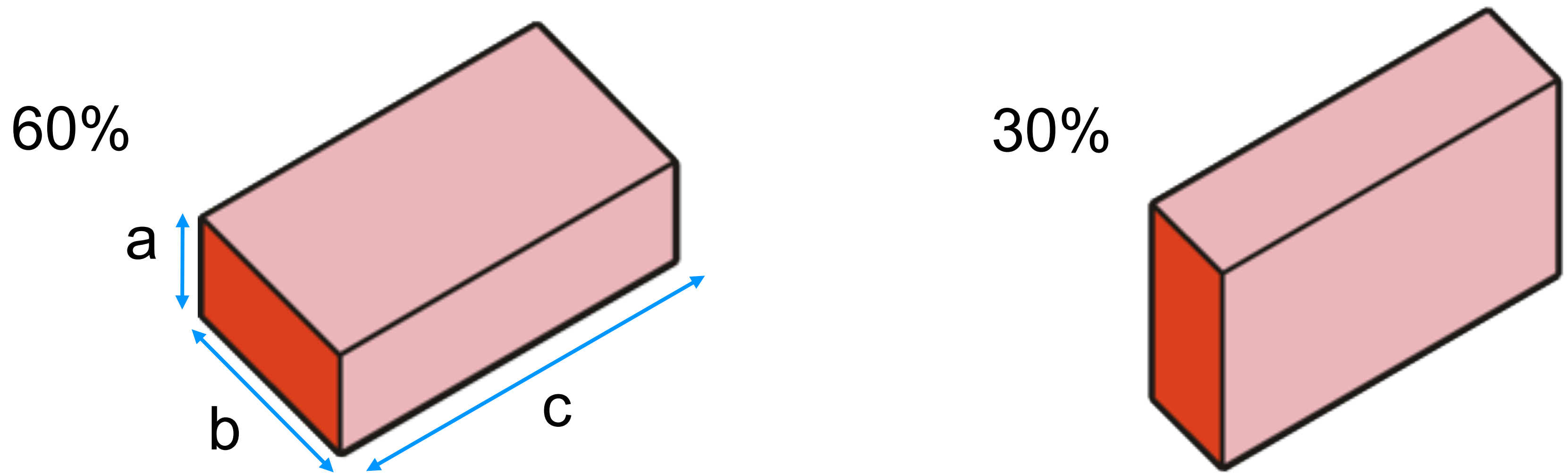
010

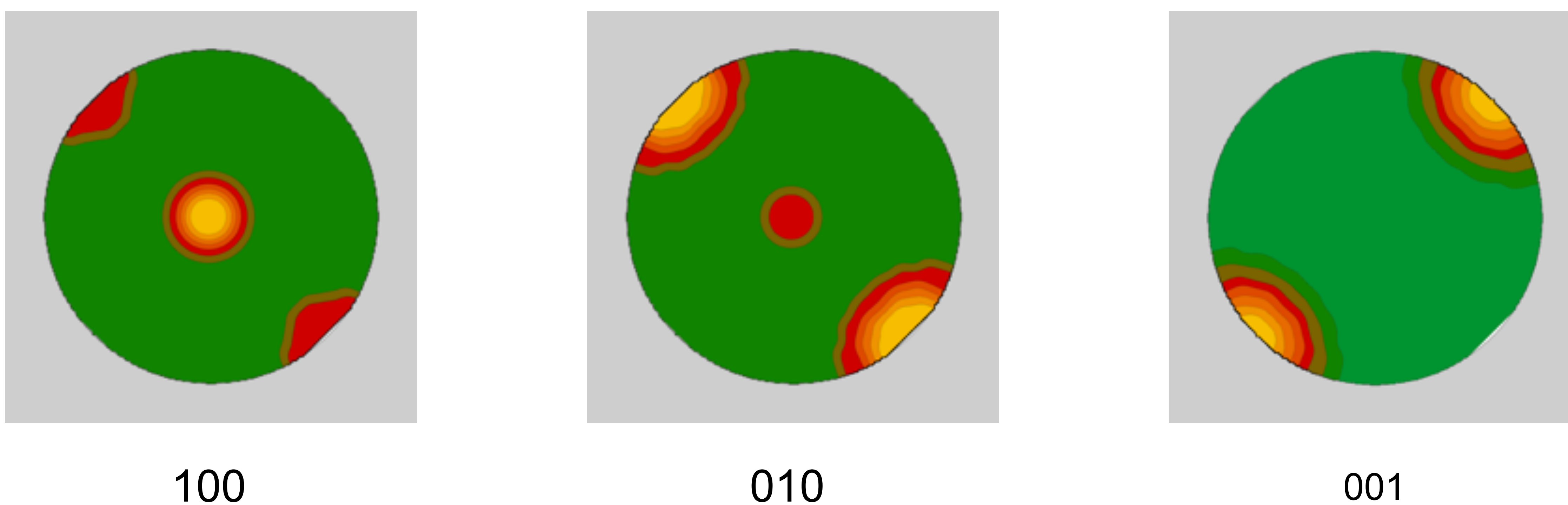


001

Pole figures are normalized $\rightarrow$ average value = 1

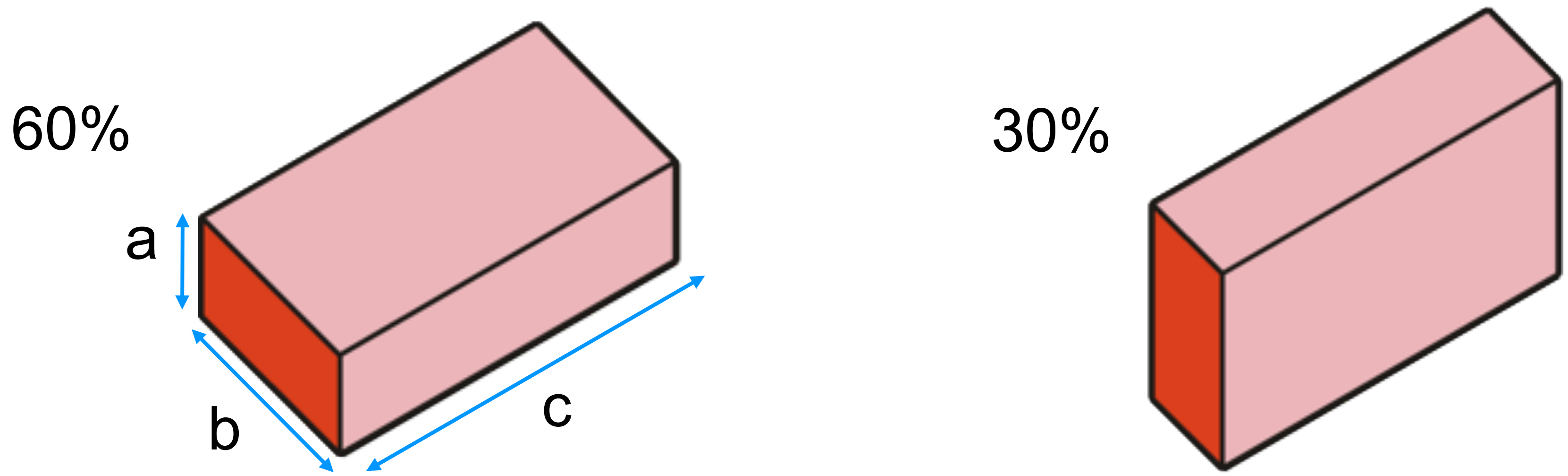
Texture Analysis

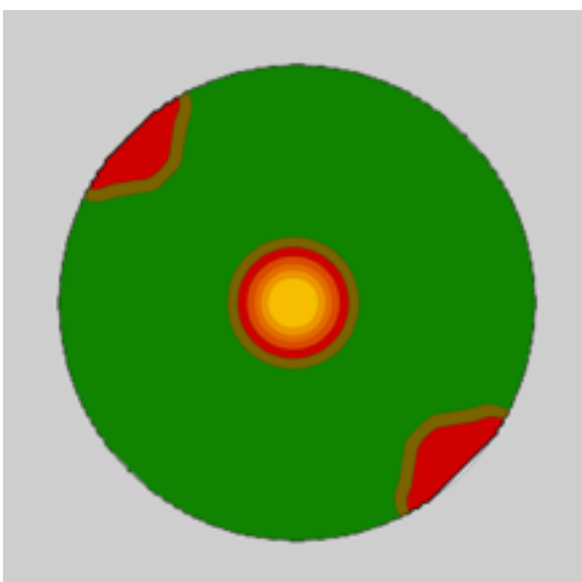




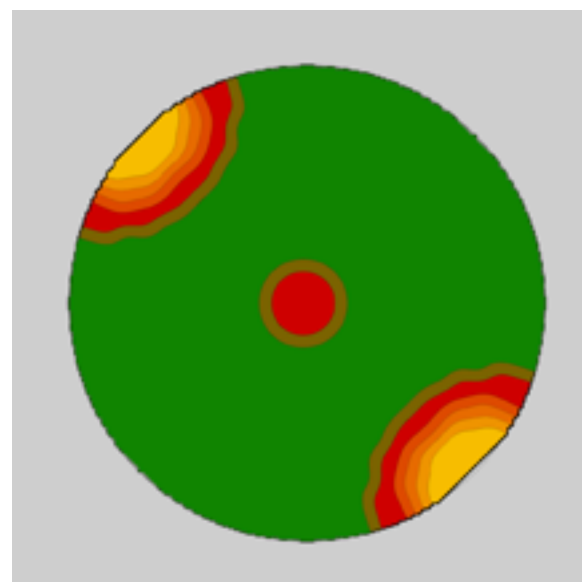
Pole figures are normalized → average value = 1
Calculate orientation distribution function (ODF) from these pole figures

Texture Analysis

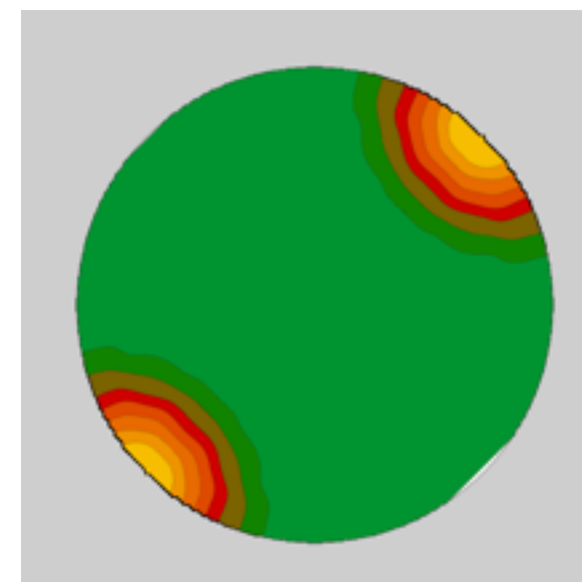




100



010



001

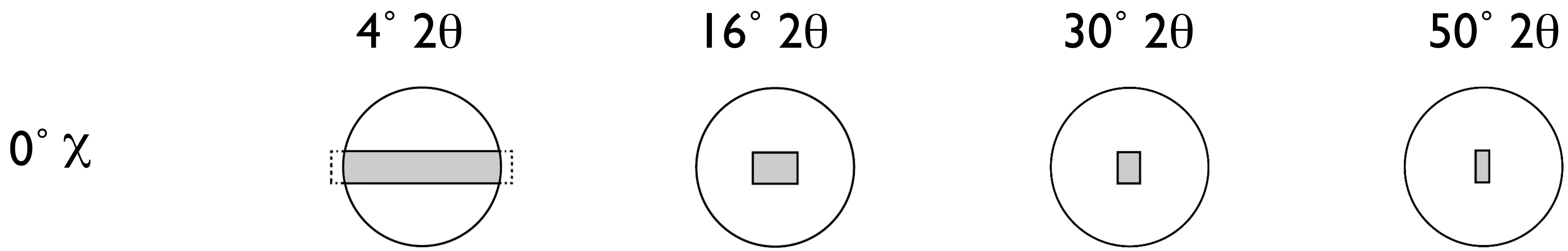
Pole figures are normalized $\rightarrow$ average value = 1

Calculate orientation distribution function (ODF) from these pole figures

From the ODF one can calculate the pole figures for any reflection

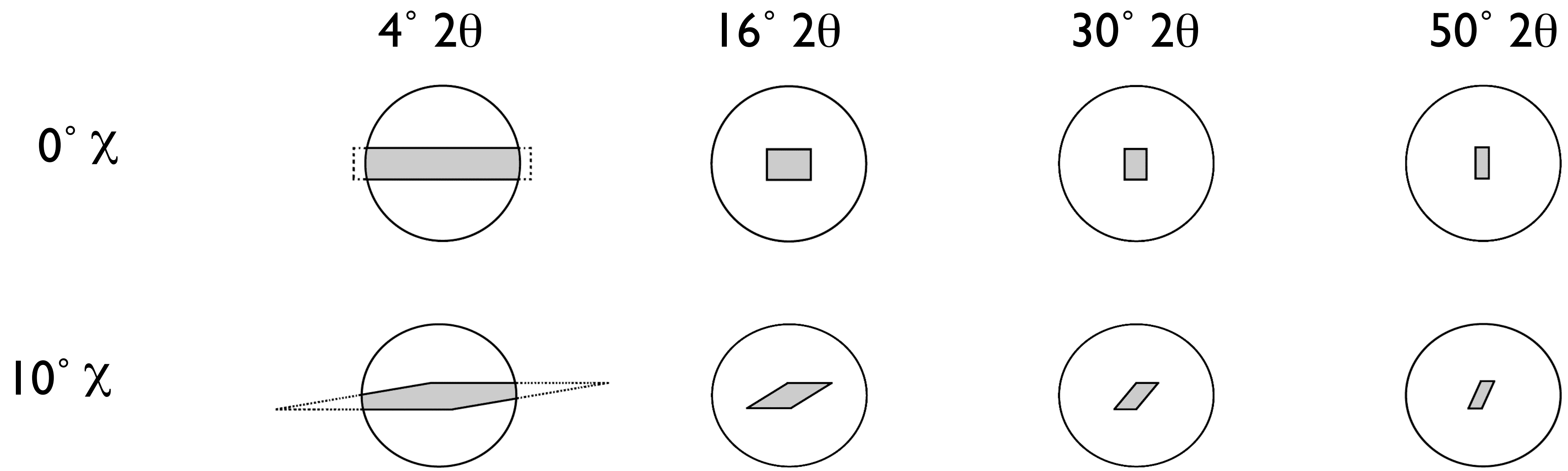
Effect of Tilt Angle in Reflection Mode

Footprint of the X-ray beam on sample



Effect of Tilt Angle in Reflection Mode

Footprint of the X-ray beam on sample



Effect of Tilt Angle in Reflection Mode

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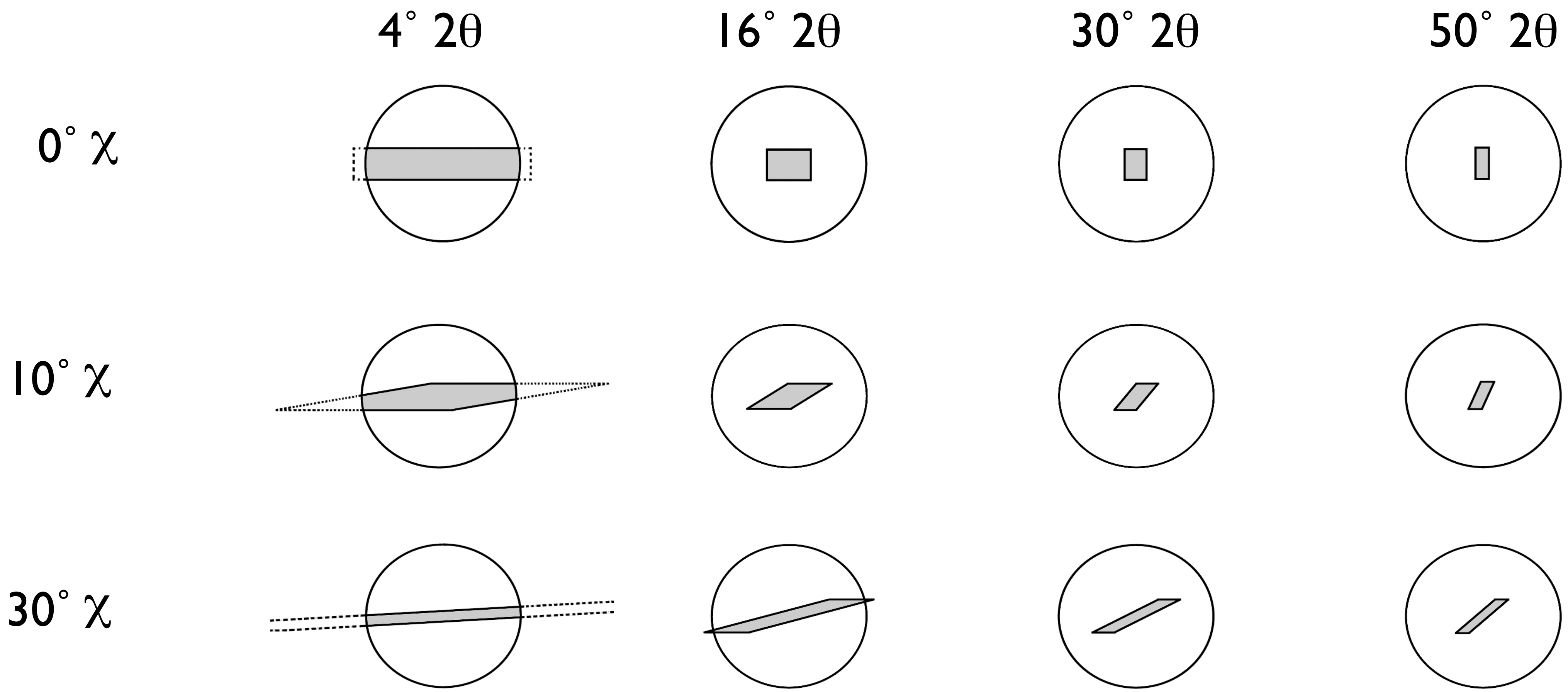
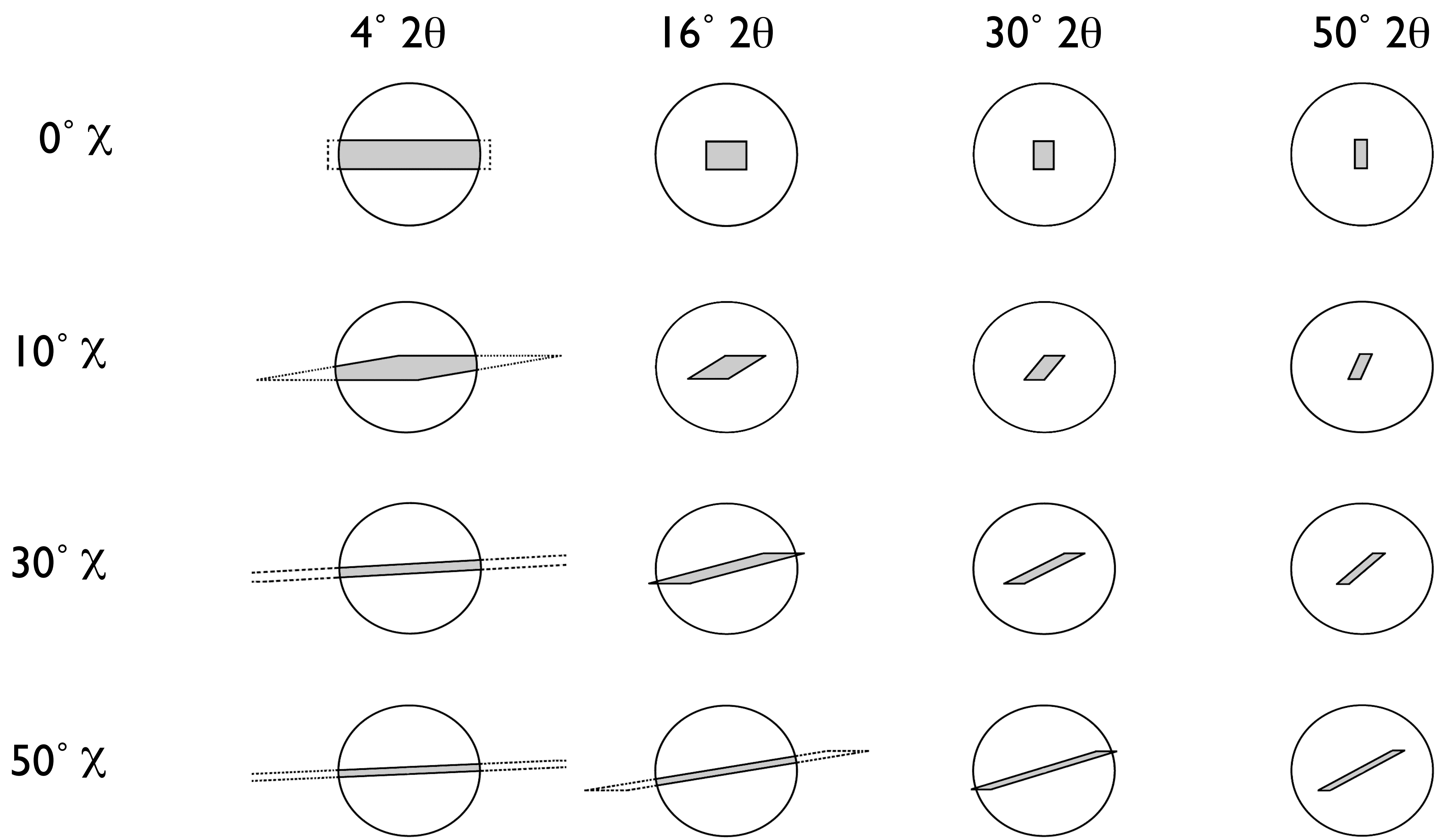


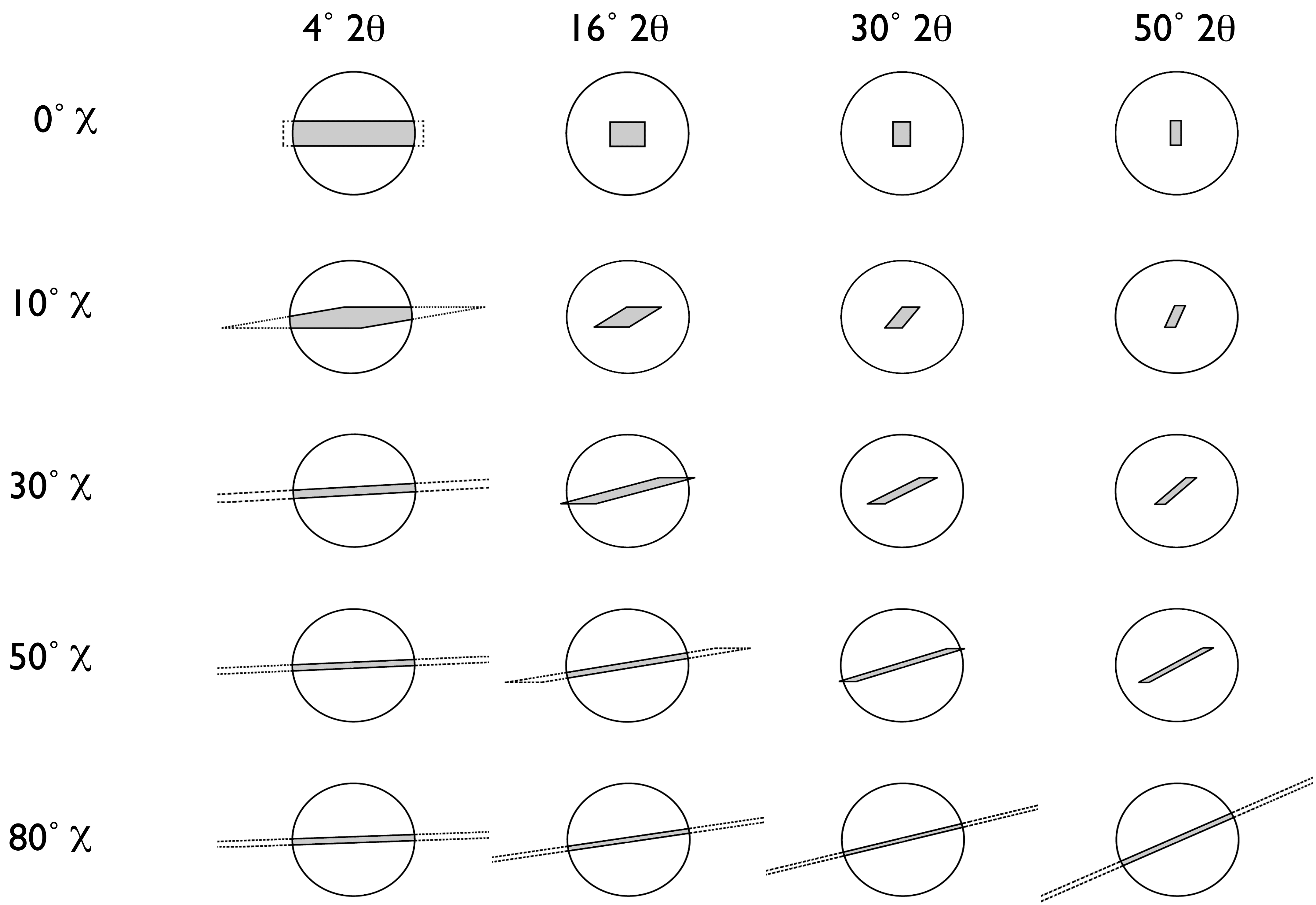
Effect of Tilt Angle in Reflection Mode

Footprint of the X-ray beam on sample

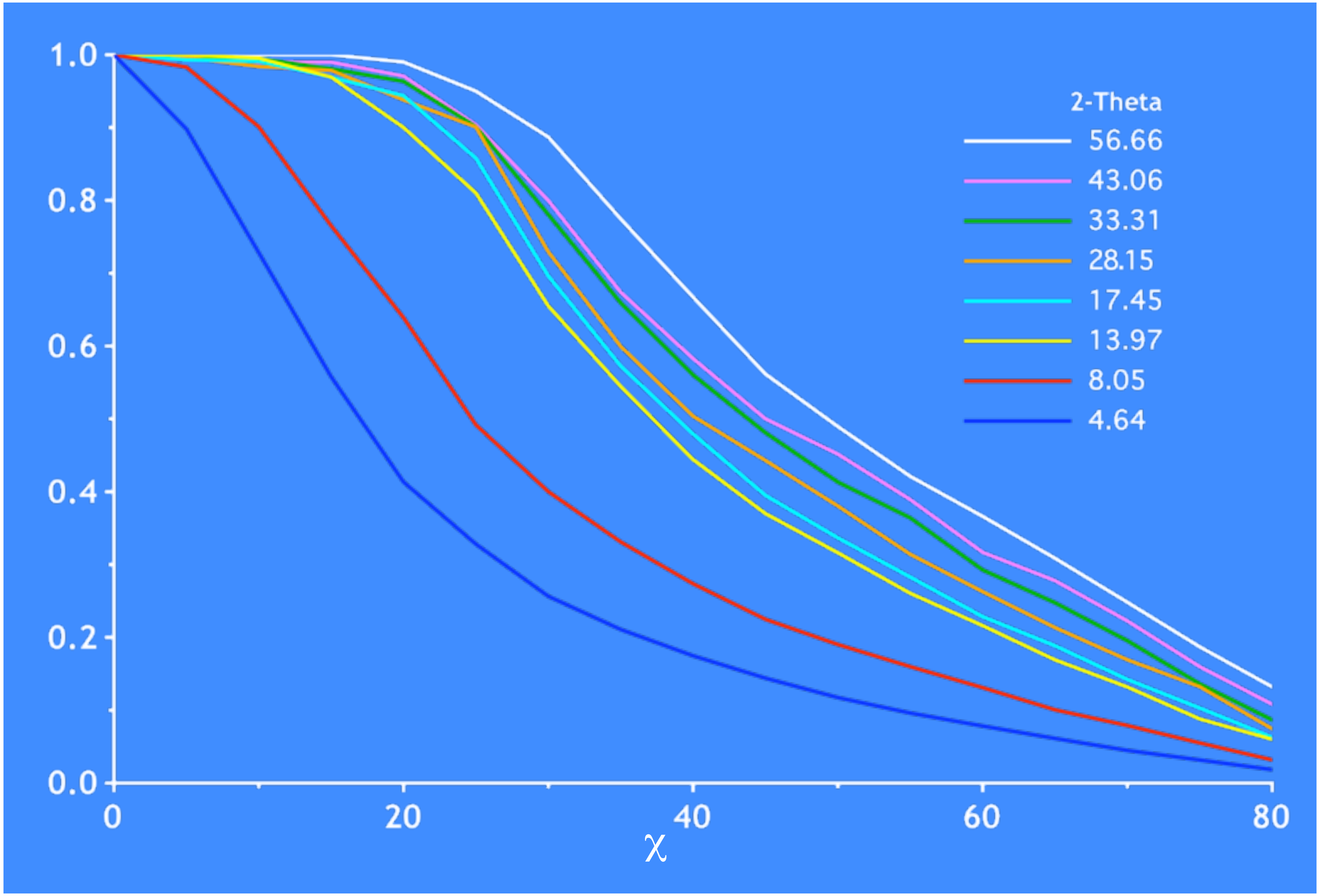


Effect of Tilt Angle in Reflection Mode

Footprint of the X-ray beam on sample

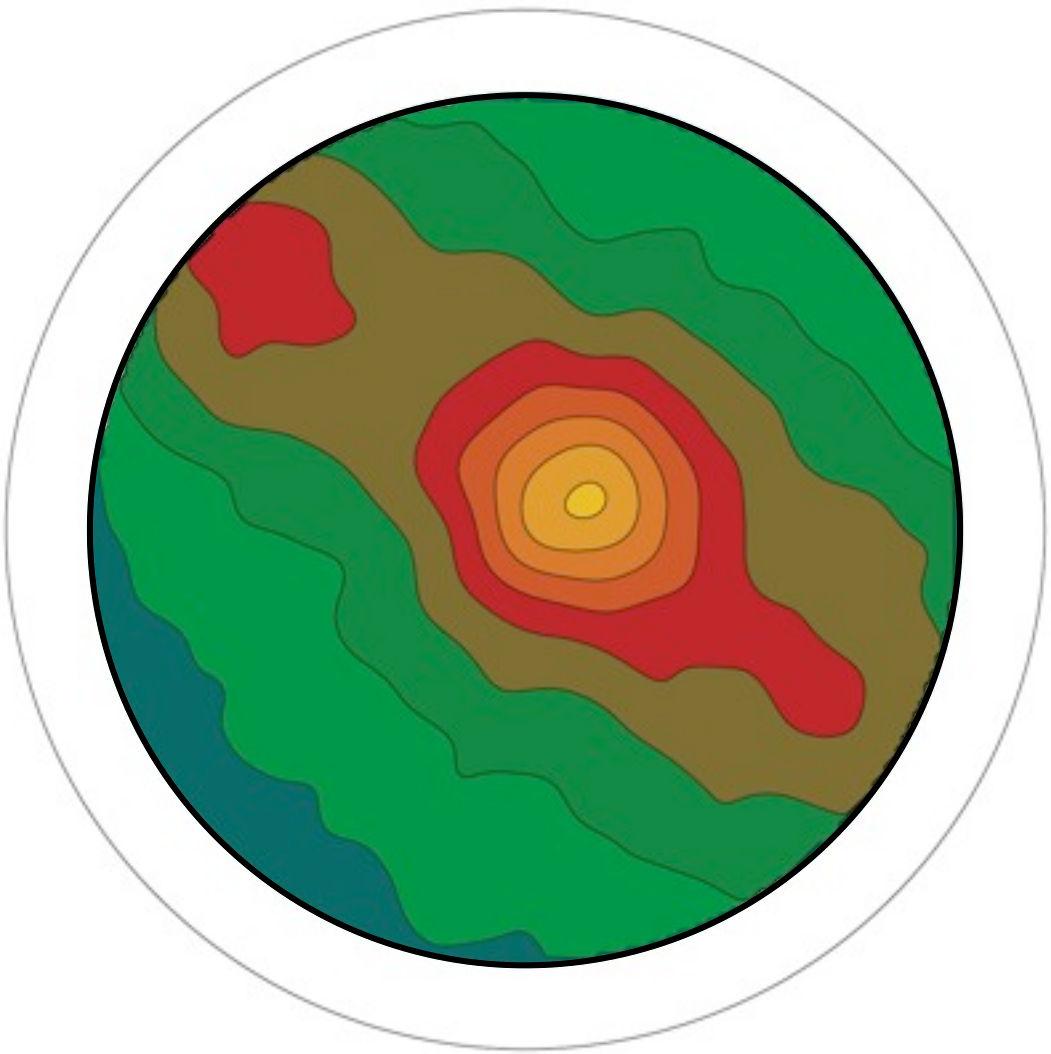


Tilt Angle Correction in Reflection Mode



Effect of Tilt Angle Correction in Reflection Mode

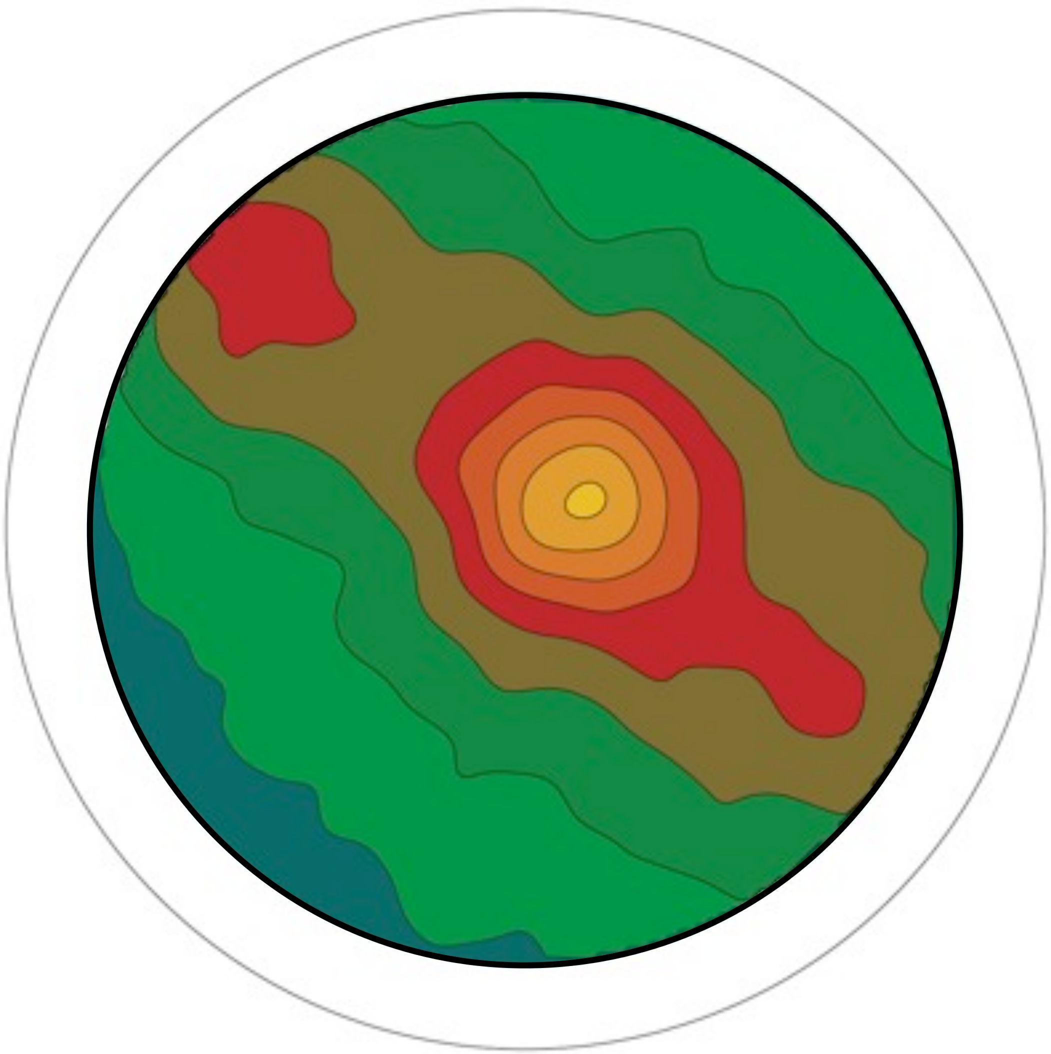
Pole figure for the 102 Reflection of ZSM-5



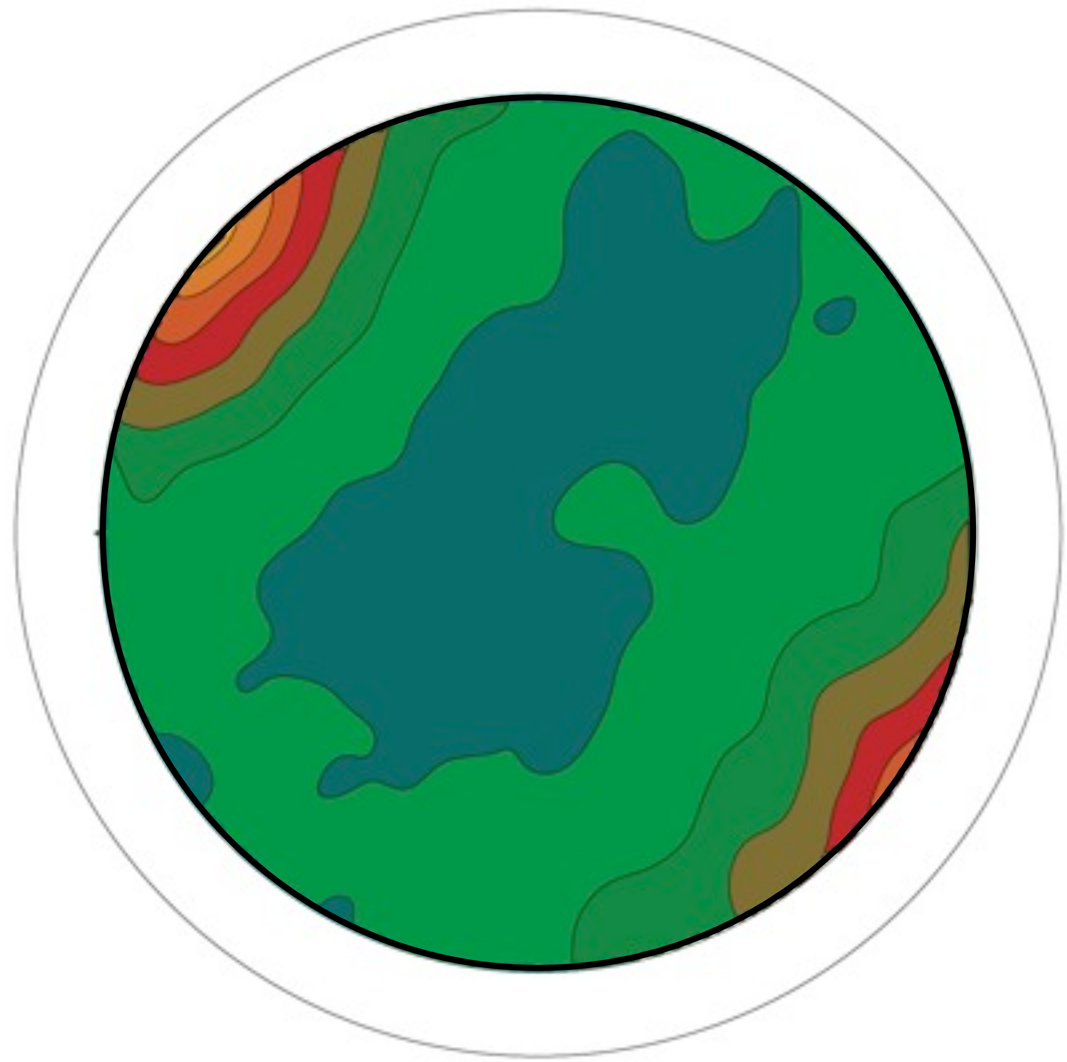
no tilt correction

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

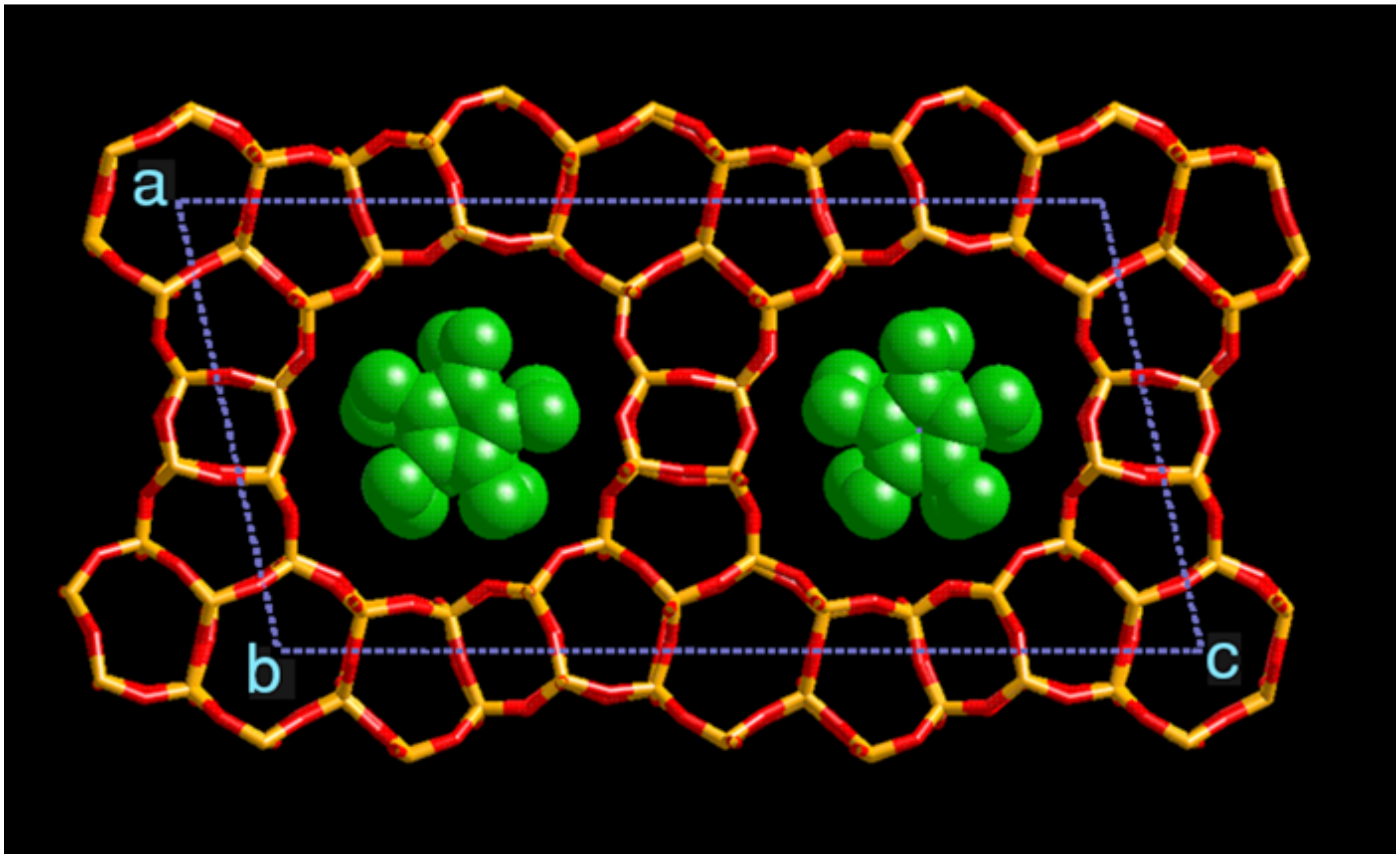
Space Group	$P2_1/c$
a	14.9701 Å
b	8.4761 Å
c	30.0278 Å
β	102.65°

Data Collection (reflection mode)

Pole figures (for ODF)	7
Full powder patterns for intensity extraction	5

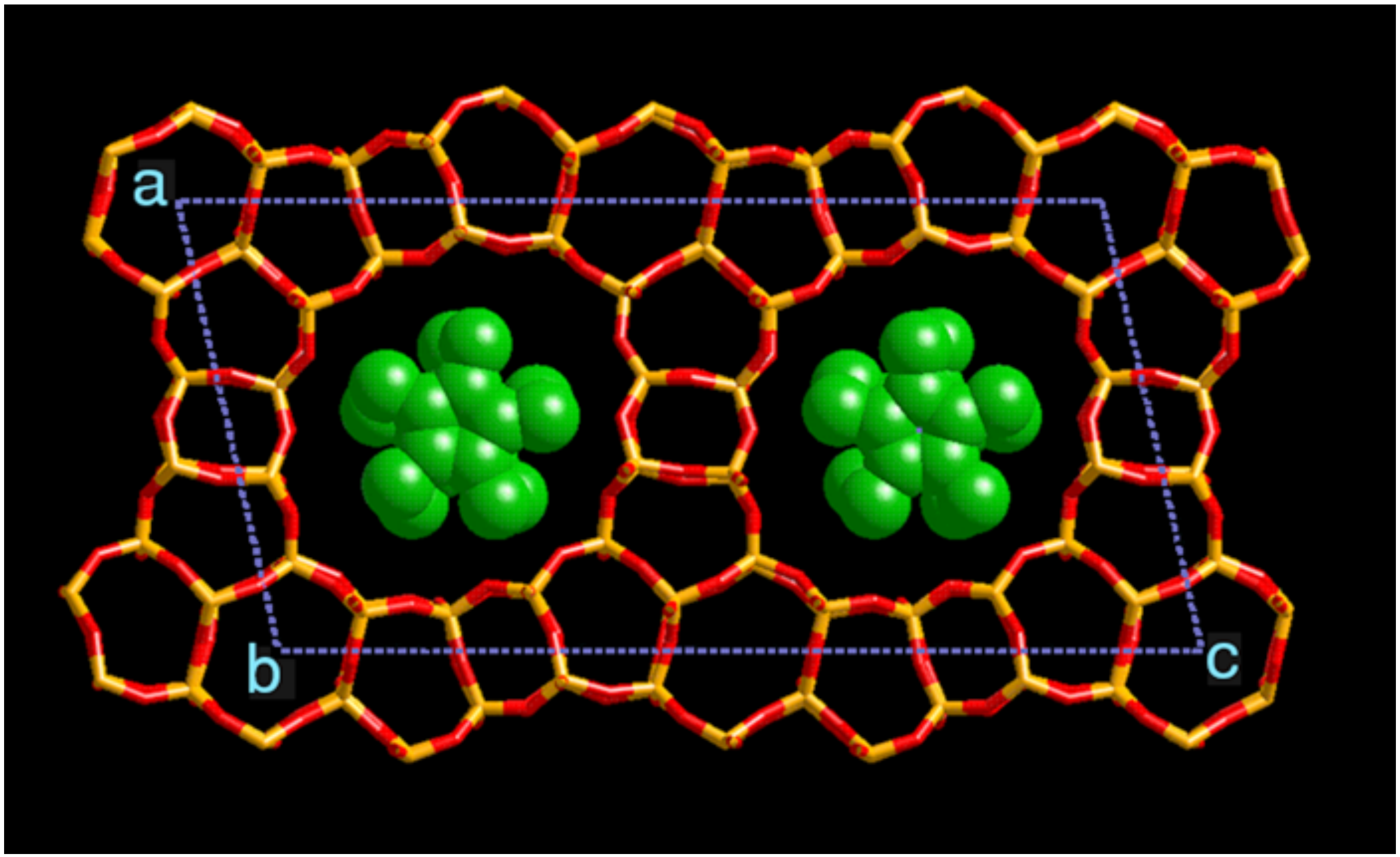
Does it work?

High-silica zeolite UTD-1F



Does it work?

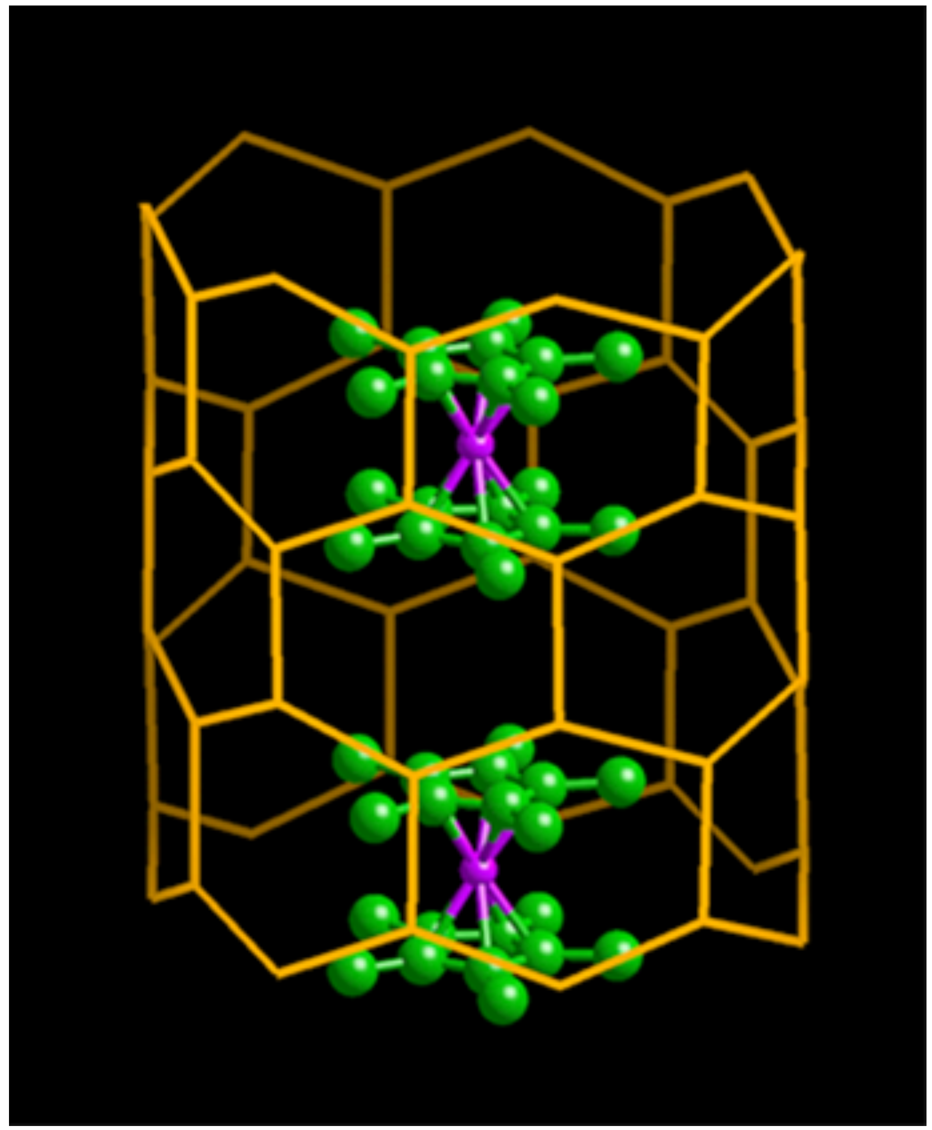
High-silica zeolite UTD-1F



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

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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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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)

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

15 O and $Co(Cp^*)_2^+$ found in difference Fourier map

Structure Refinement (Rietveld method)

non-centrosymmetric Pc

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

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

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

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

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Sample

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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

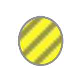
→ ca. 3 days per sample

Transmission mode - experimental setup

Area detector

Transmission mode - experimental setup

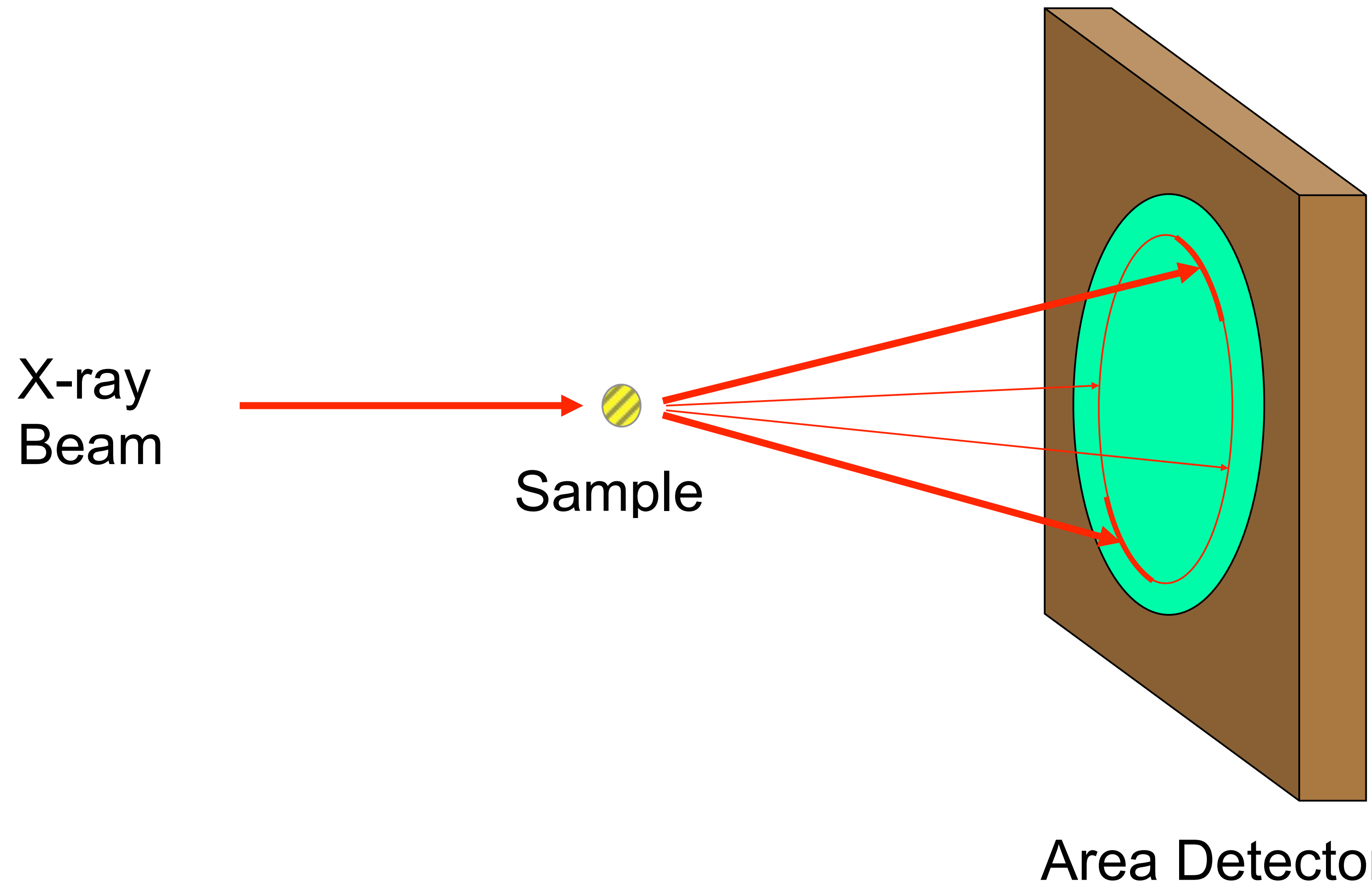
Area detector



Sample

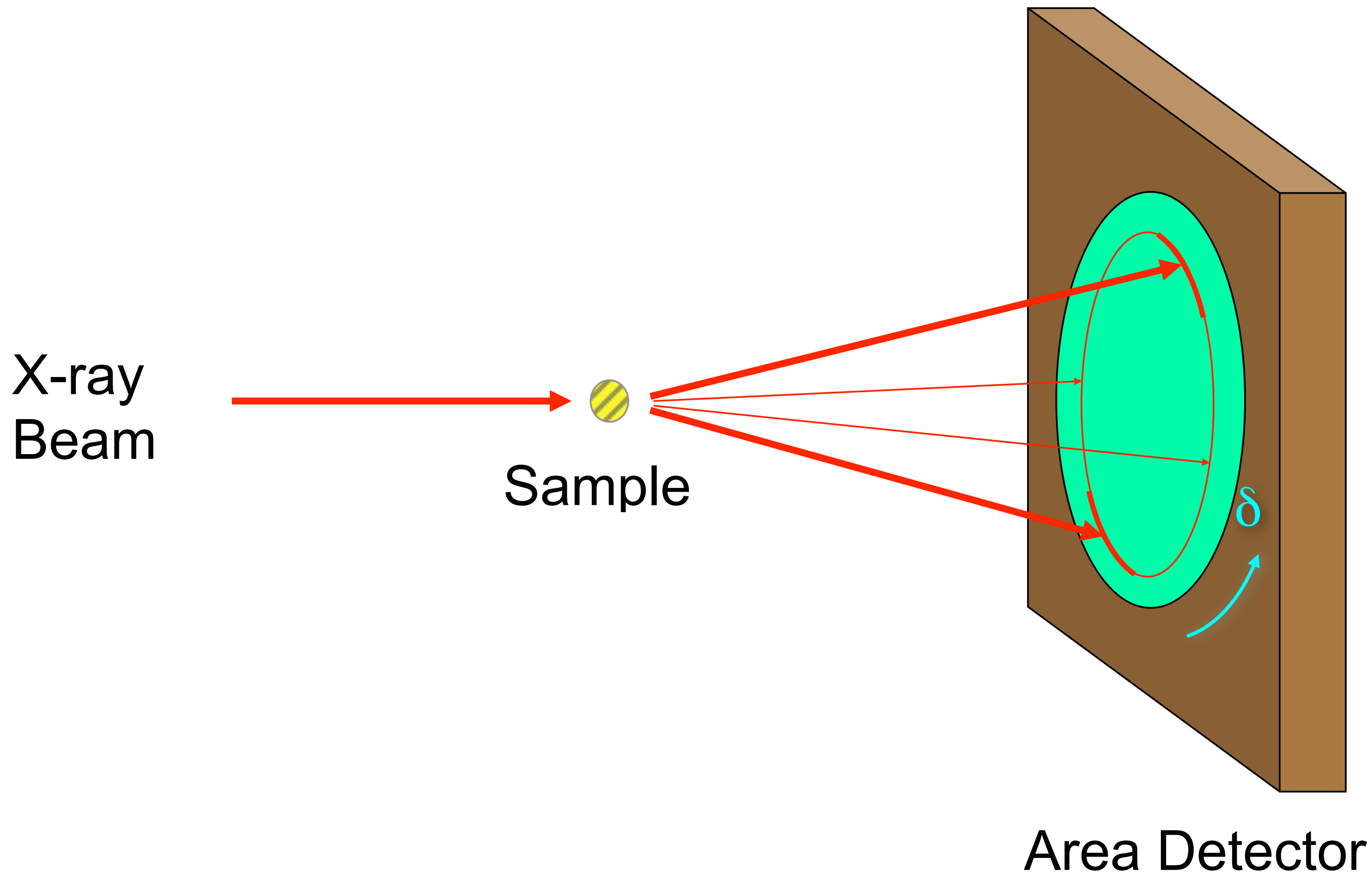
Transmission mode - experimental setup

Area detector



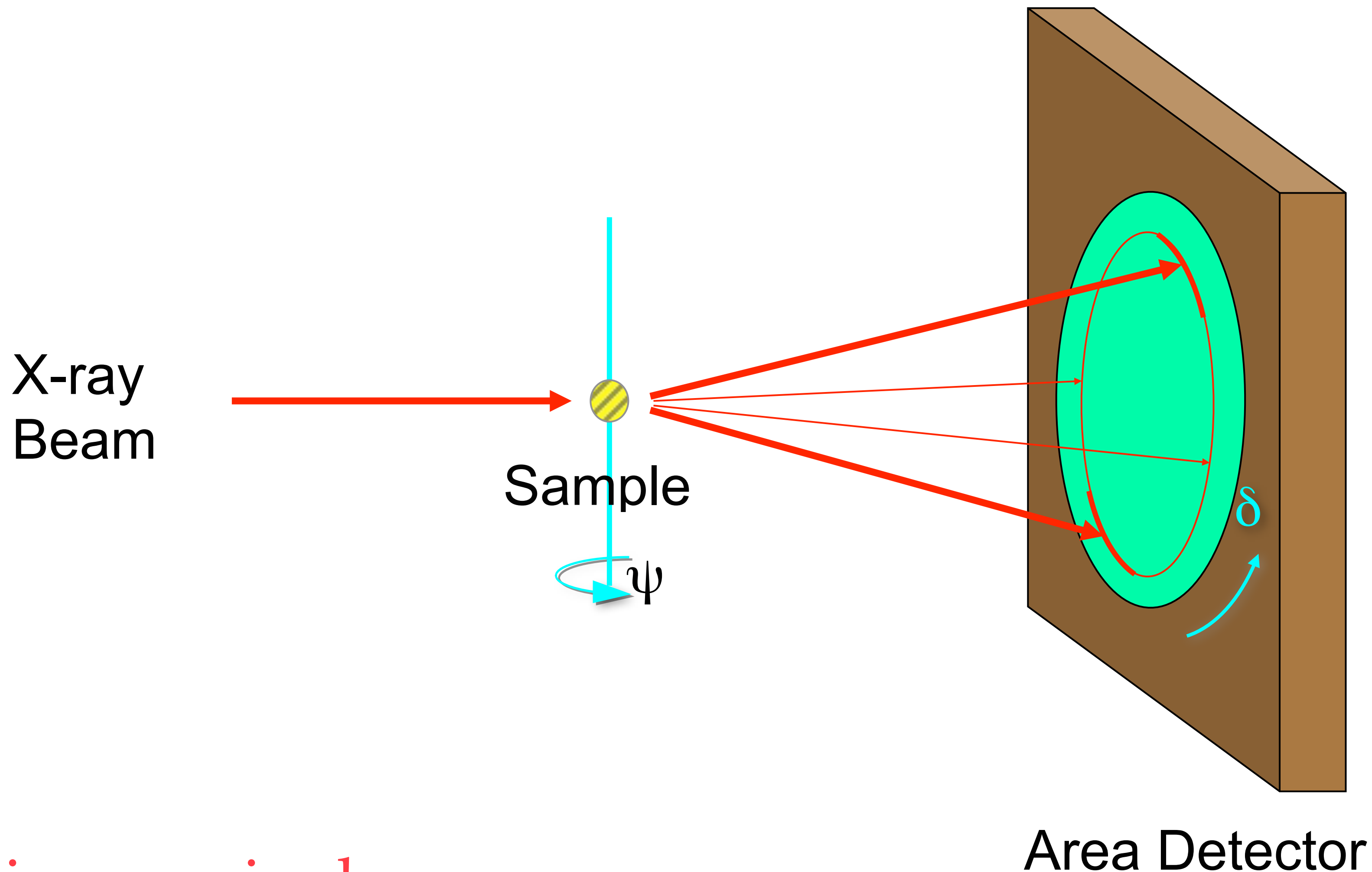
Transmission mode - experimental setup

Area detector



Transmission mode - experimental setup

Area detector



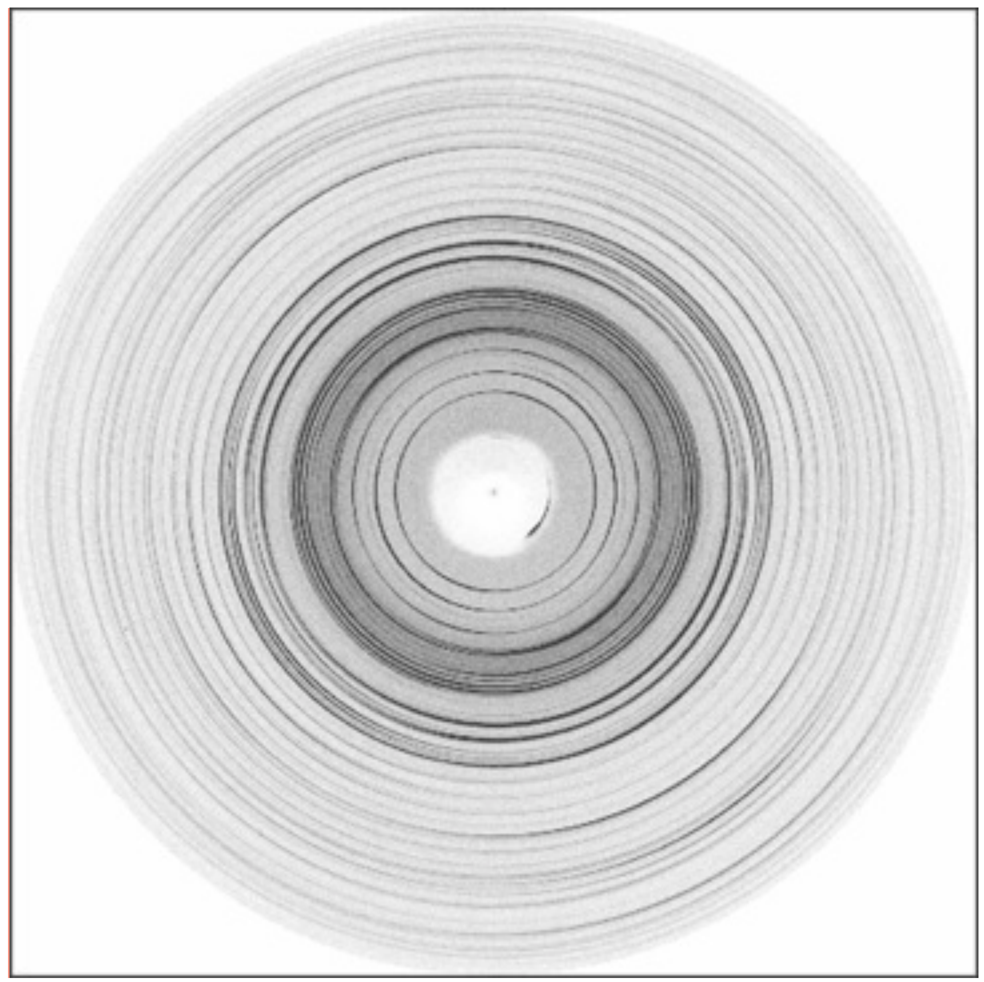
Only one rotation required
5° steps

Transmission mode with area detector

Data analysis

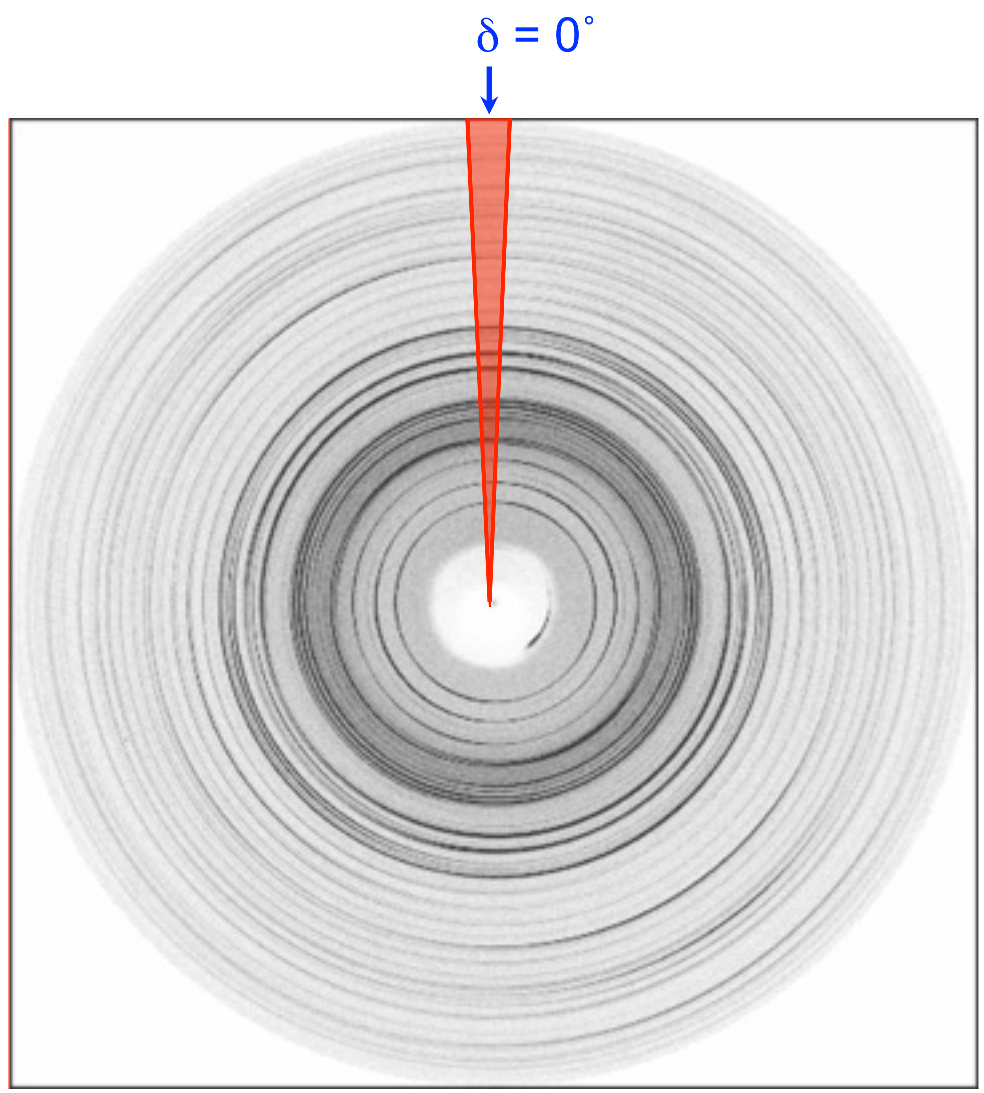
Transmission mode with area detector

Data analysis



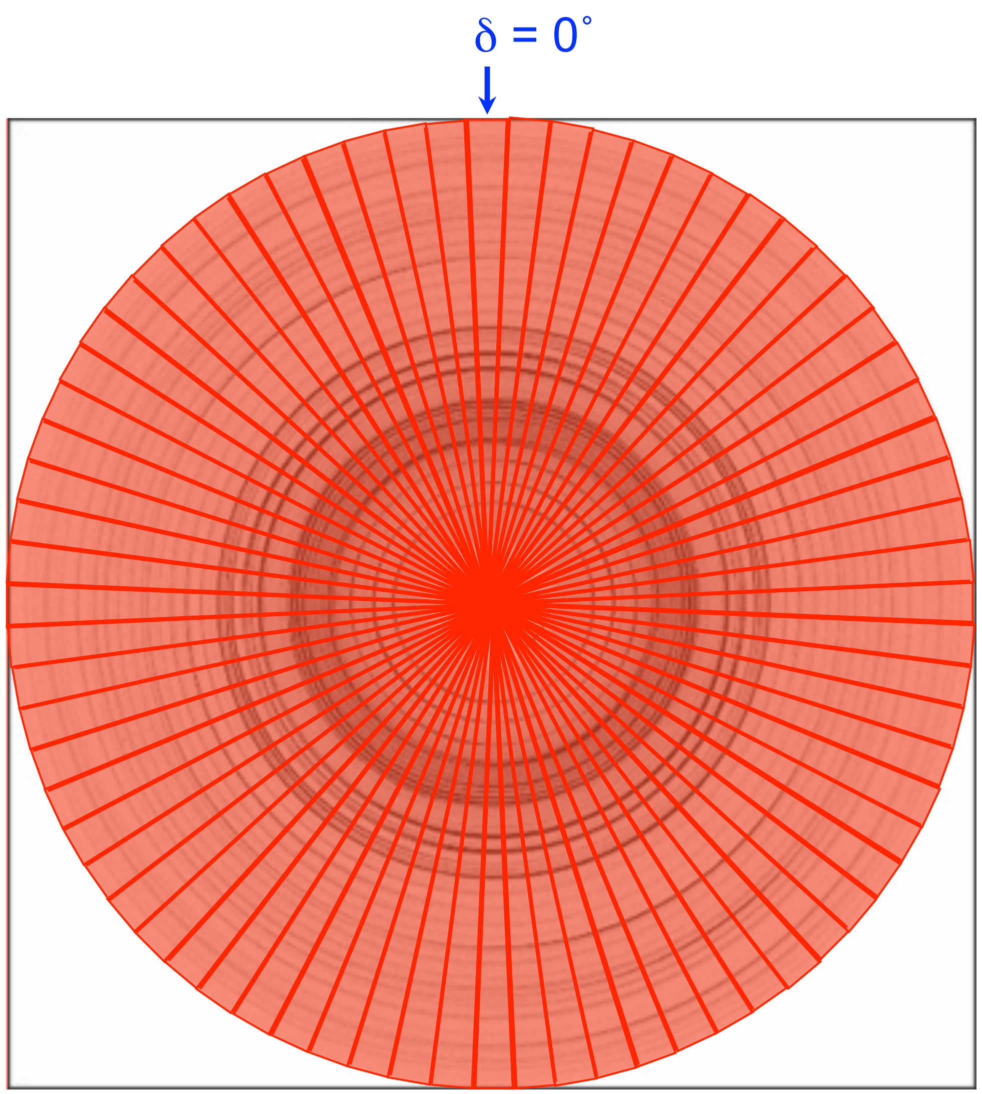
Transmission mode with area detector

Data analysis



Transmission mode with area detector

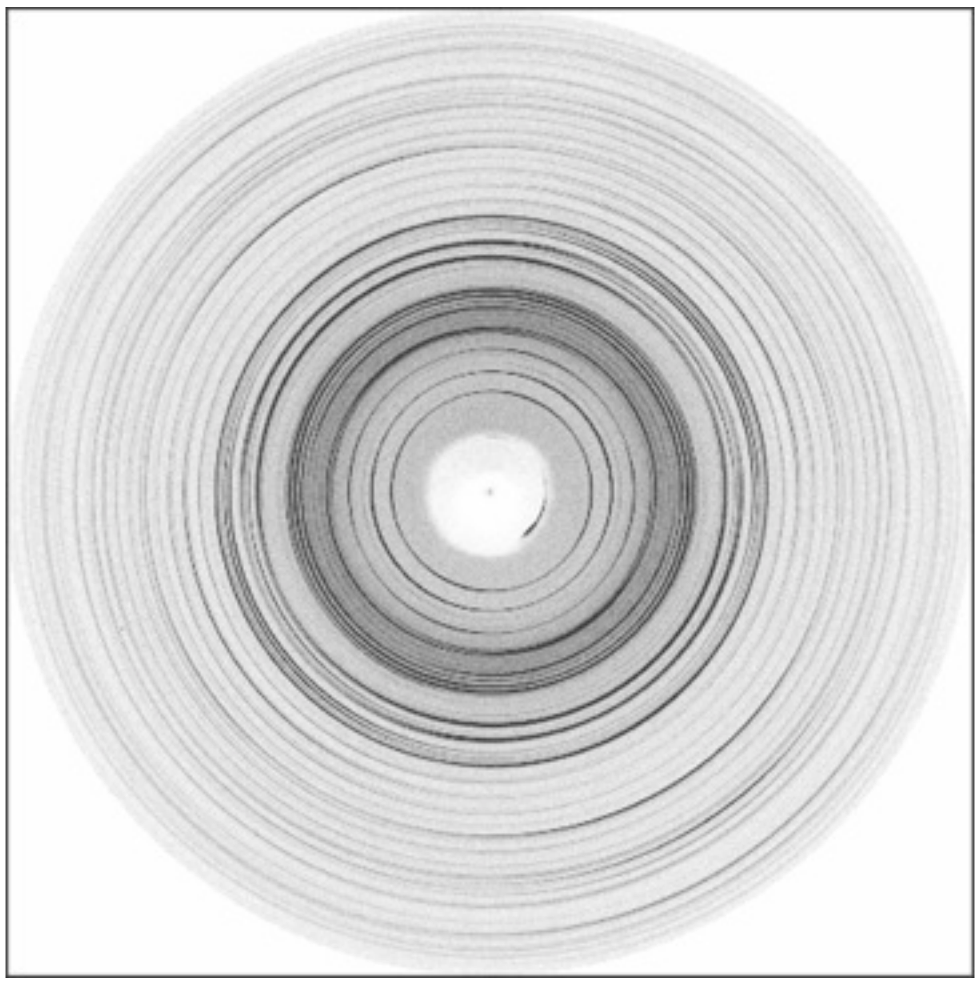
Data analysis



72 sectors

Transmission mode with area detector

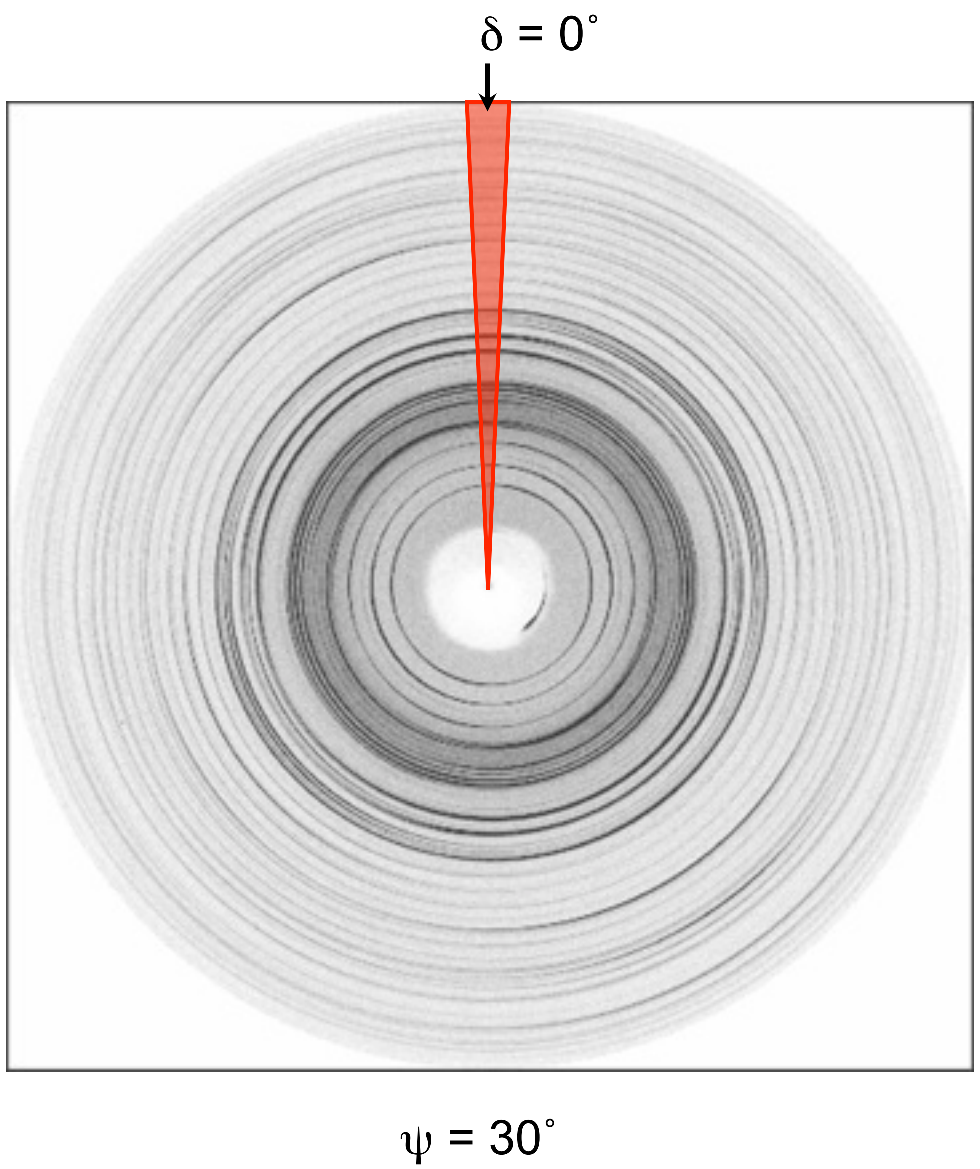
Data analysis

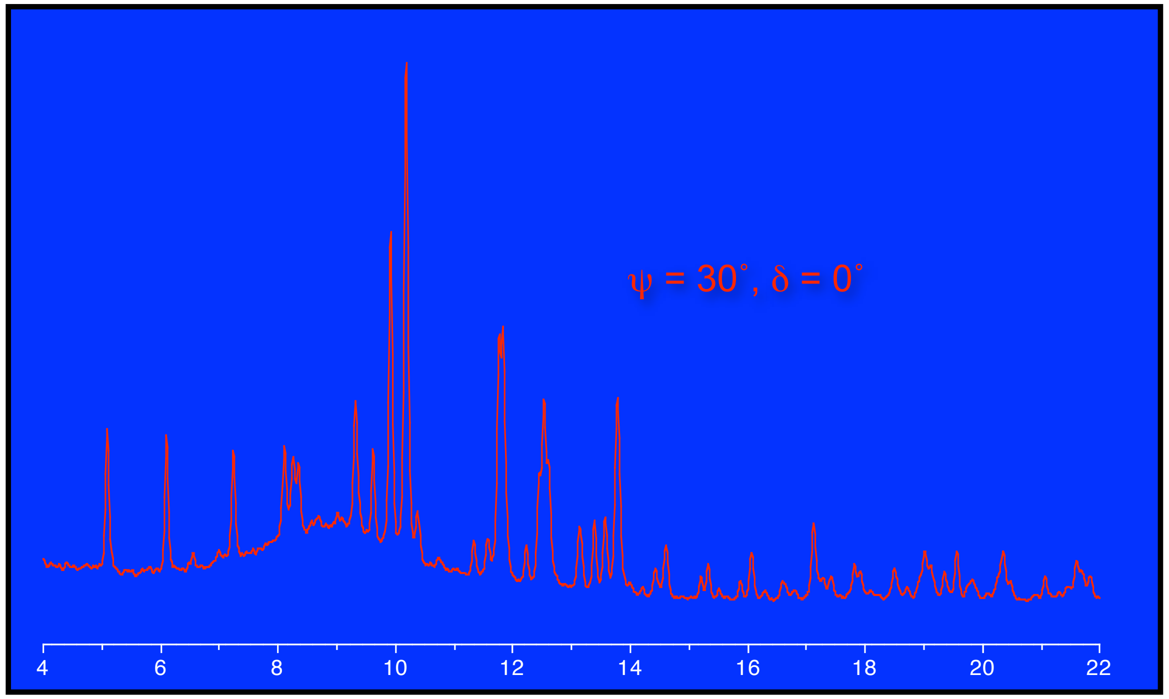


$\psi = 30^{\circ}$

Transmission mode with area detector

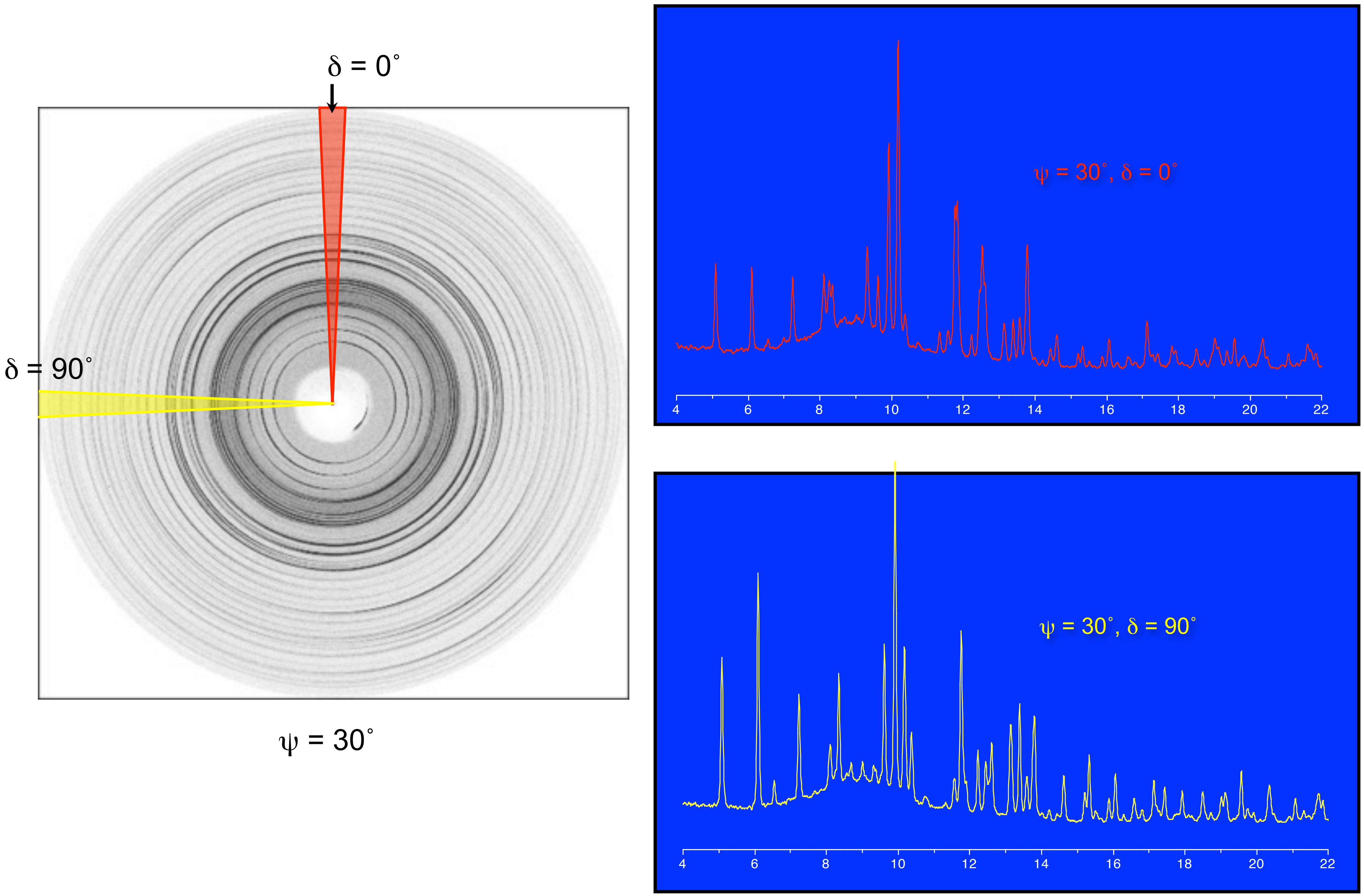
Data analysis





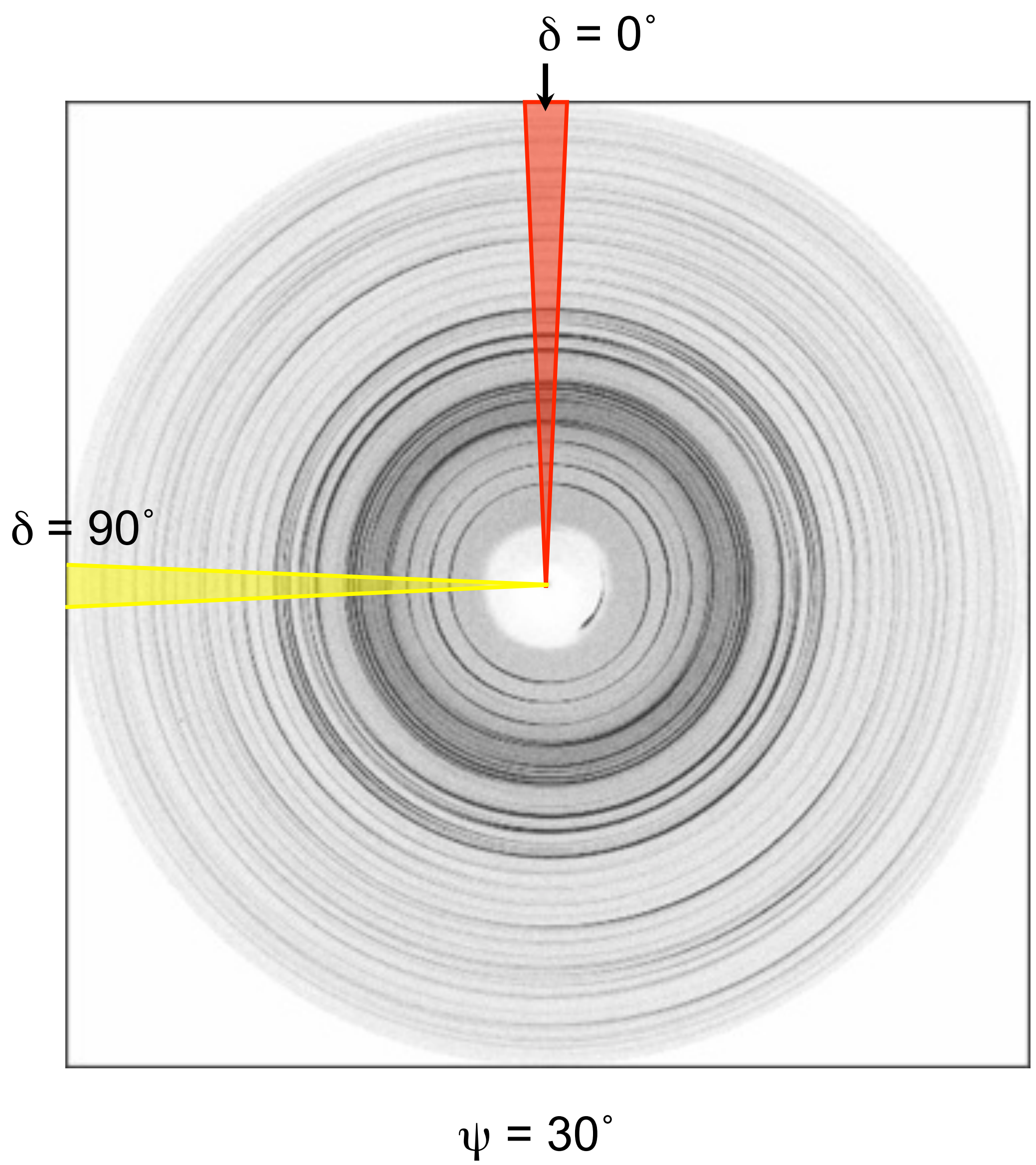
Transmission mode with area detector

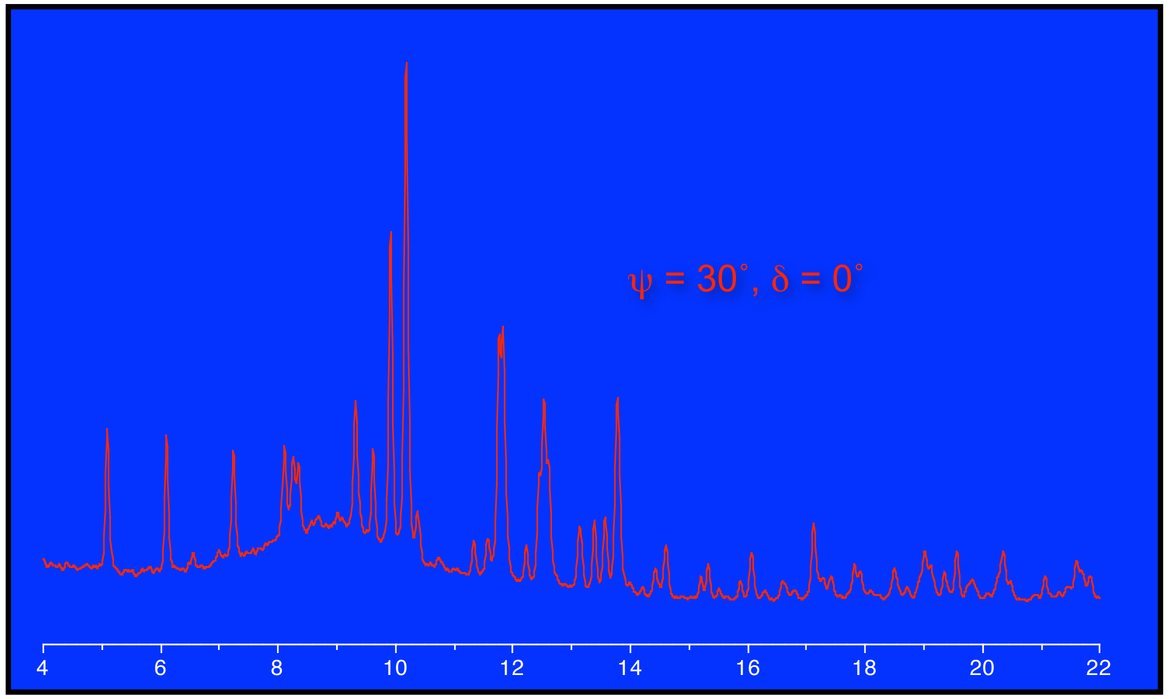
Data analysis

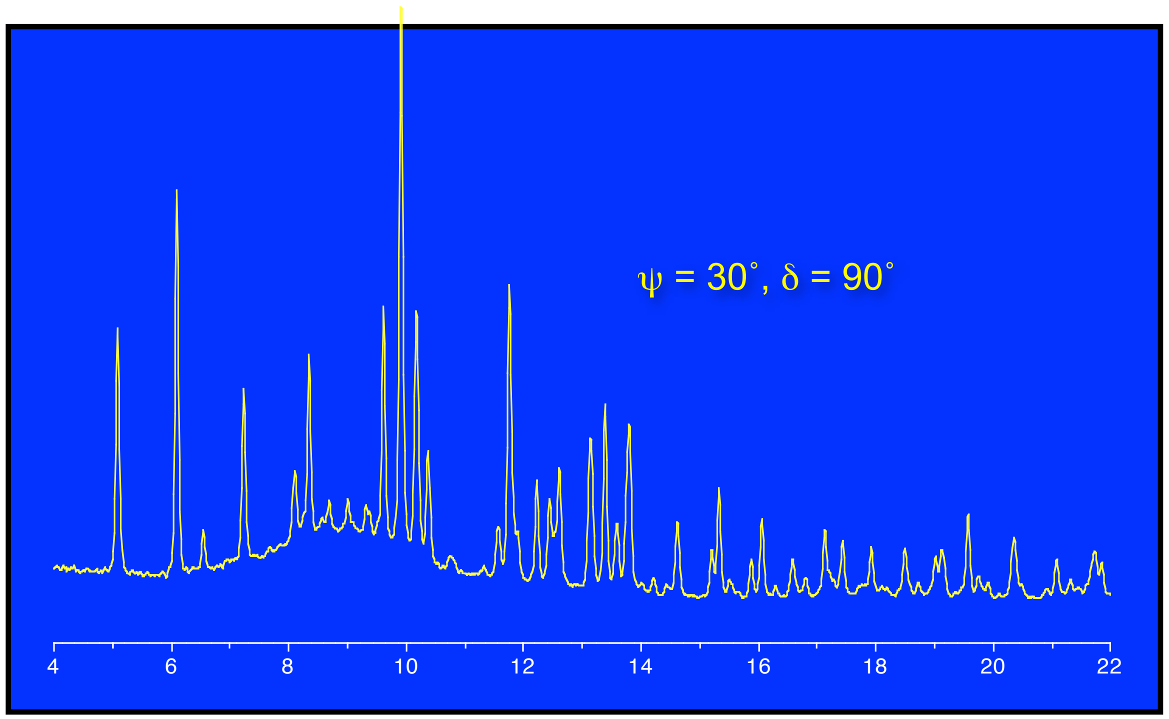


Transmission mode with area detector

Data analysis







extract 1296 unique patterns
with good statistics

Preparing a textured sample

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mix sample in a dissolved polymer (polystyrene)

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evaporate solvent till mixture becomes viscous

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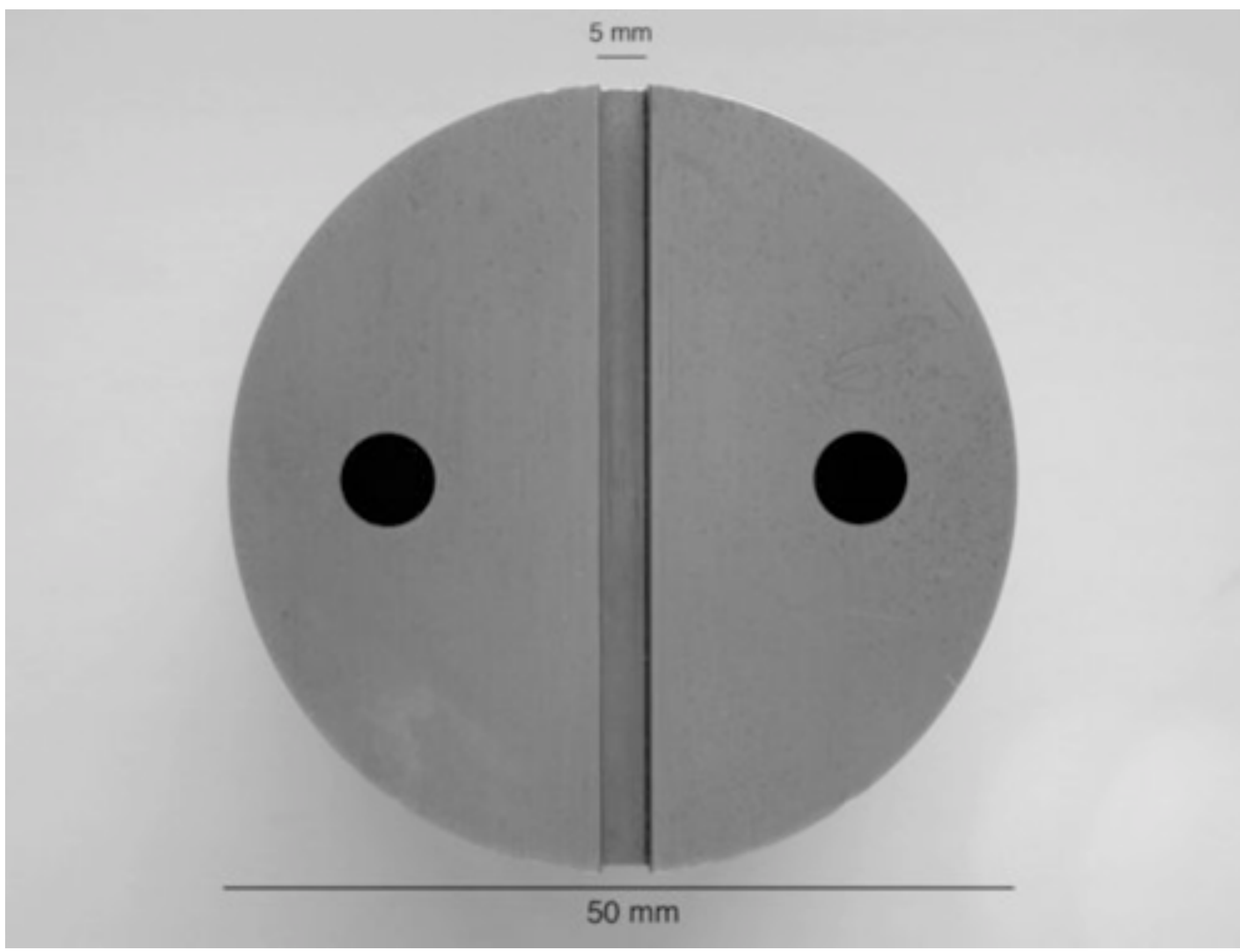

Preparing a textured sample

mix sample in a dissolved polymer (polystyrene)
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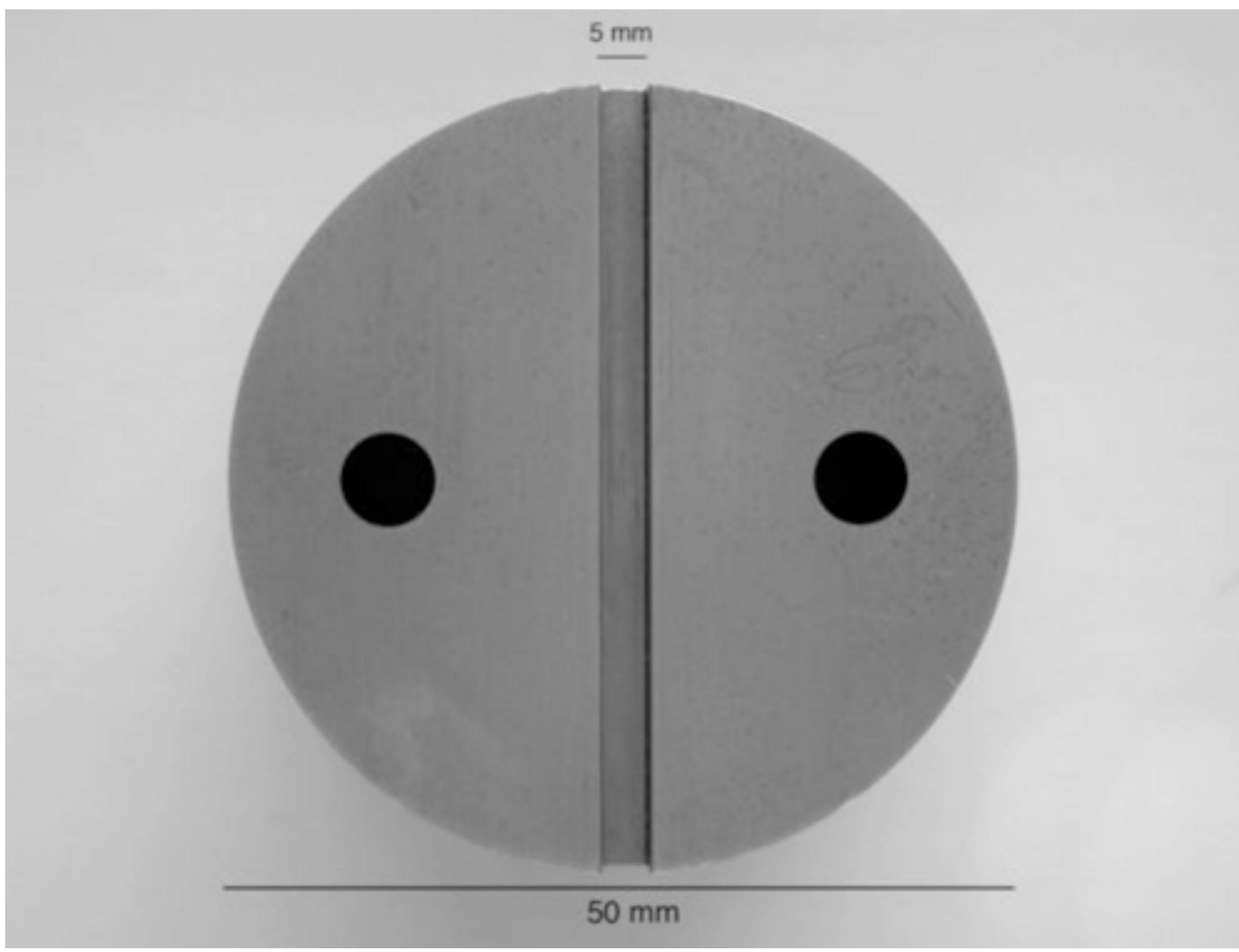
put in center of groove in die and press with top part
open and remove film from die and fold



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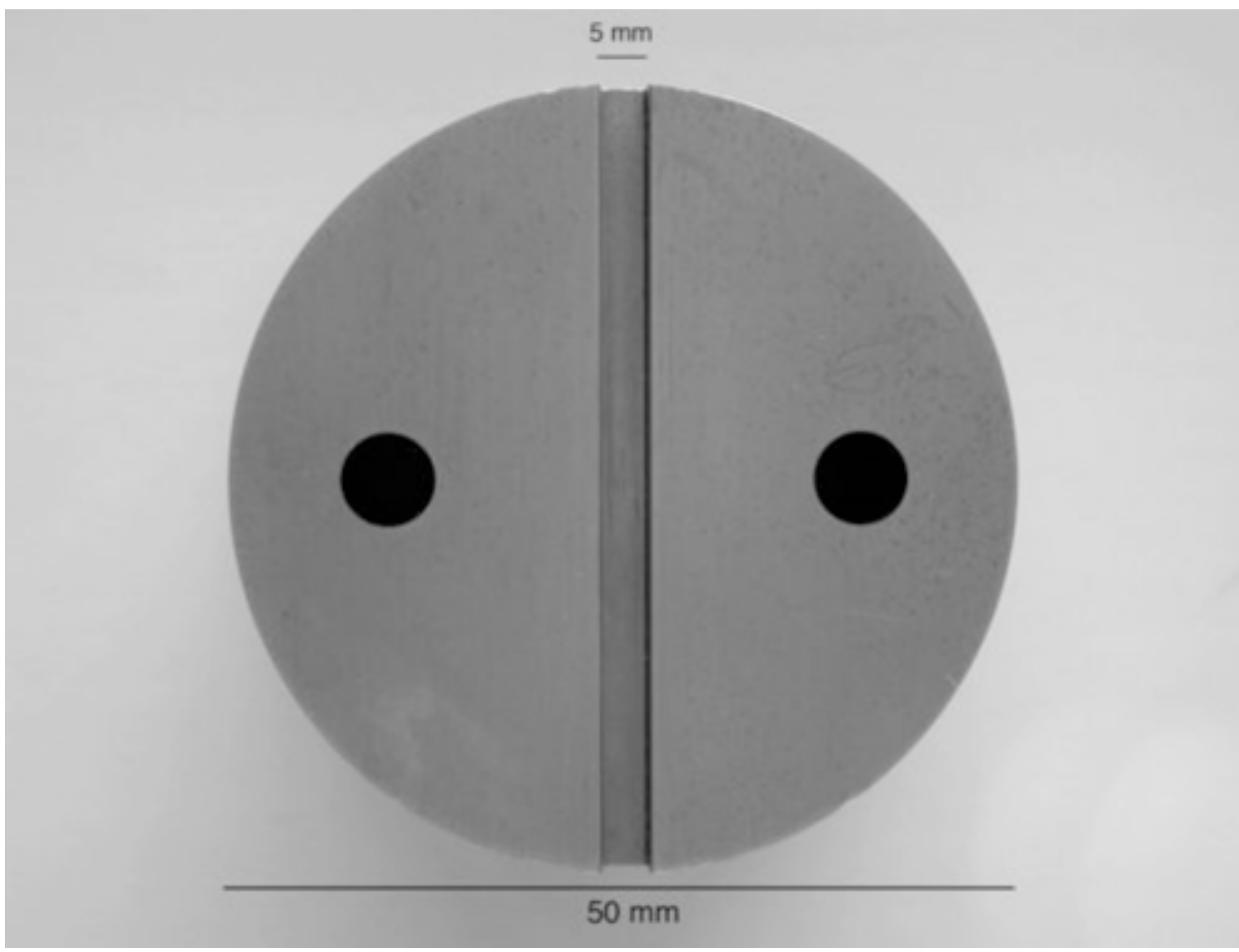
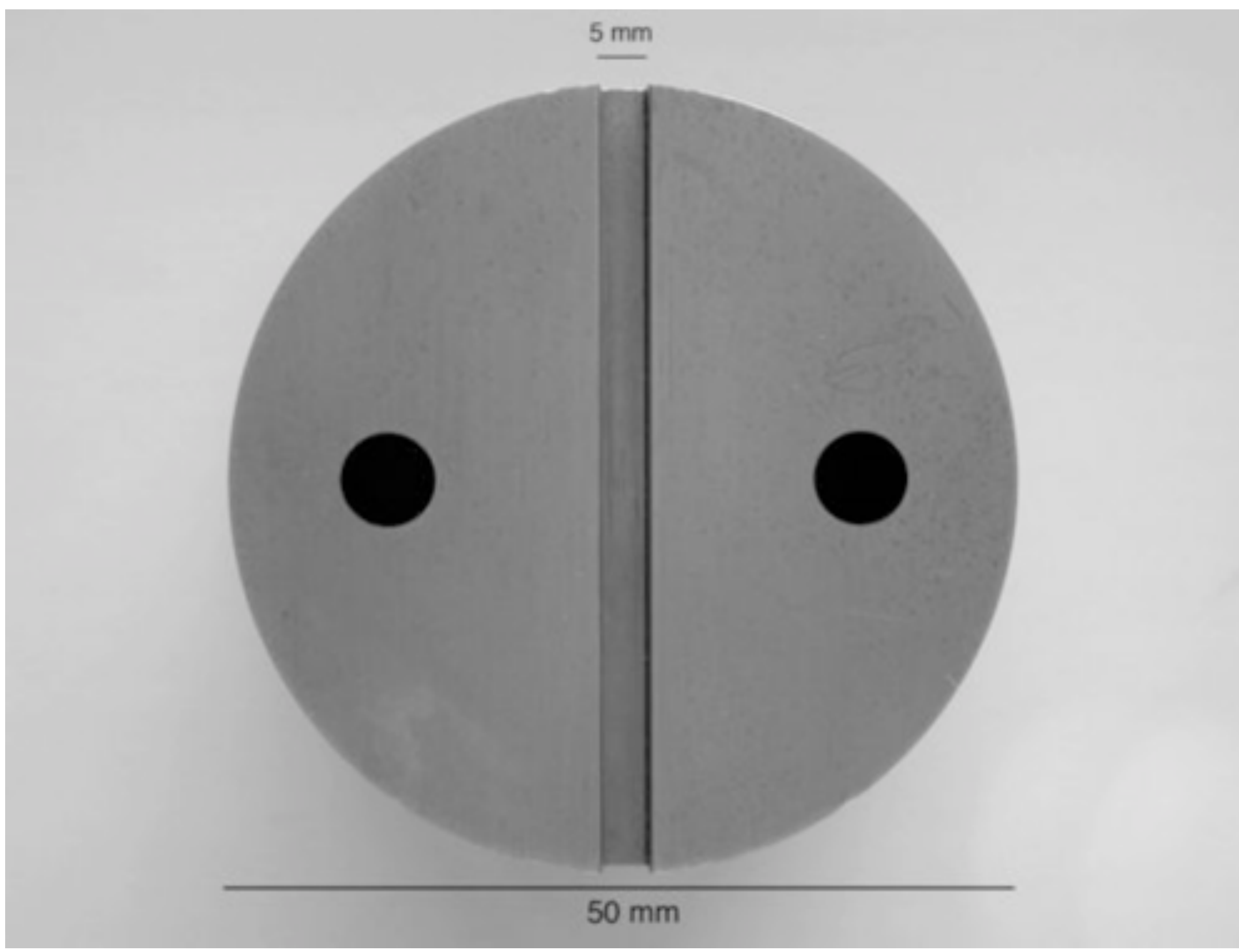


Preparing a textured sample

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

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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
No tilt correction required
Good counting statistics

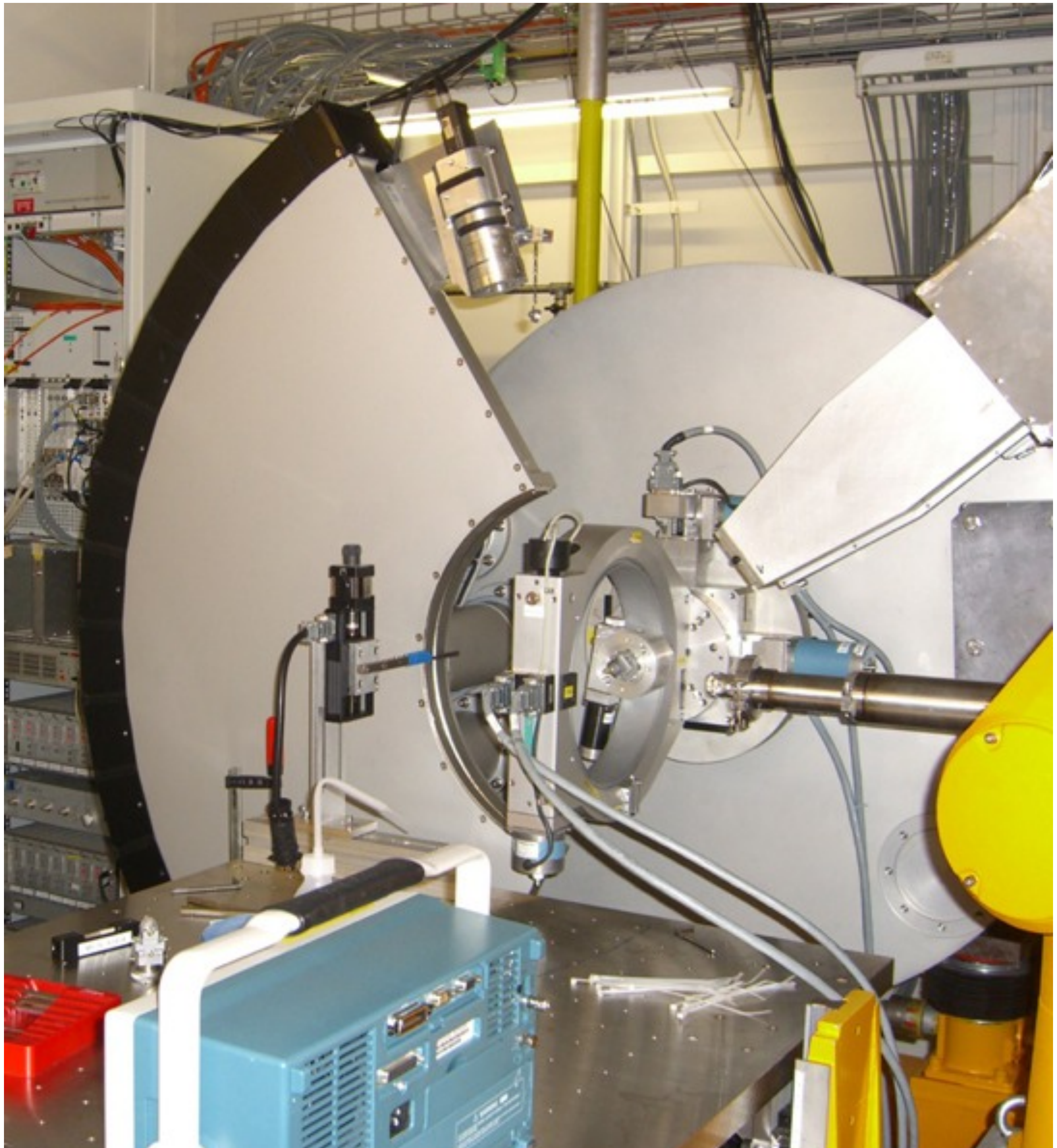
Cons

broader peaks
restricted 2θ range

Put detector further away
Resolution limited by pixel size
reduces 2θ range

Transmission mode - experimental setup

1D detector

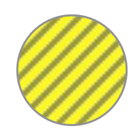


SLS MS beam line

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

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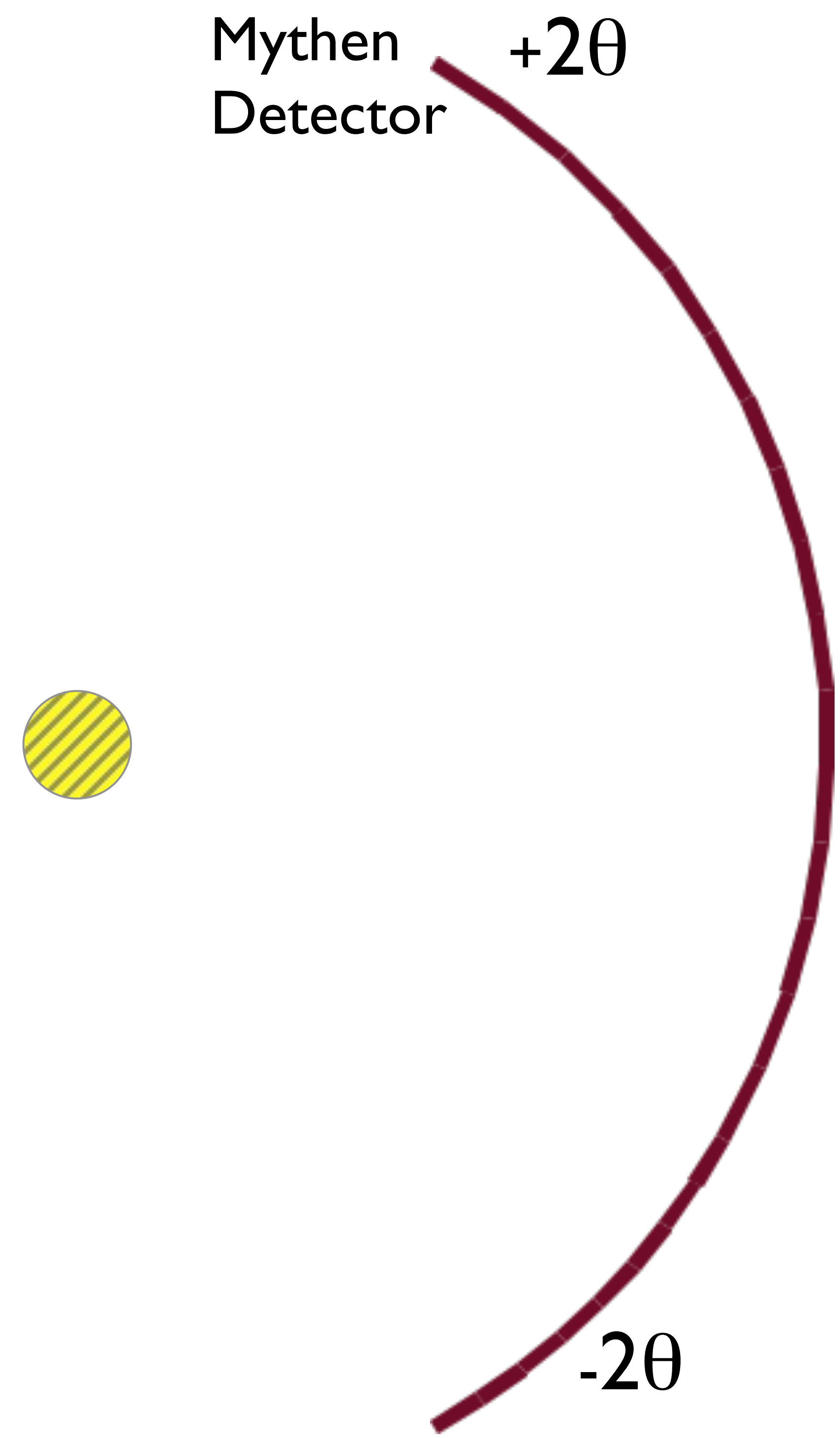

Transmission mode - experimental setup

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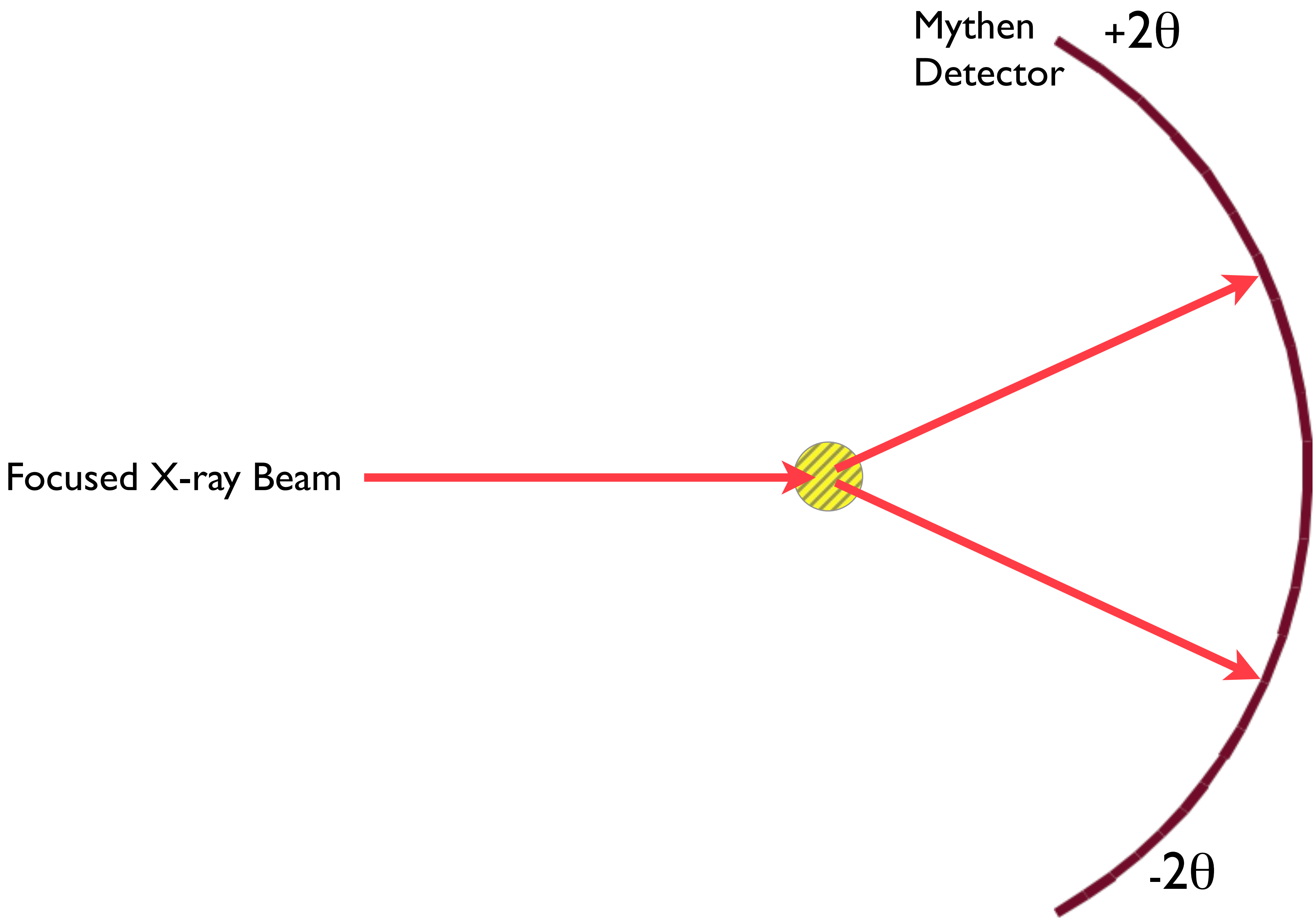

Transmission mode - experimental setup

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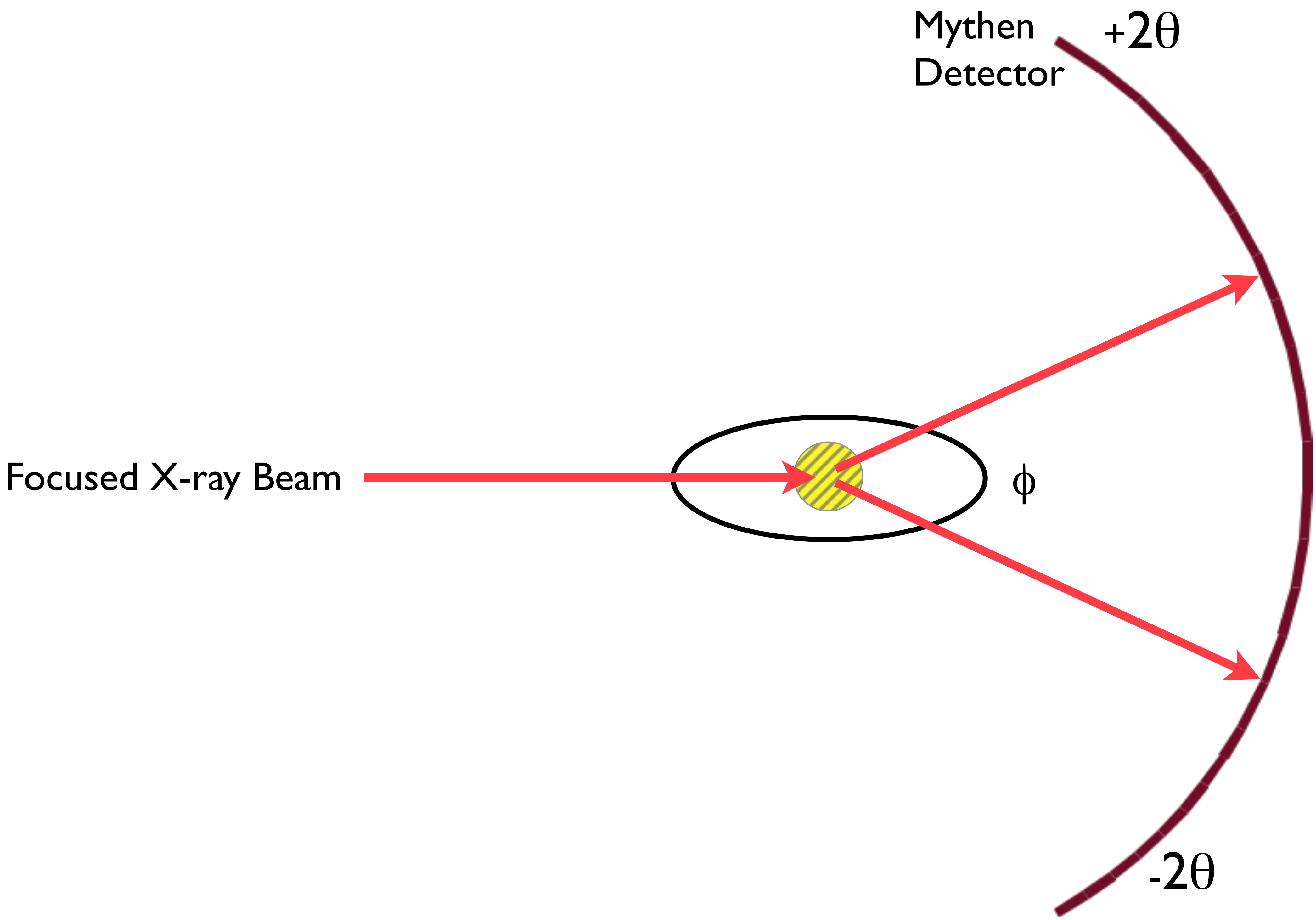

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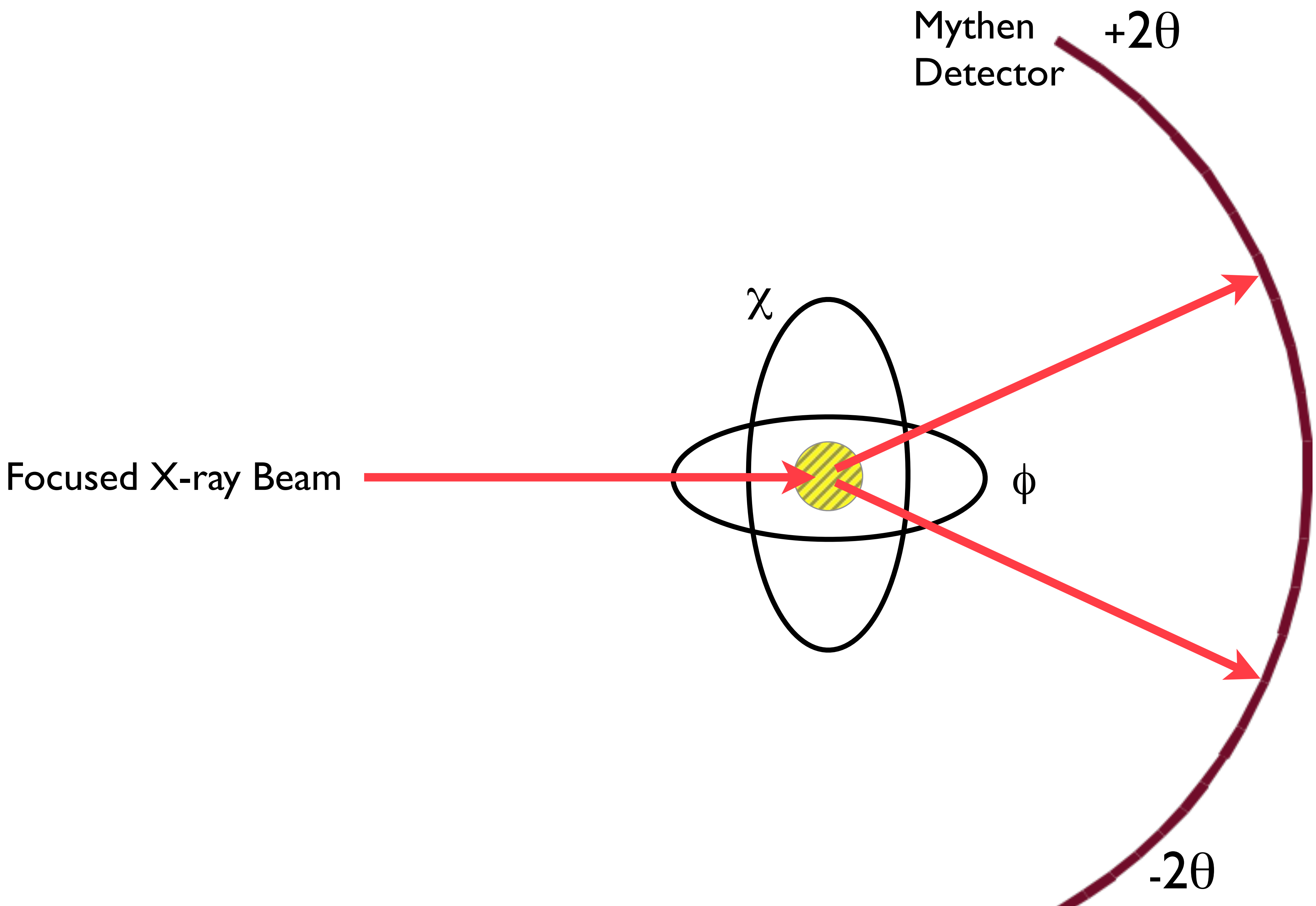
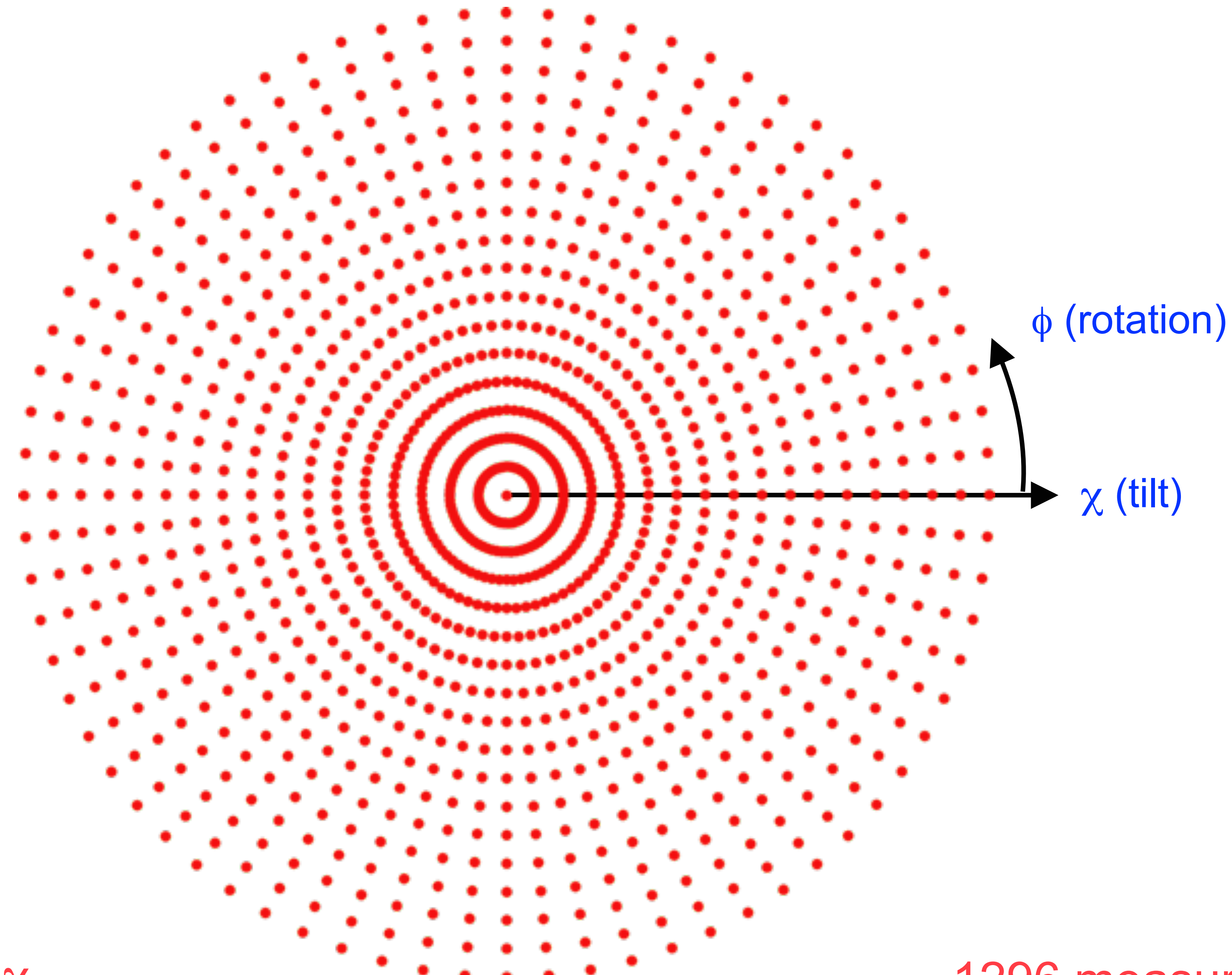


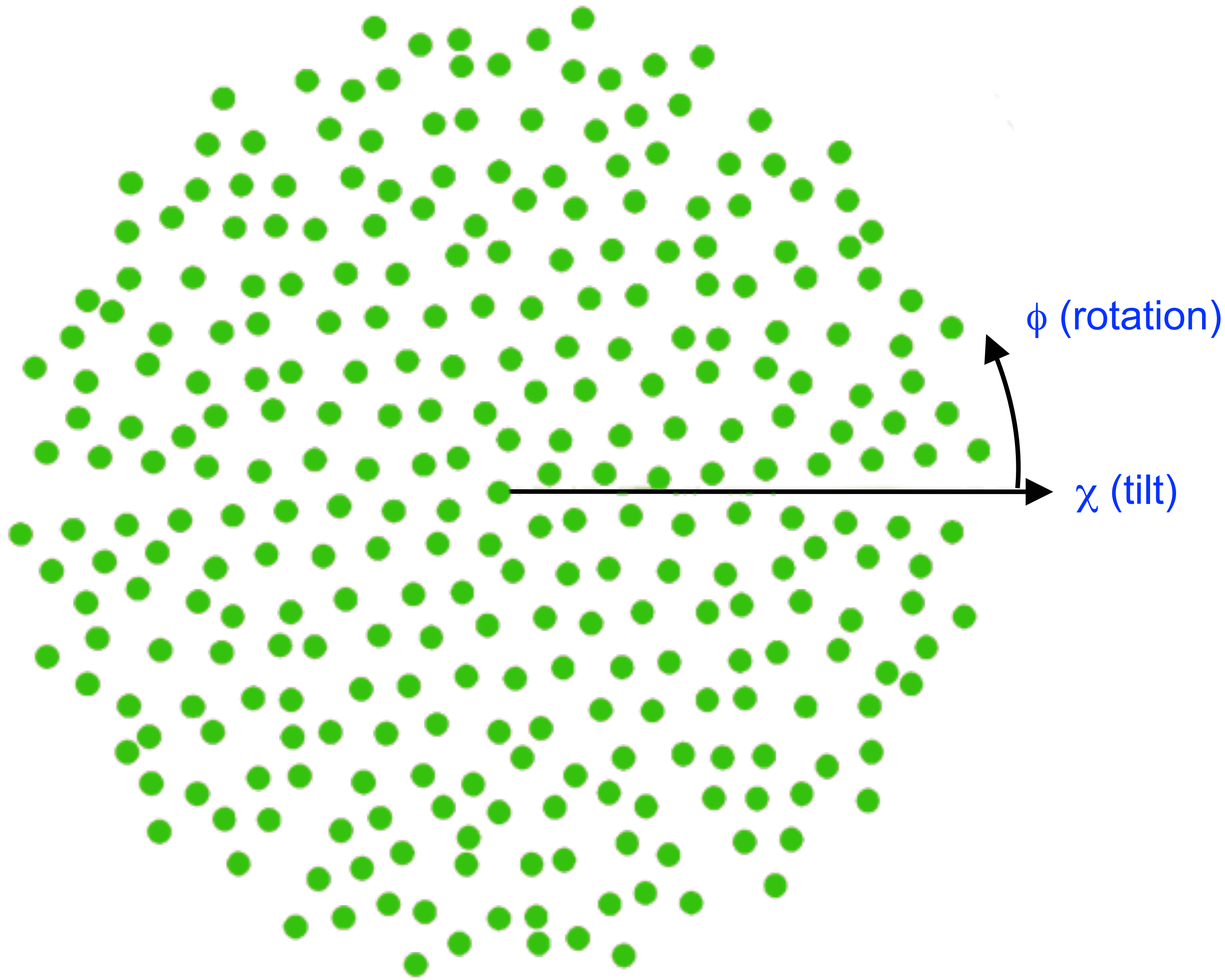
Texture Analysis



every 5° in ϕ and χ

1296 measurements

Texture Analysis



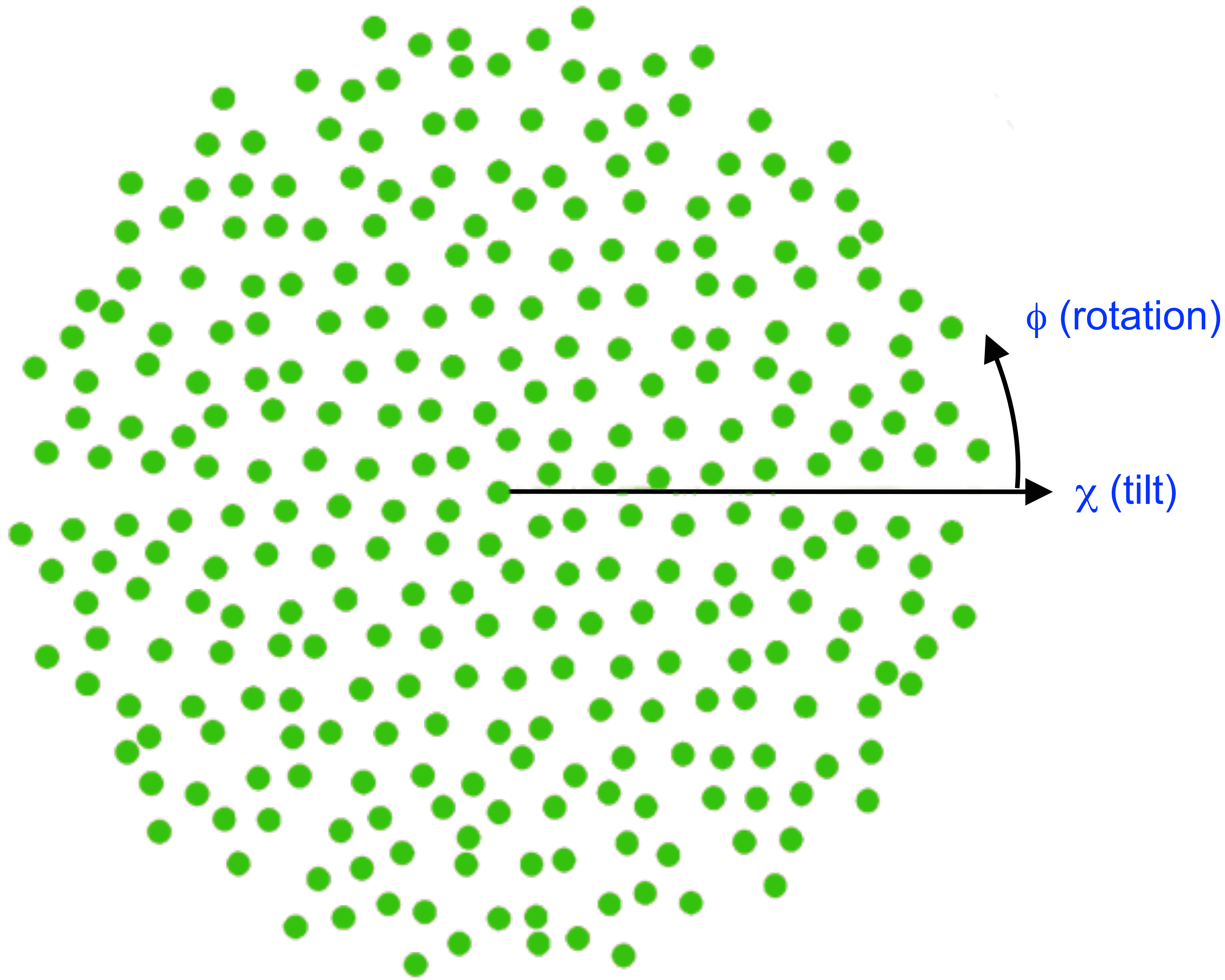
optimized coverage

302 measurents

MAUD software

Texture Analysis

shorter data collection time

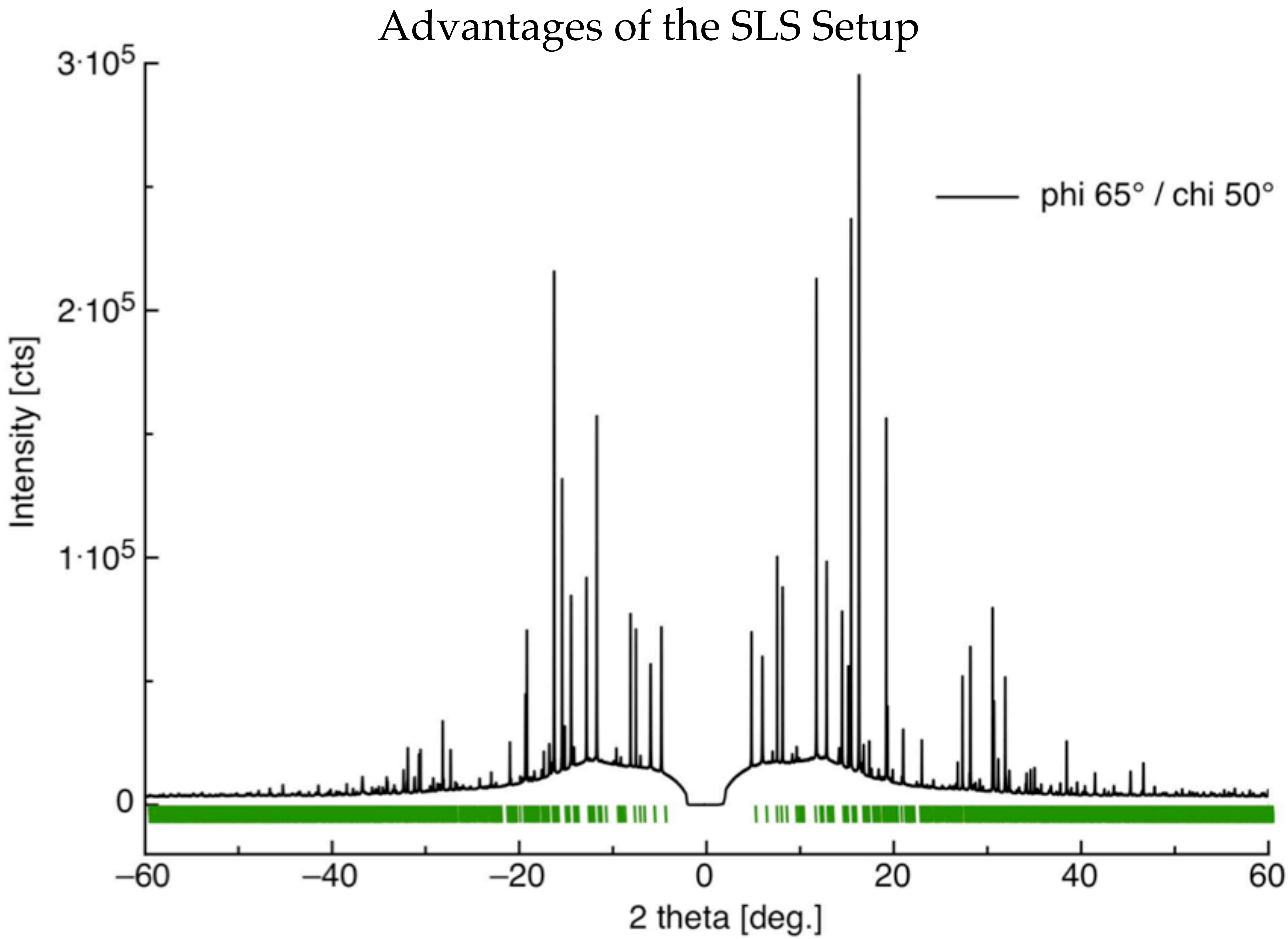


optimized coverage

302 measurents

MAUD software

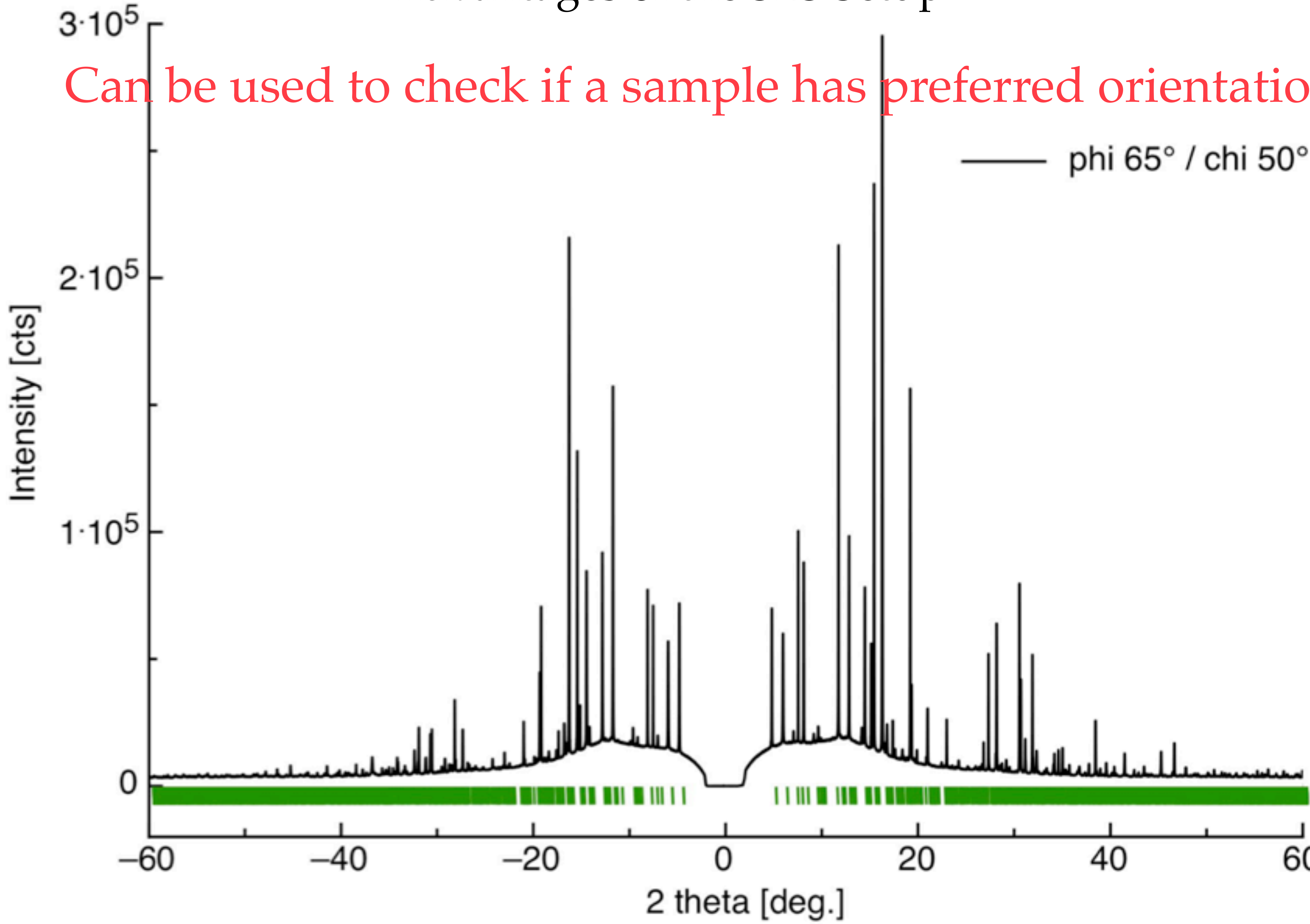
Transmission mode



Transmission mode

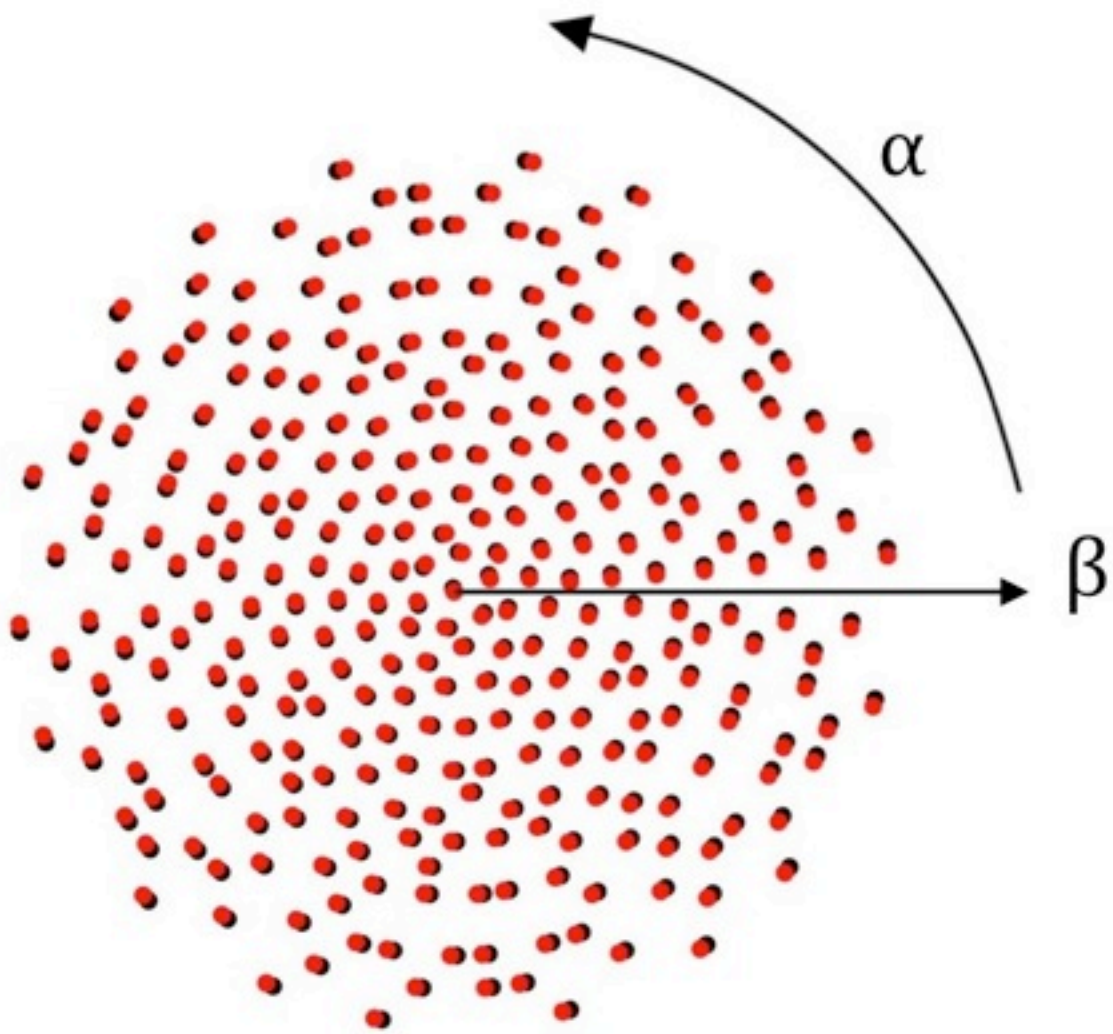
Advantages of the SLS Setup

Can be used to check if a sample has preferred orientation

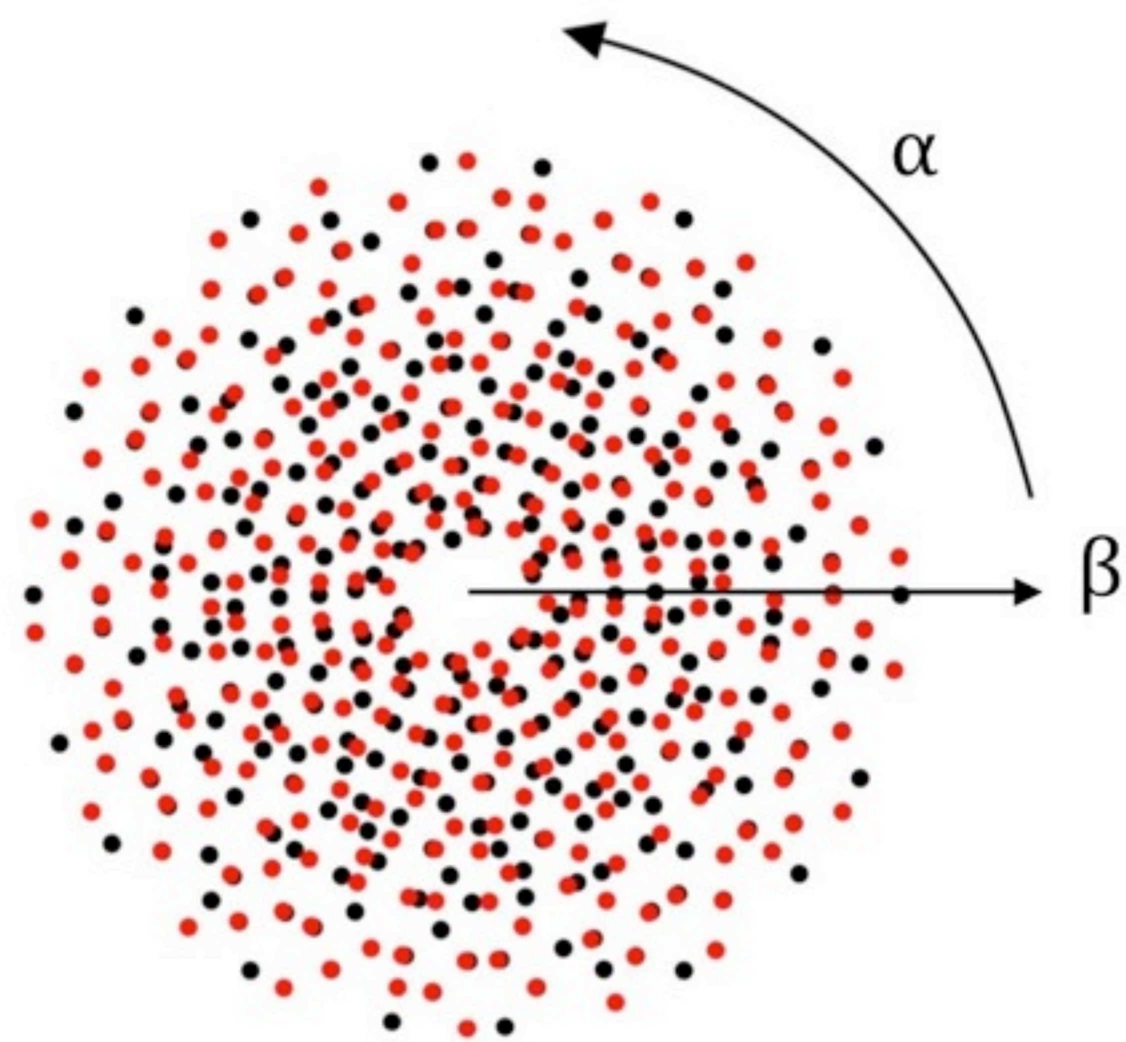


Transmission mode

Advantages of the SLS Setup



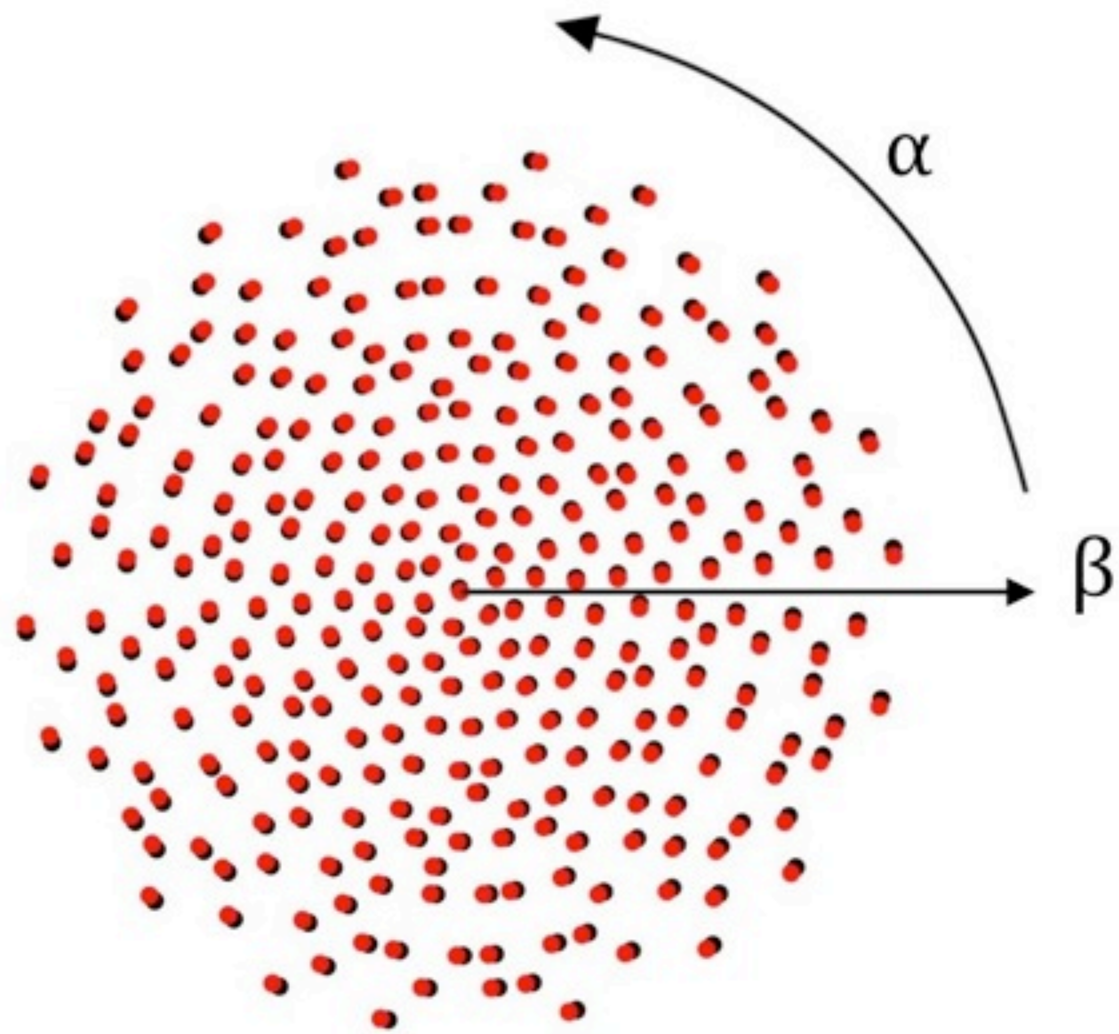
$1^{\circ}\ 2\theta$



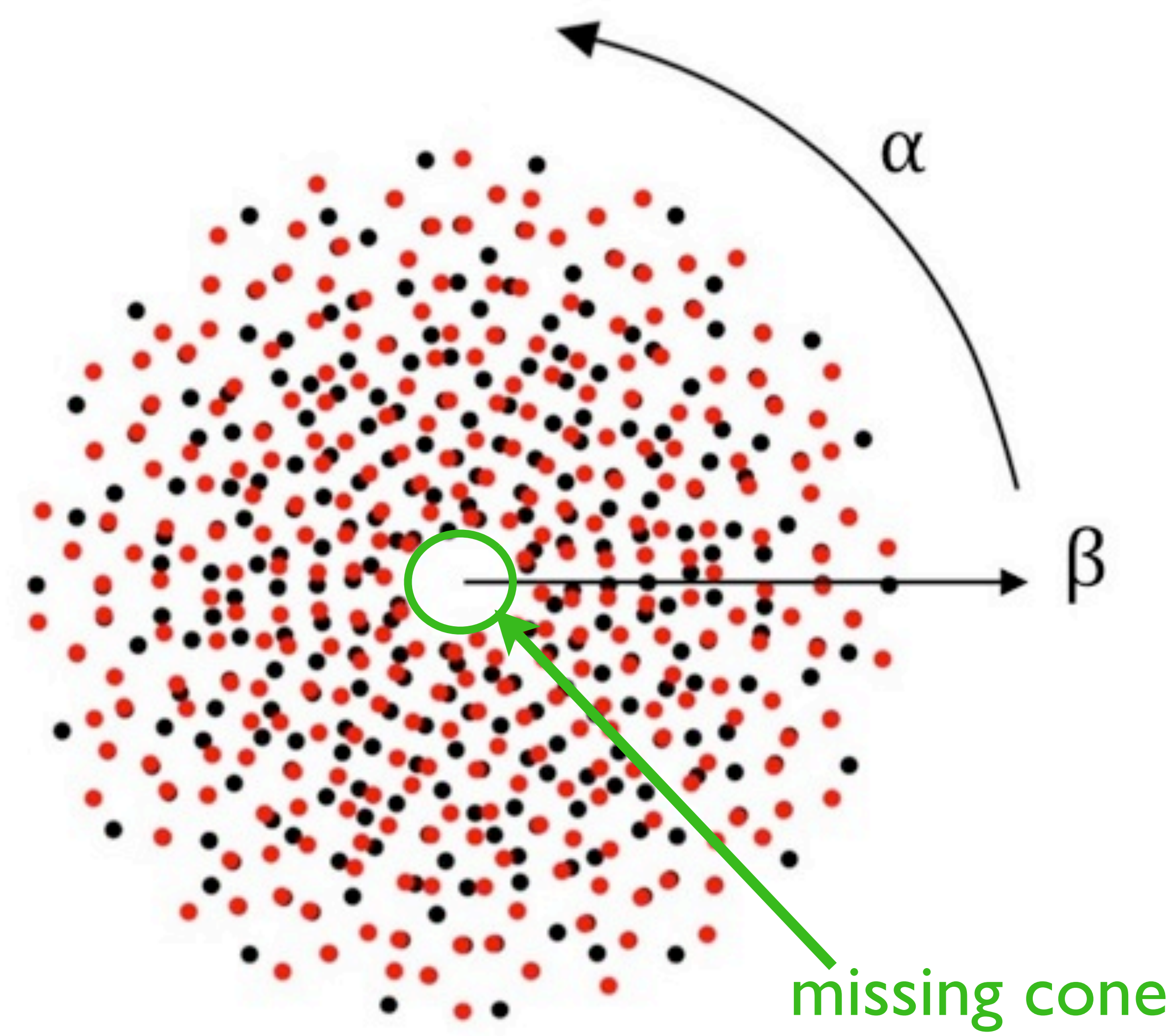
$30^{\circ}\ 2\theta$

Transmission mode

Advantages of the SLS Setup



1° 2θ



30° 2θ

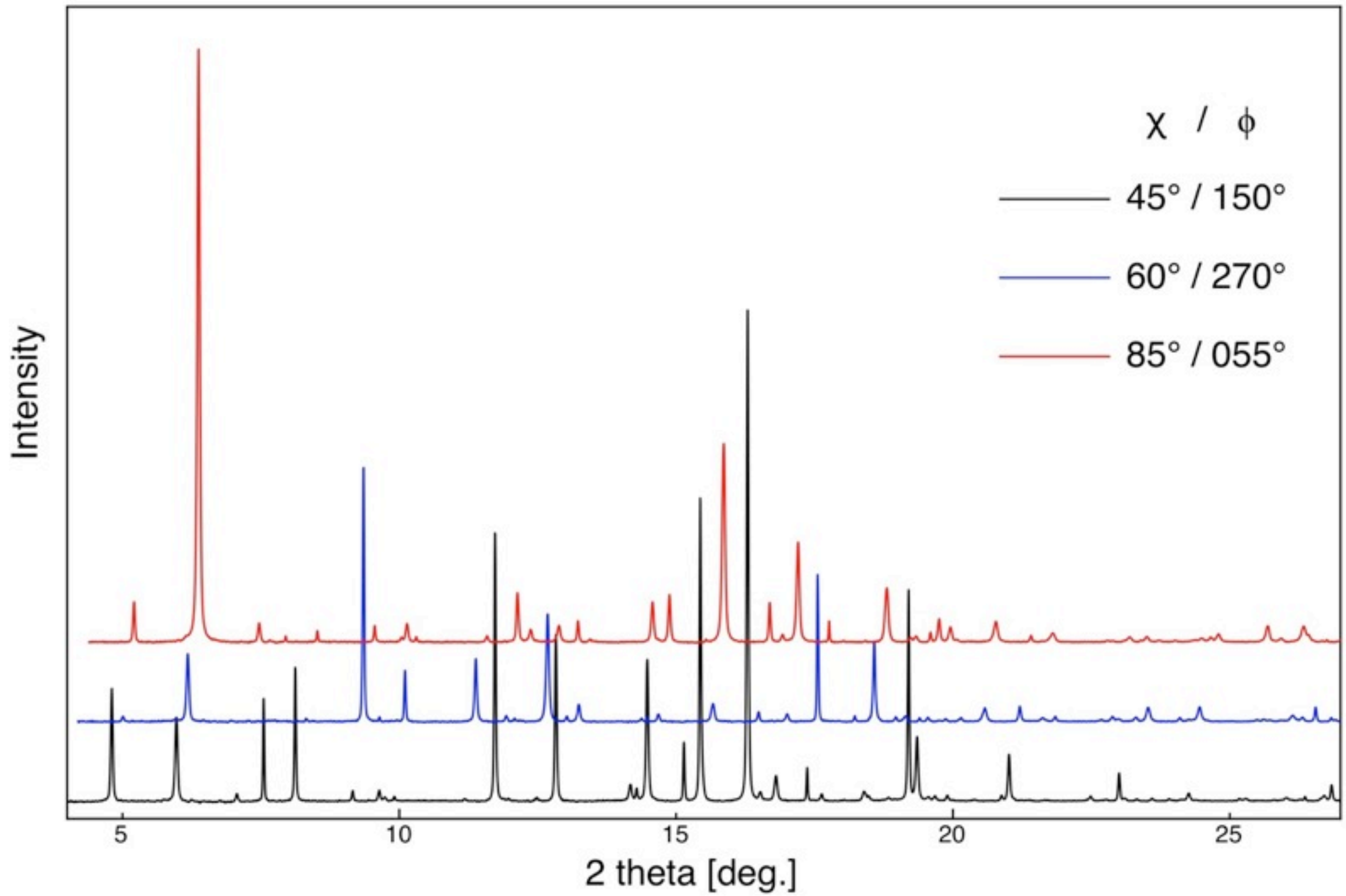
Transmission mode

Advantages of the SLS Setup (Mythen detector)

- High resolution
- Large angular range
- Very fast, 2-10 sec per pattern → 300 patterns (10-50 min)
- Good counting statistics
- 120° 2θ range → 2 patterns at the same time
- Local integration by oscillating sample ±2.5° in δ and ψ
- Helpful beamline staff

Test Example $ZrPO_4$ -pyr

Some powder patterns



Transmission mode

Analysis Procedure

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- Prepare textured sample (using sheer forces in polymer matrix)

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- Prepare textured sample (using sheer forces in polymer matrix)
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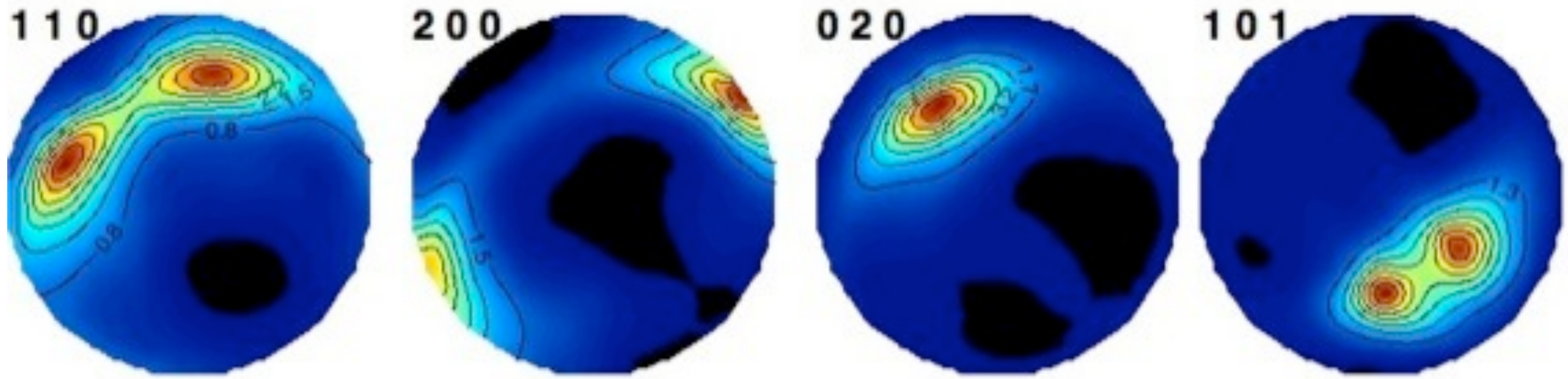
- De-convolute overlapping reflections using selected patterns
- Solve structure using direct methods

Test Example $ZrPO_4$ -pyr

Polfigures used for the texture determination

measured

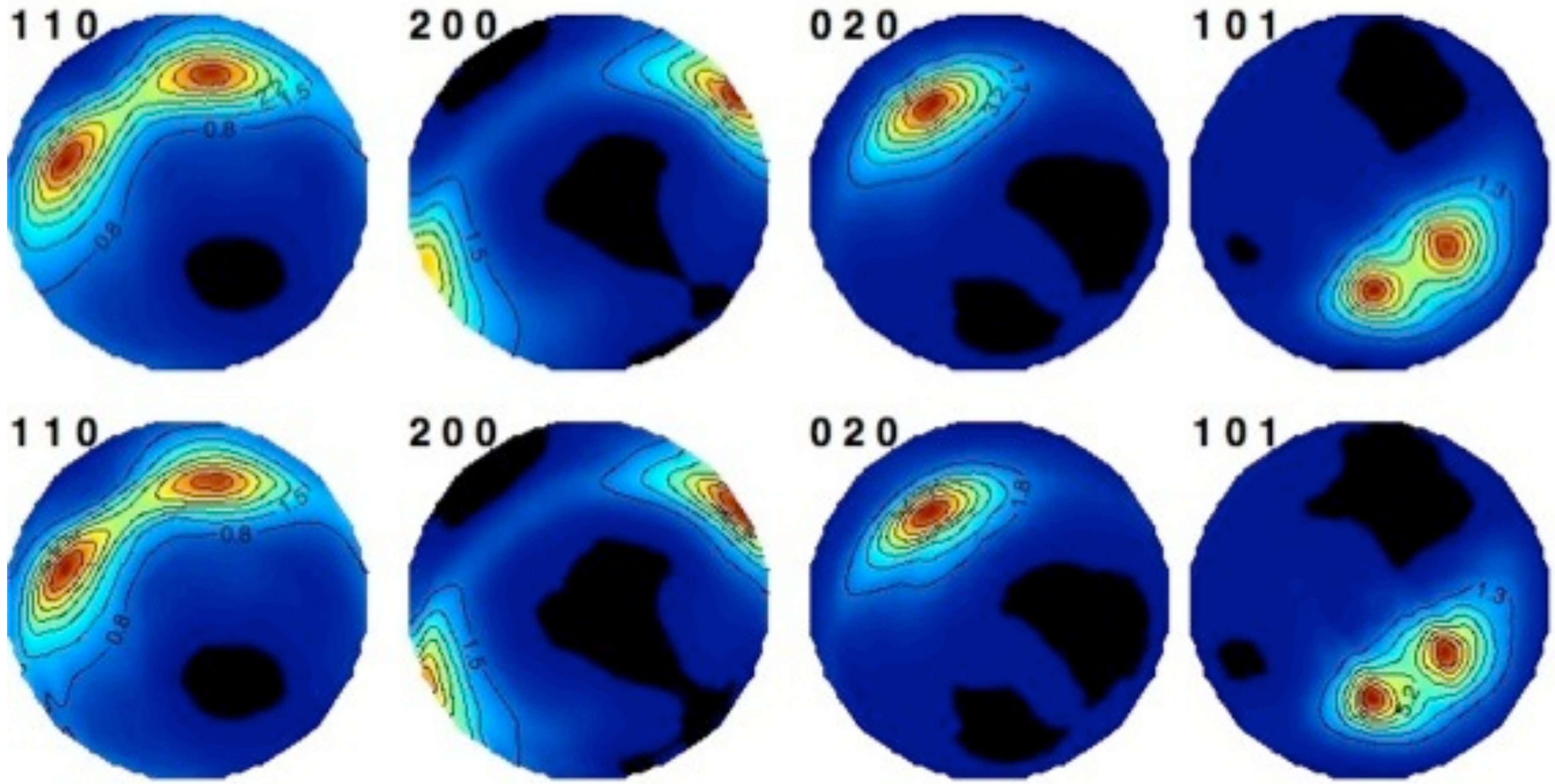


Test Example $ZrPO_4$ -pyr

Polfigures used for the texture determination

measured

calculated from ODF

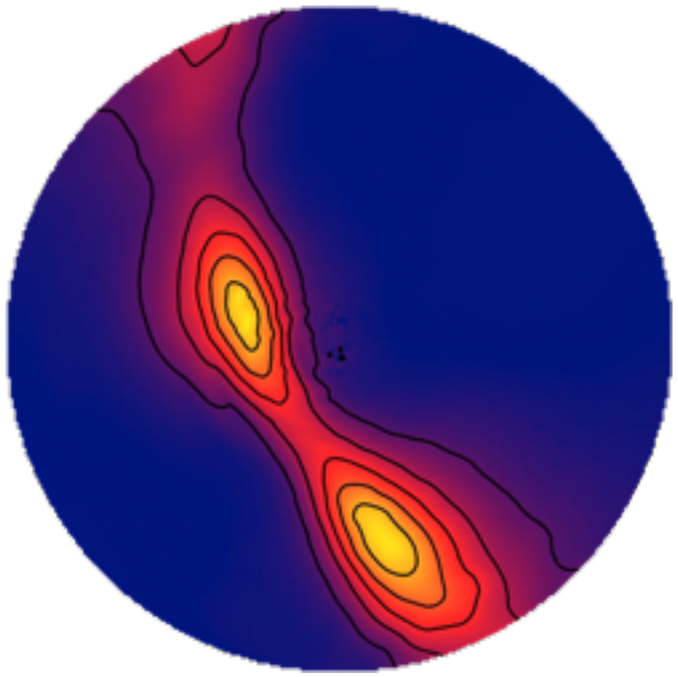


Test Example $ZrPO_4$ -pyr

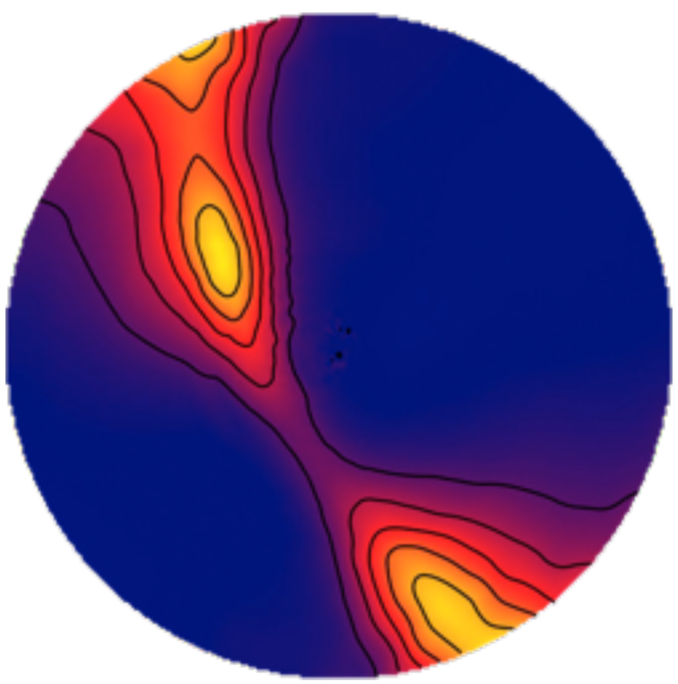
Select most useful sample orientations using all calculated pole figures

Overlapped reflections 760 and 940

760



940



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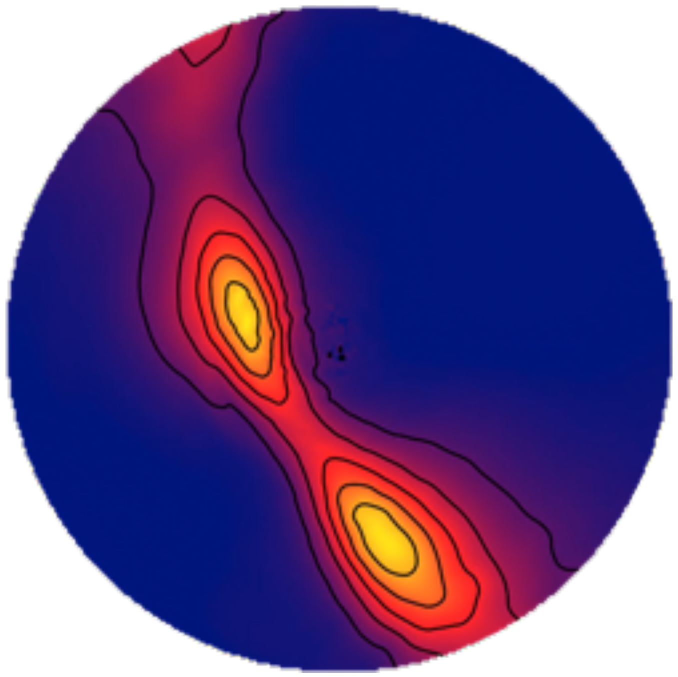
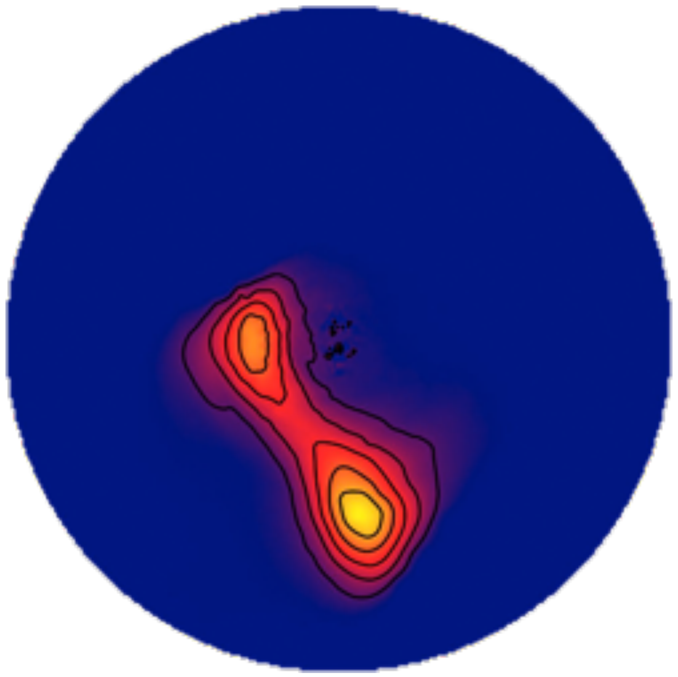


760 - 940



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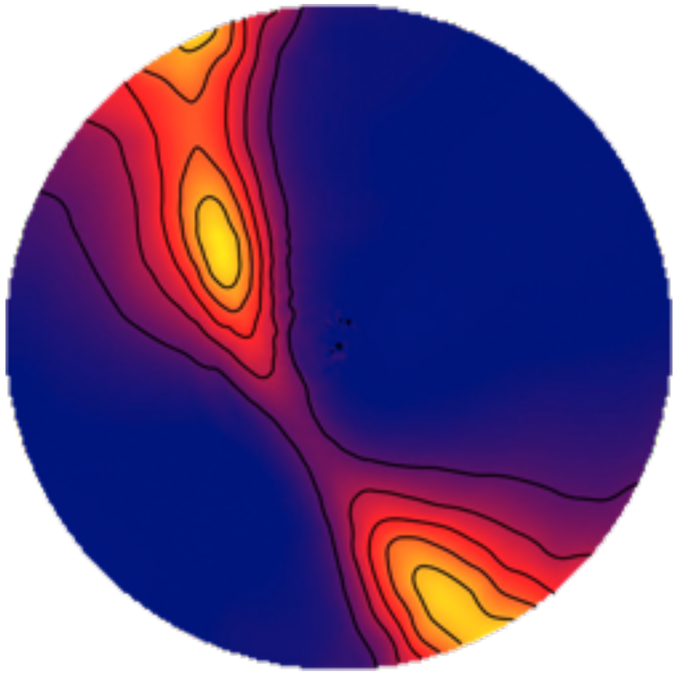

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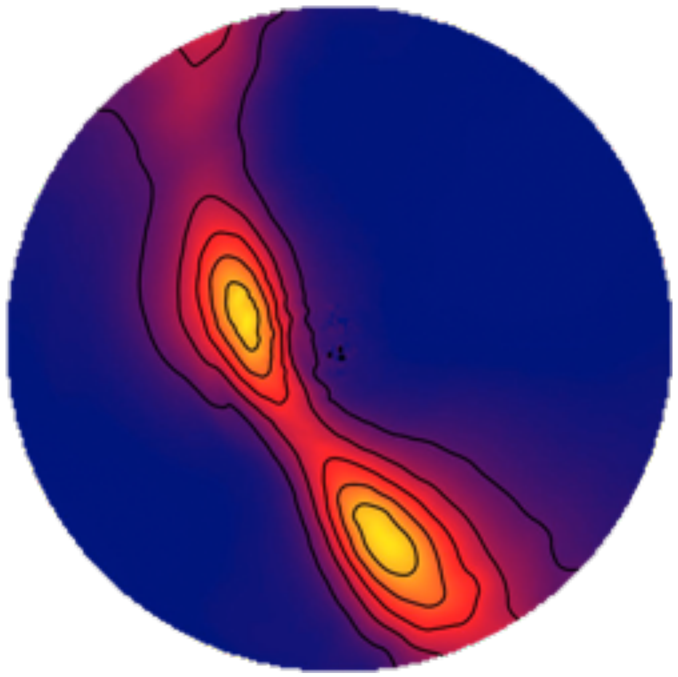

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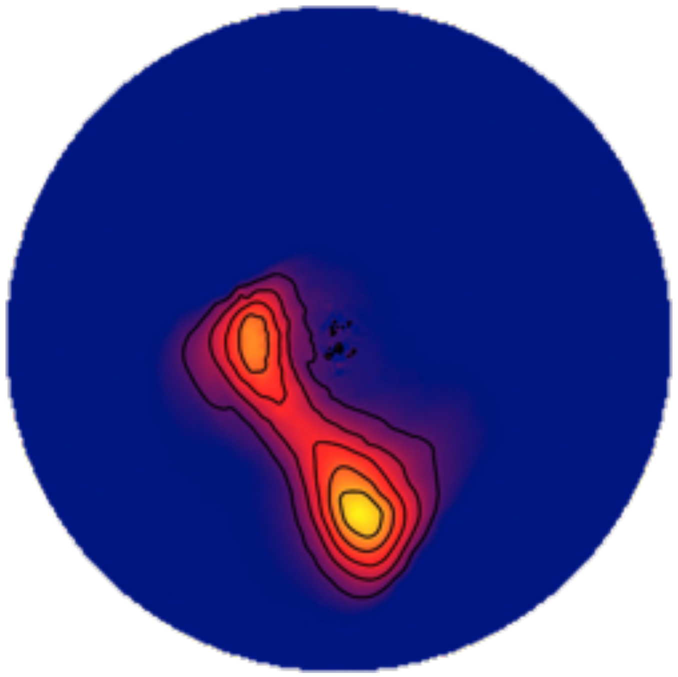

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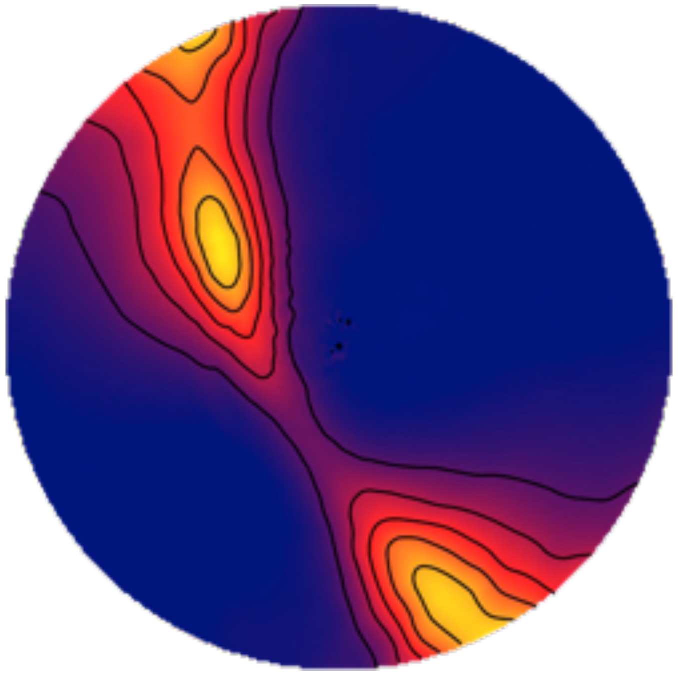
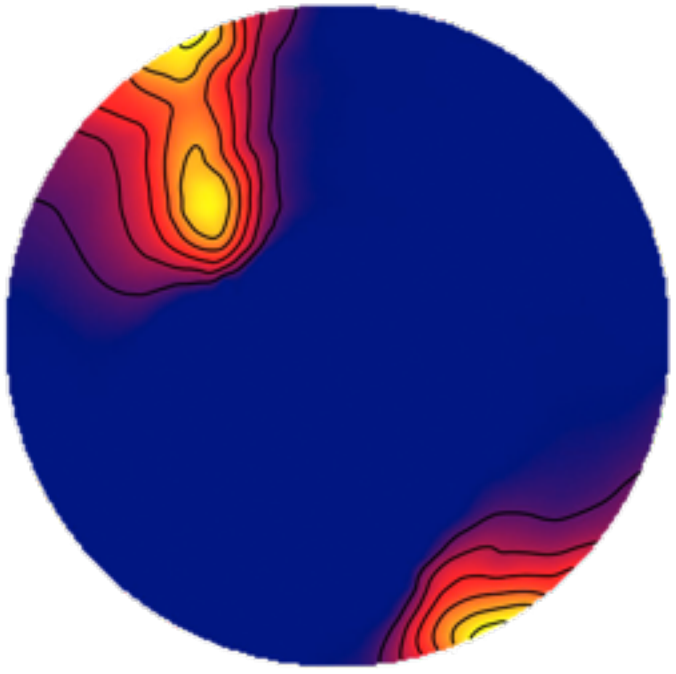


940 - 760



Test Example $ZrPO_4$ -pyr

How many different orientations are needed?

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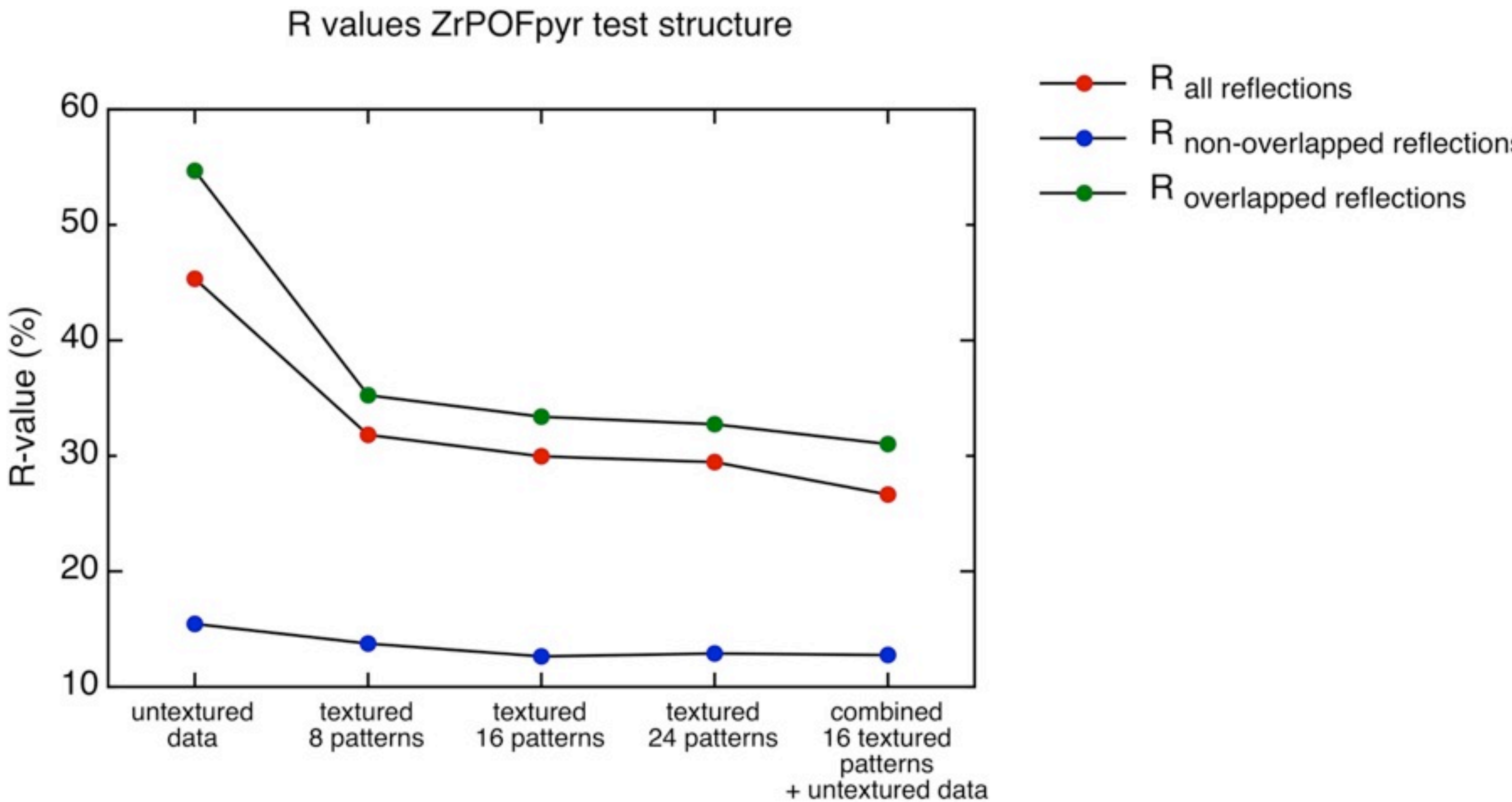
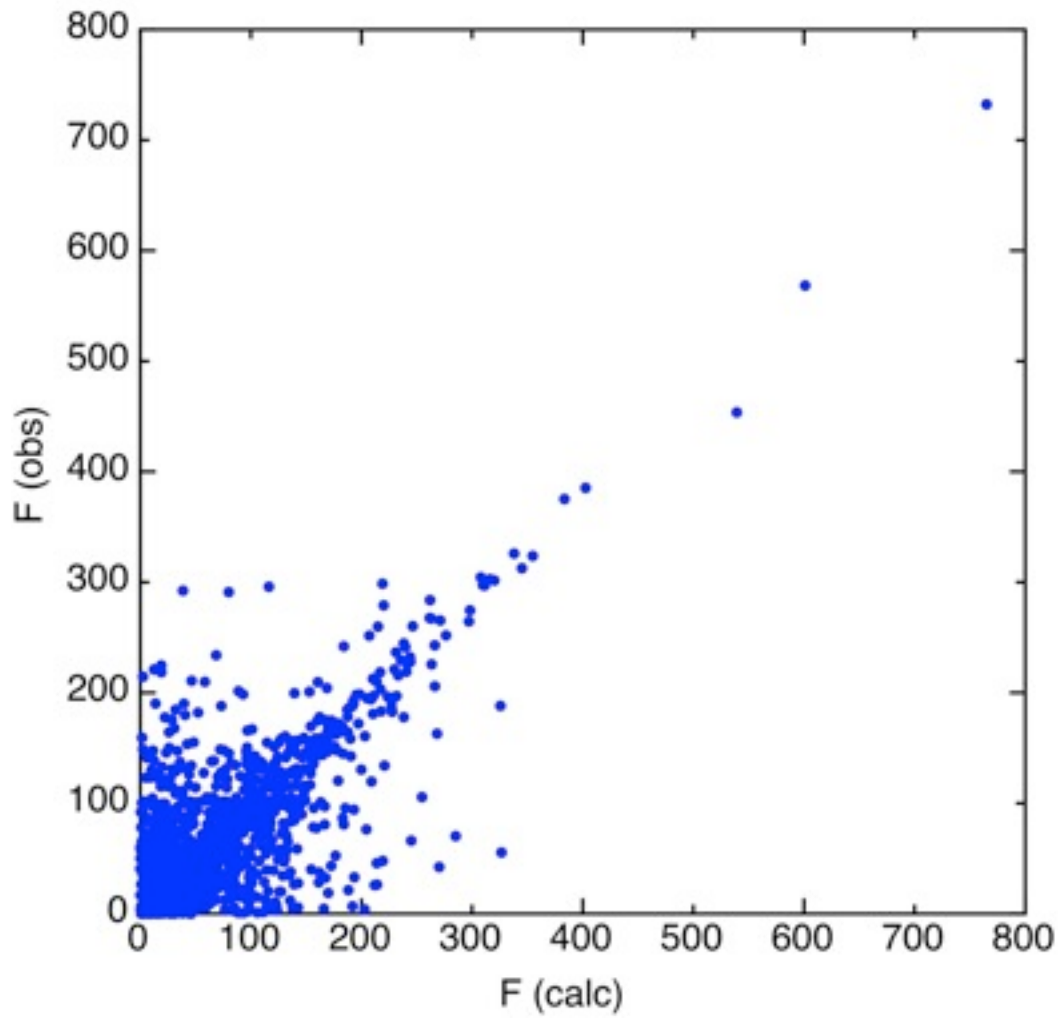


Test Example $ZrPO_4$ -pyr

F(extracted) vs. F(calculated)



untextured data
equipartinioned

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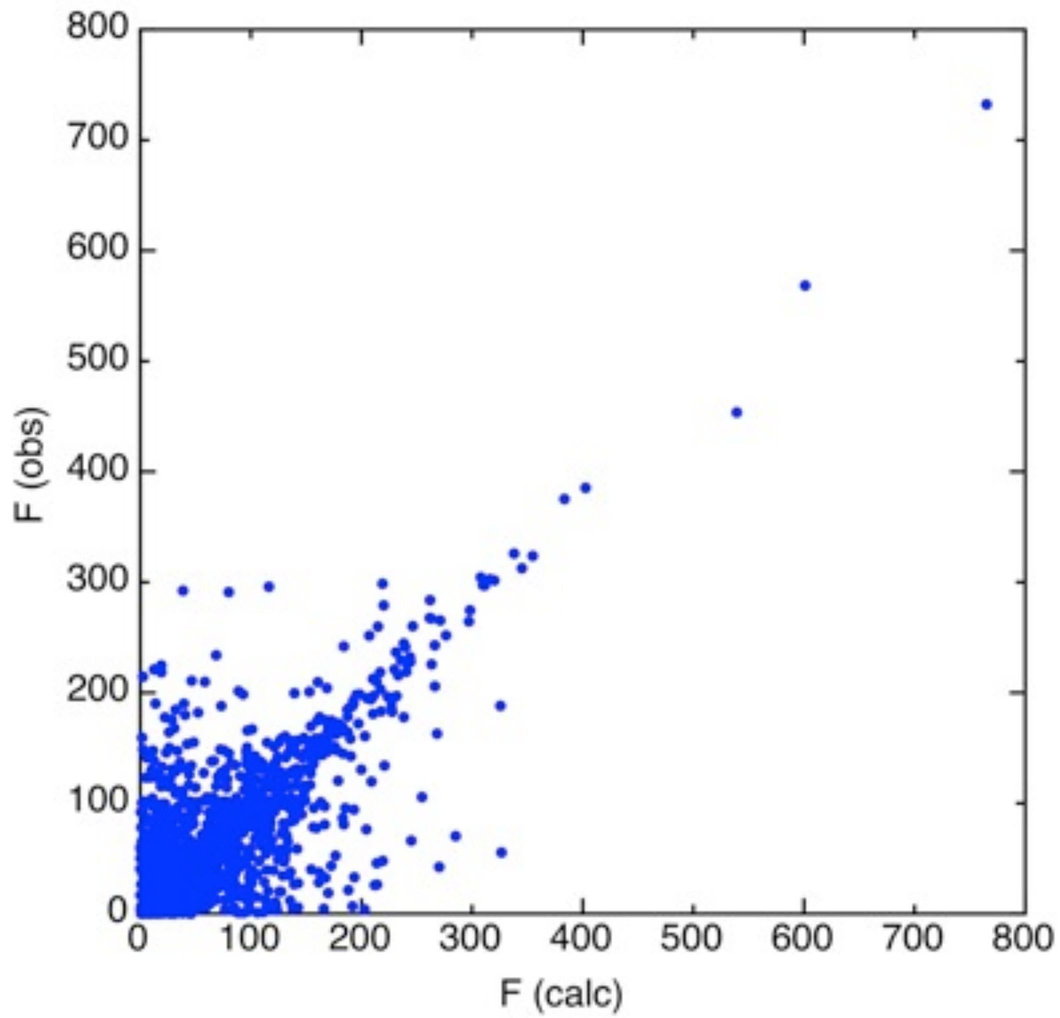

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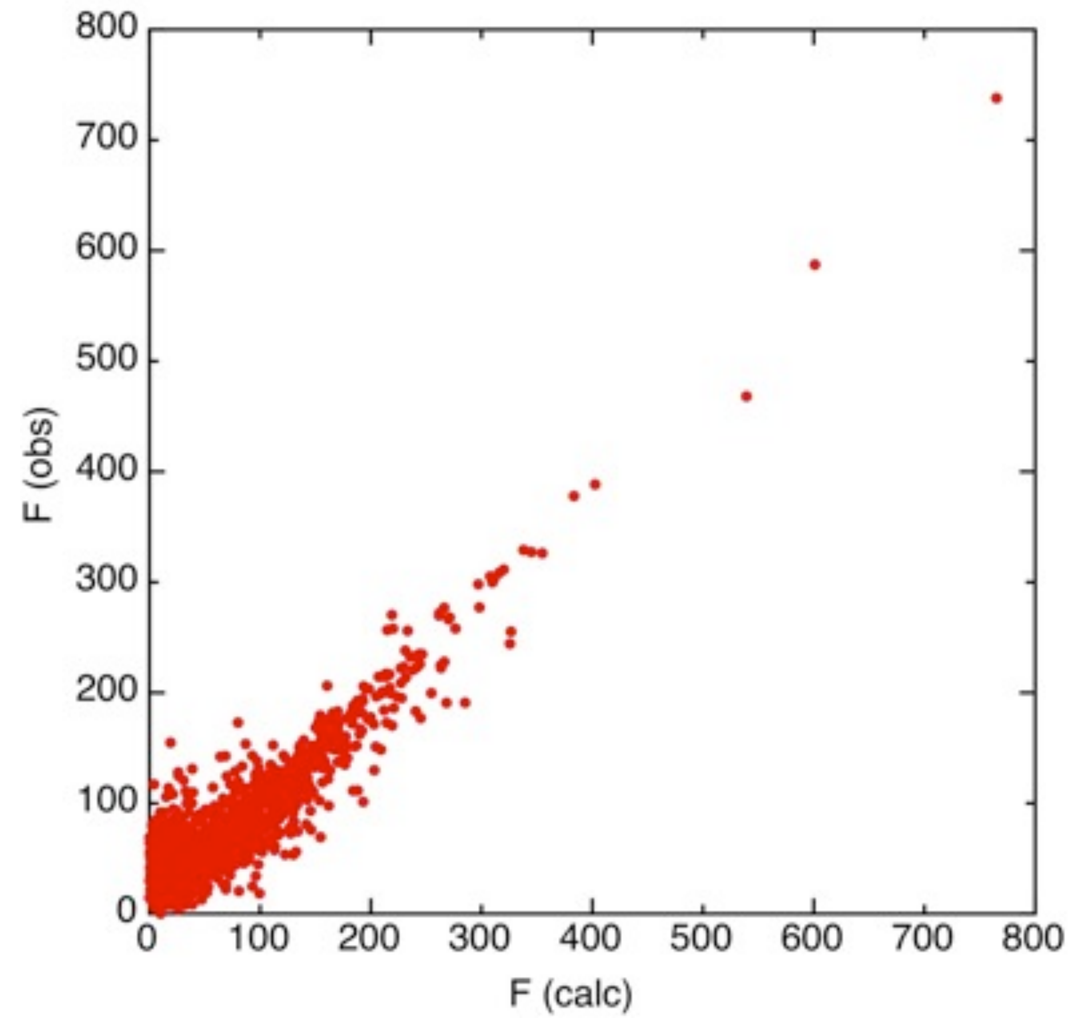
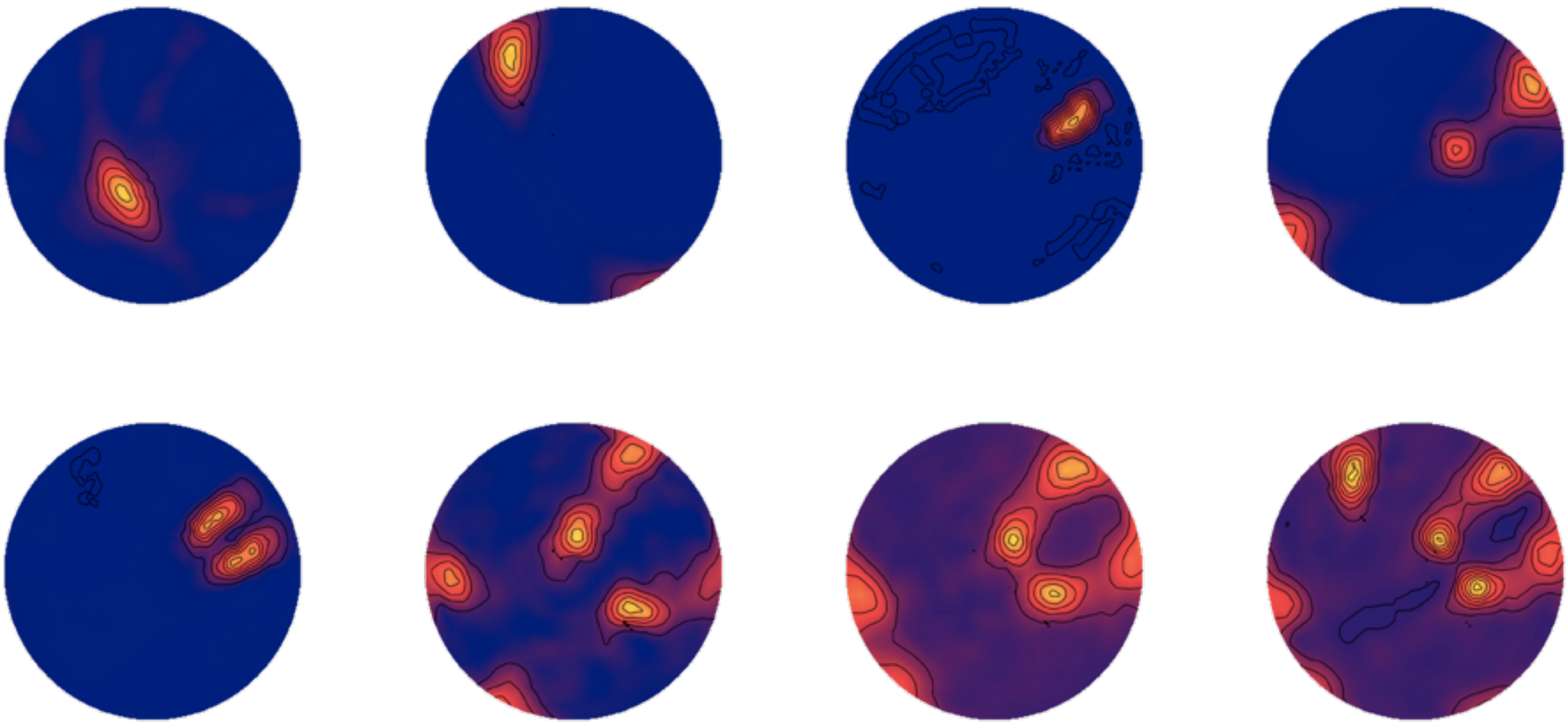


texture data

Other benefits from texture data



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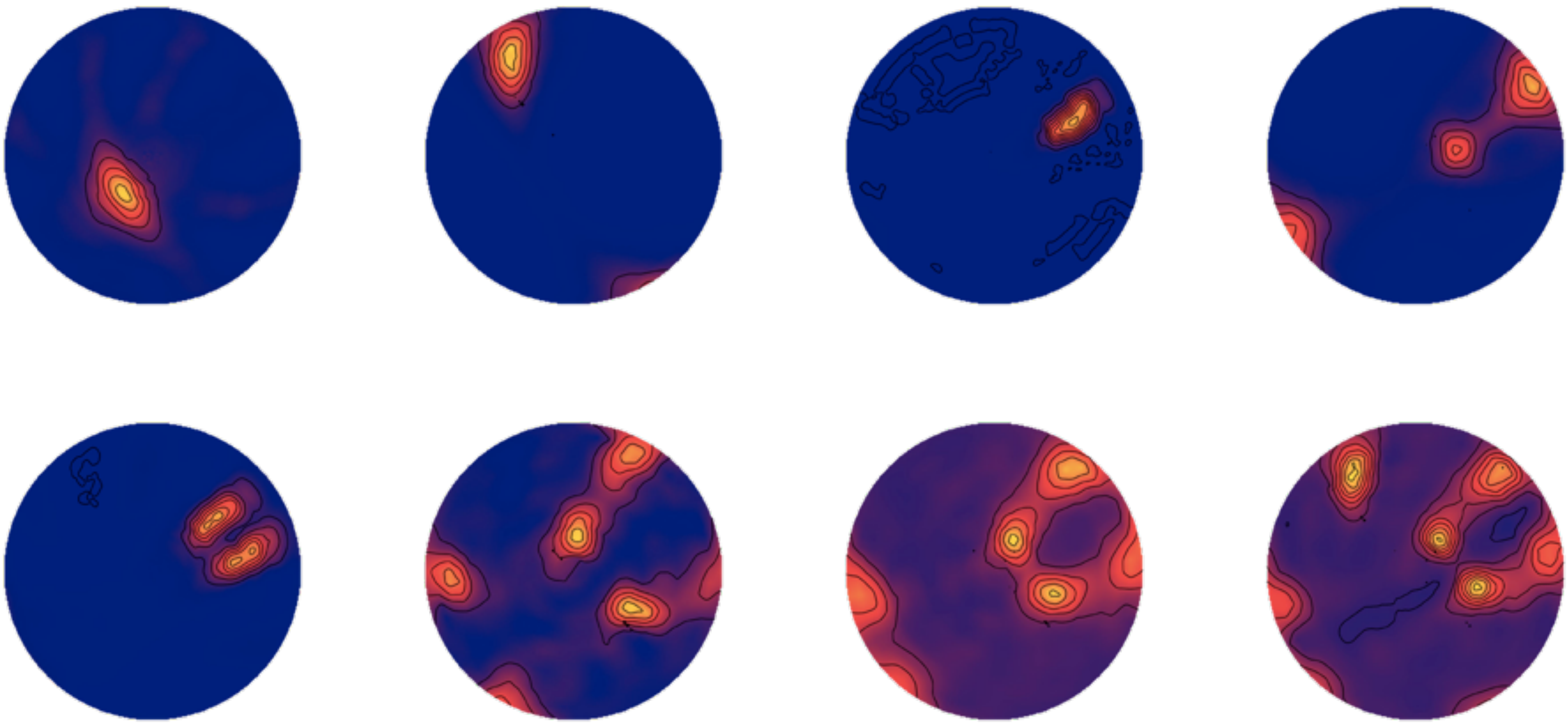

Pole figures look like a stereographic plot of a single crystal

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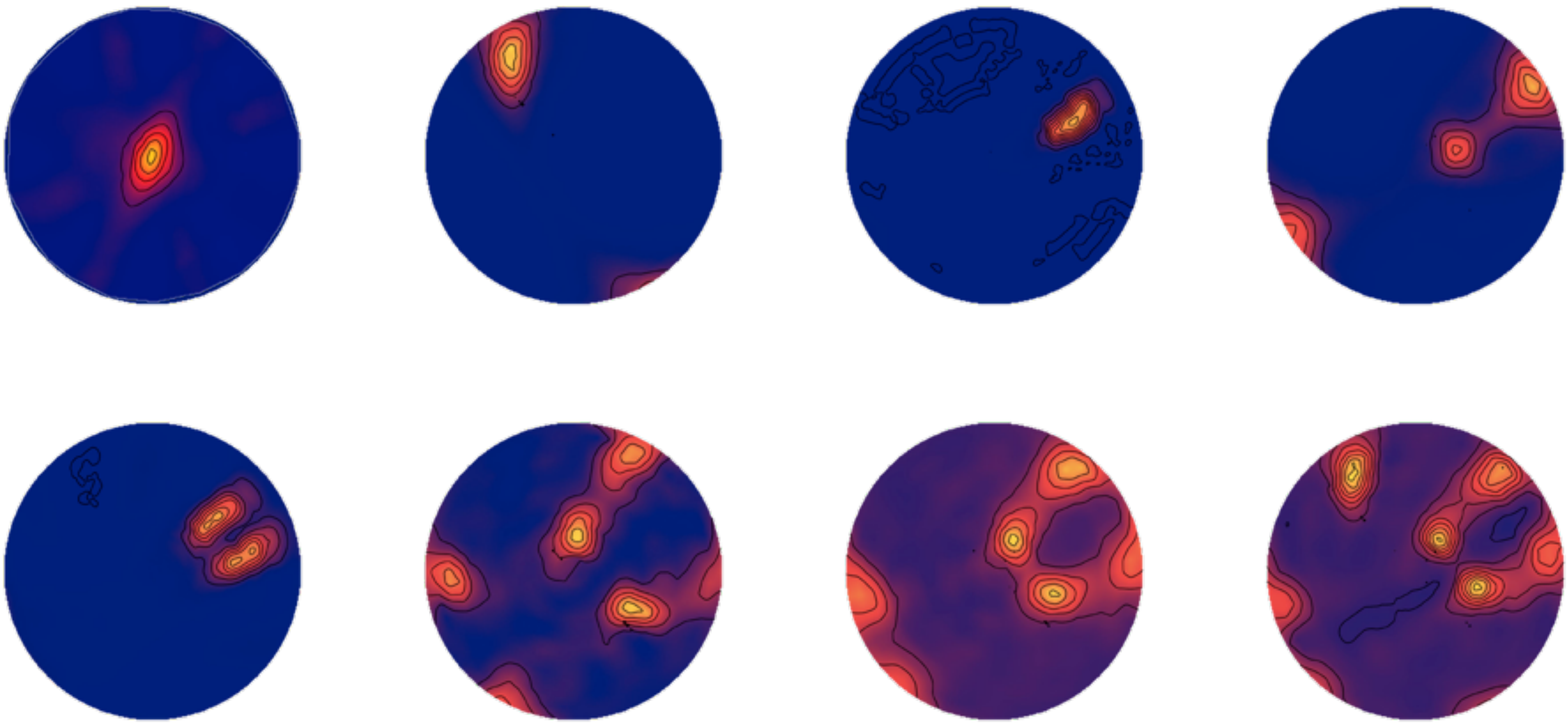

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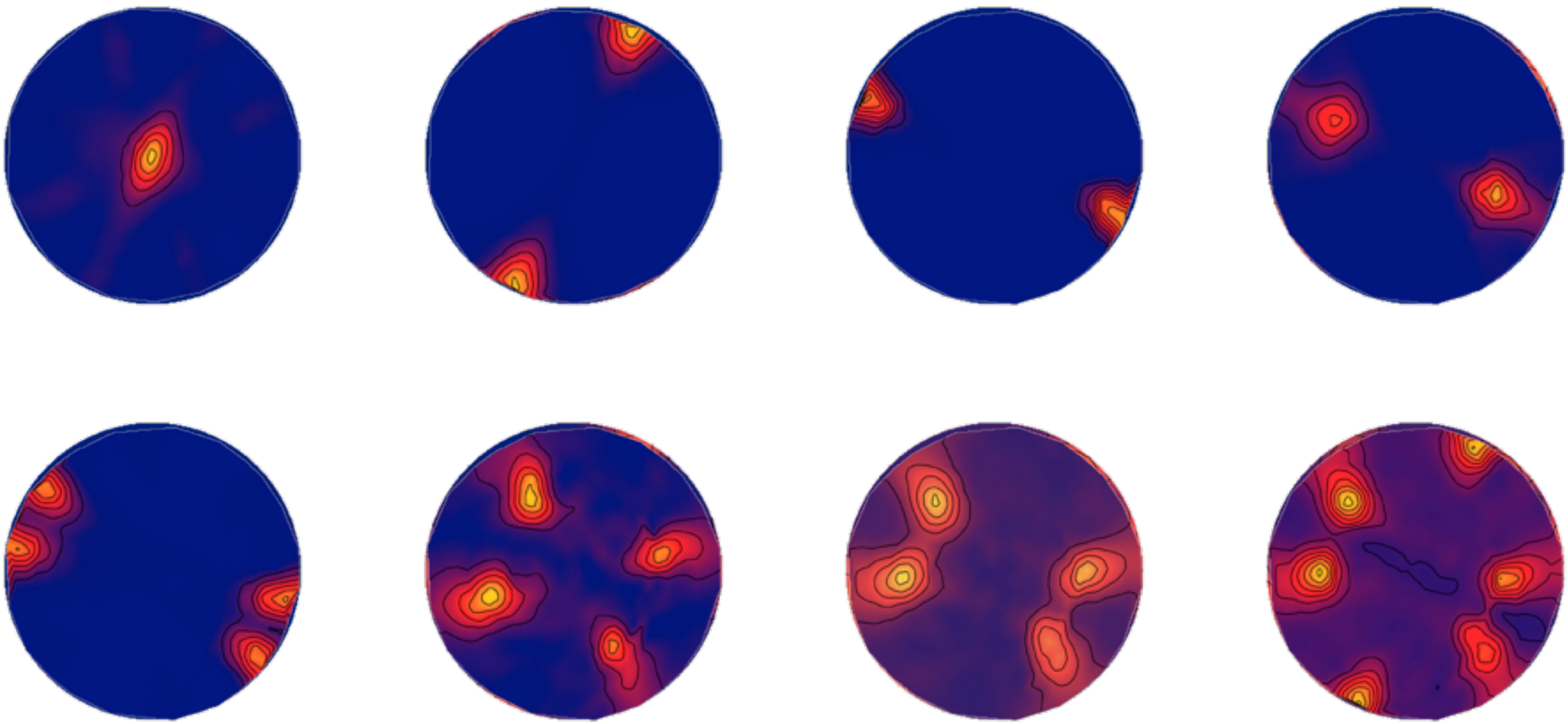

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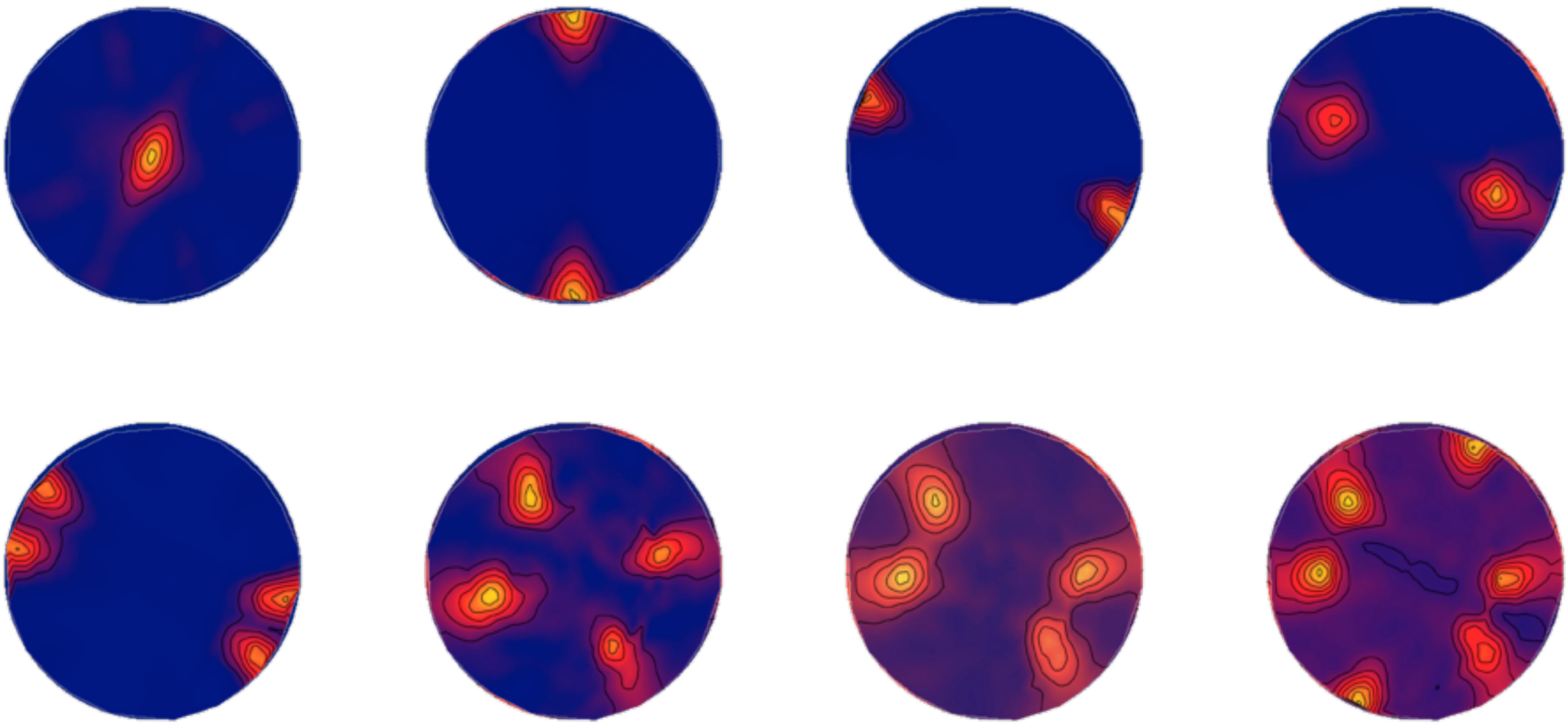

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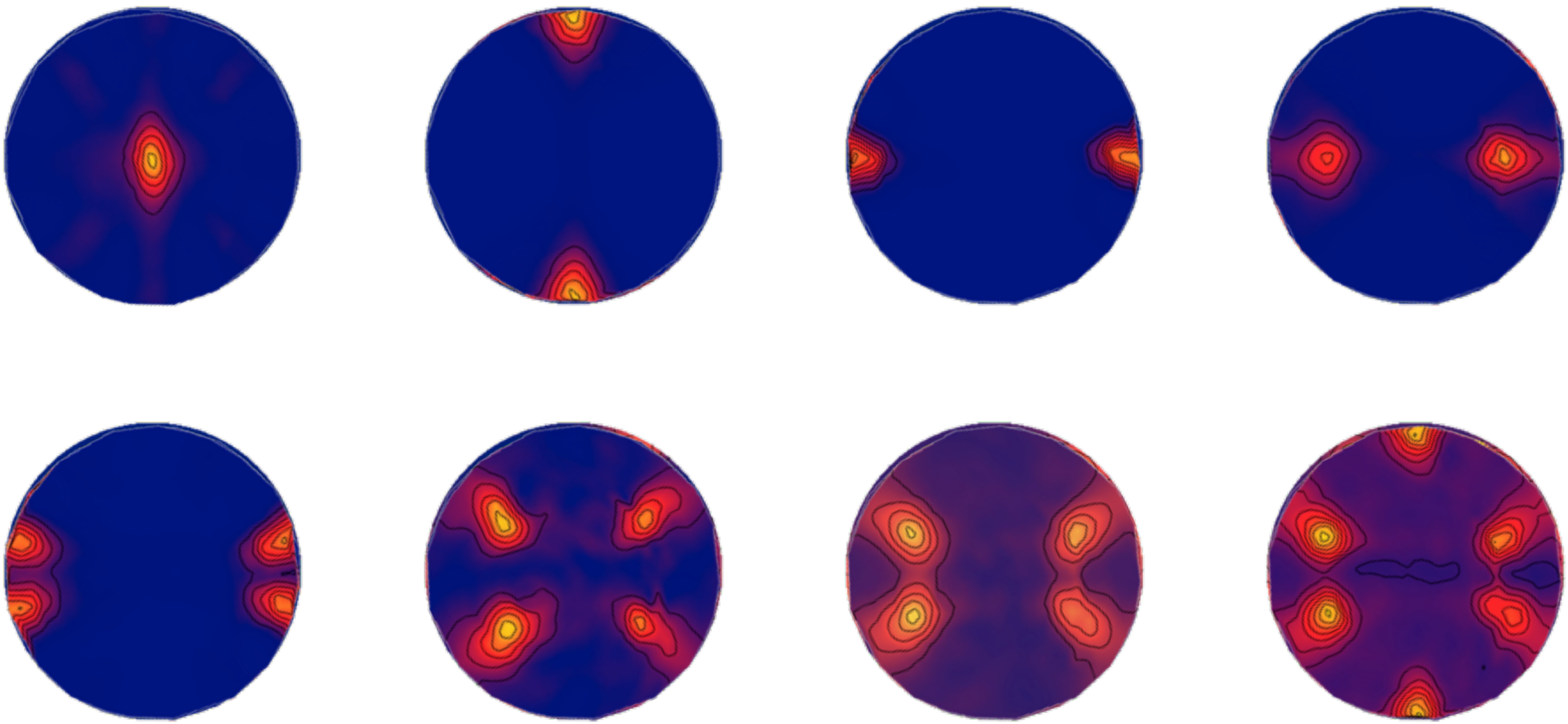

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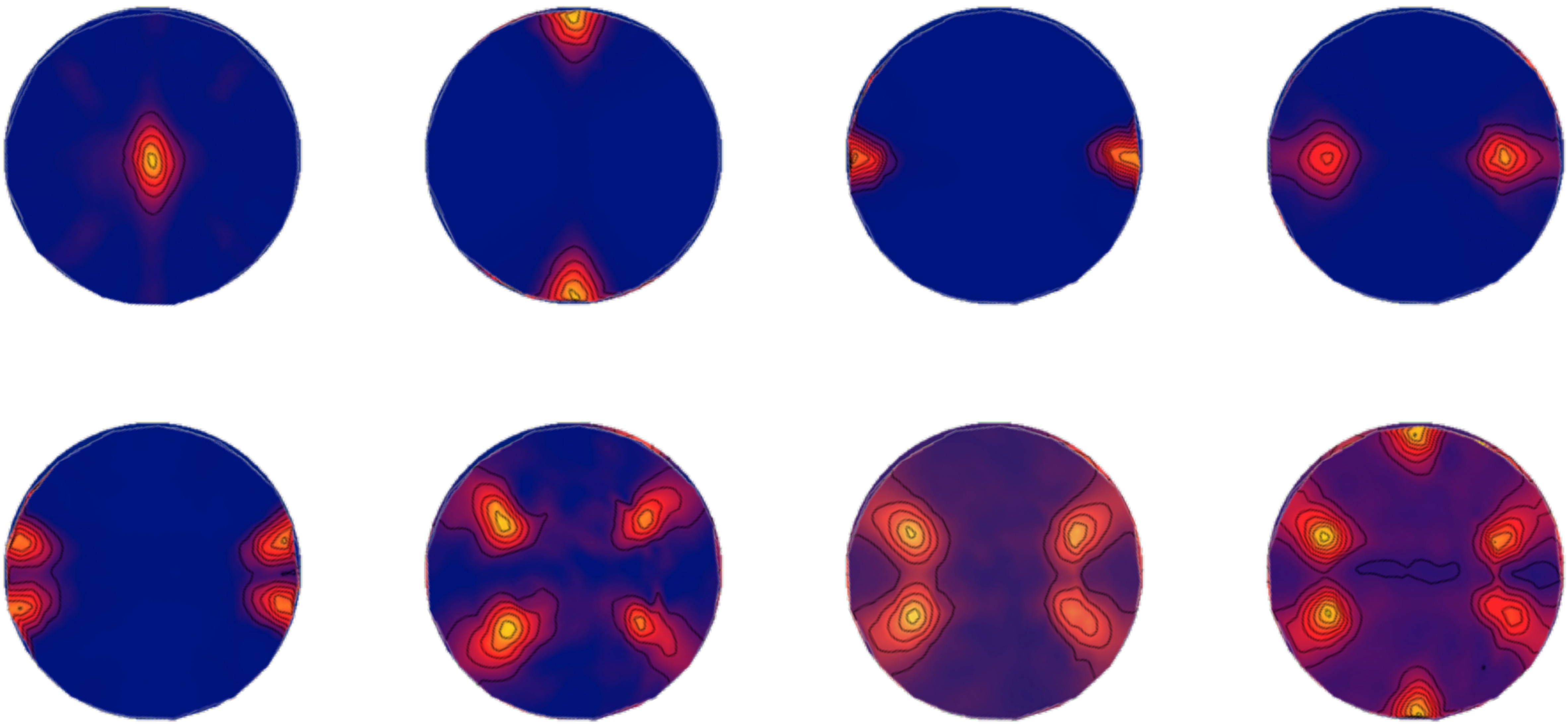
Other benefits from texture data

- Symmetry determination



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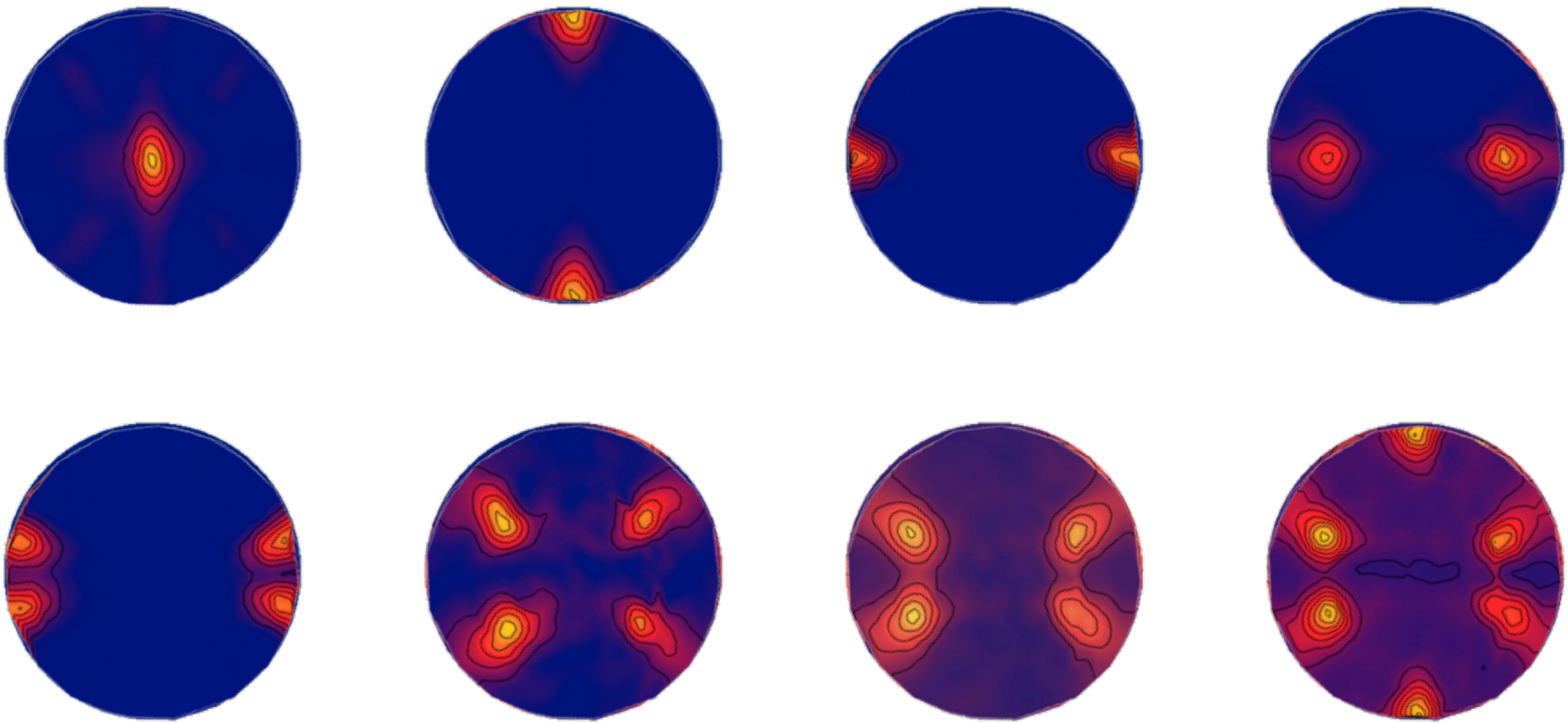
sample symmetry: mm2



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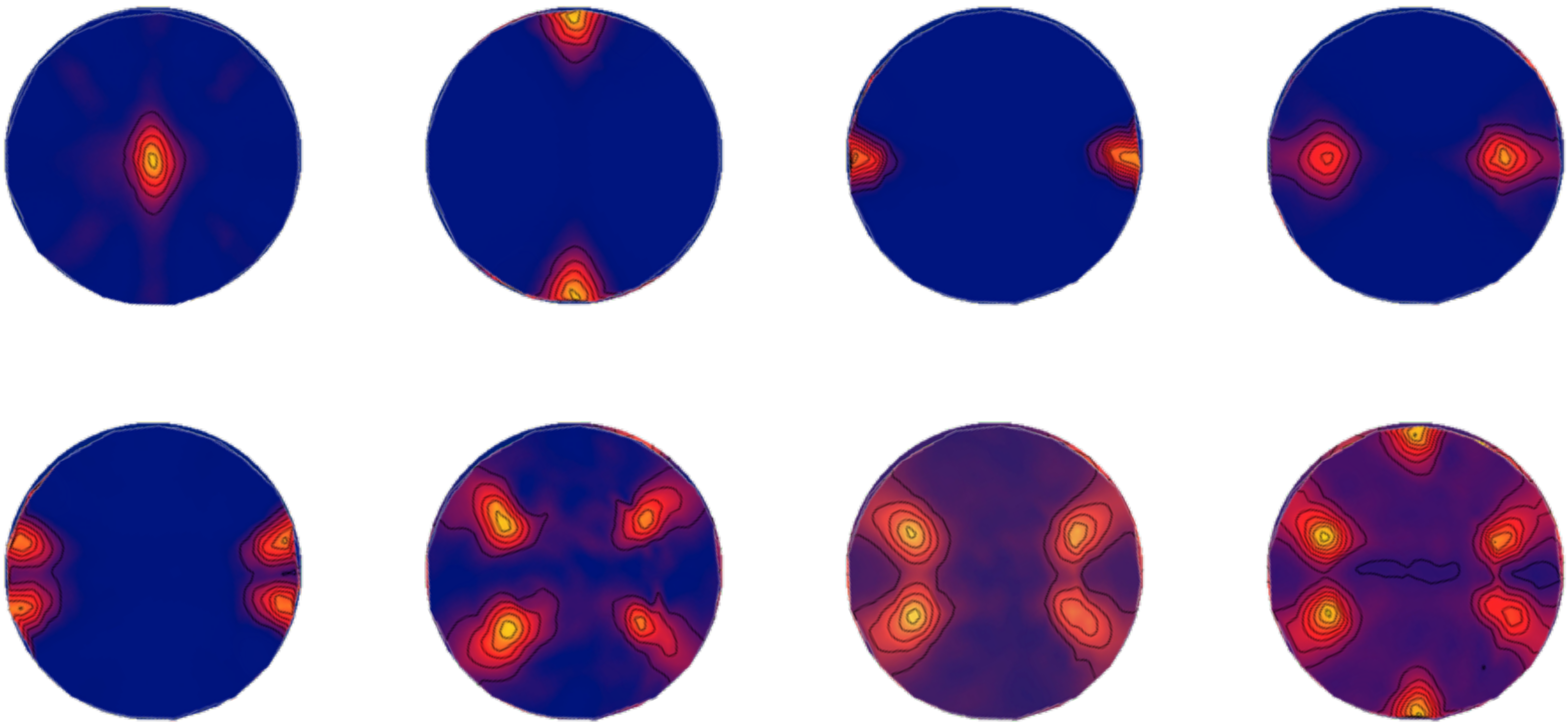
crystal symmetry: triclinic



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Other benefits from texture data

- Symmetry determination
- Indexing

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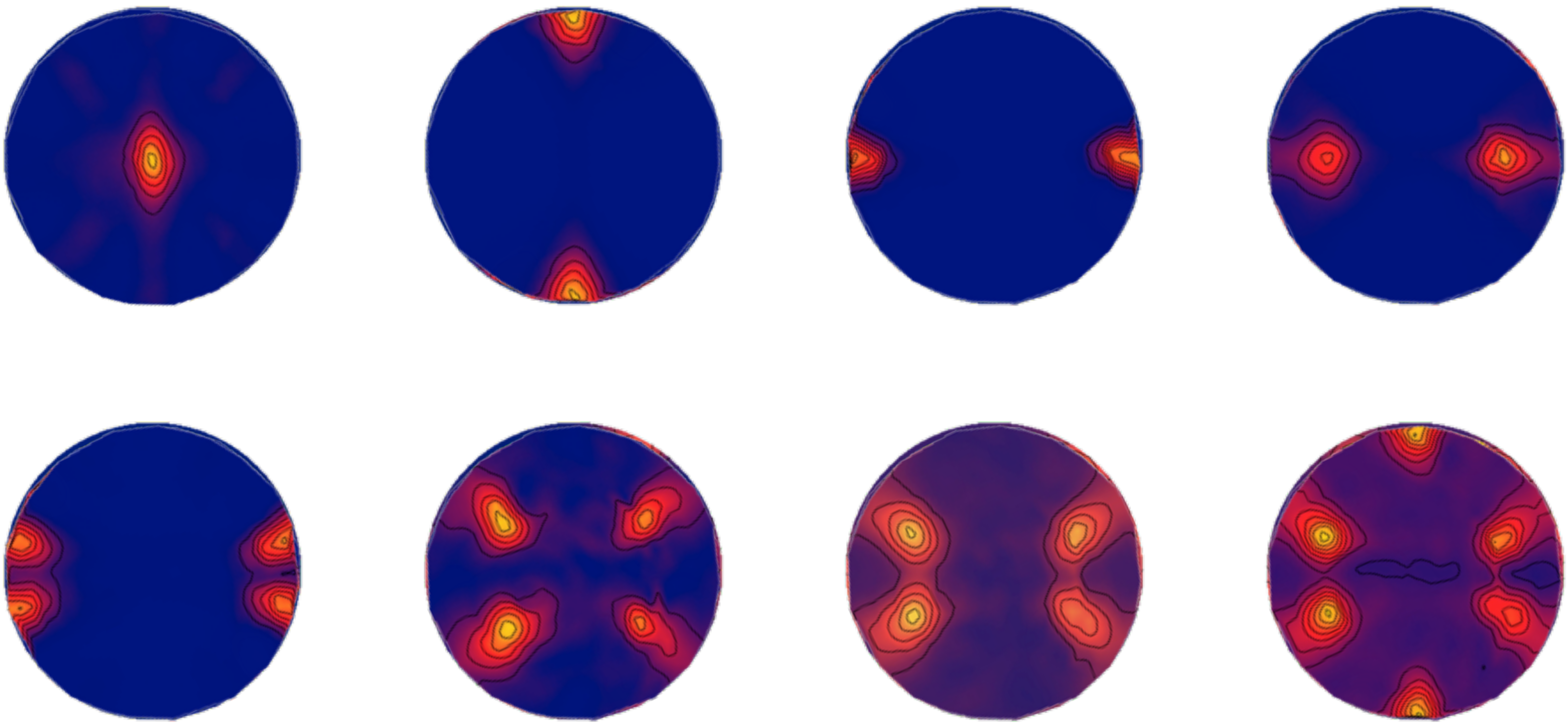

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Maxima in pole figures give direction of lattice planes → Normal of corresponding crystal face

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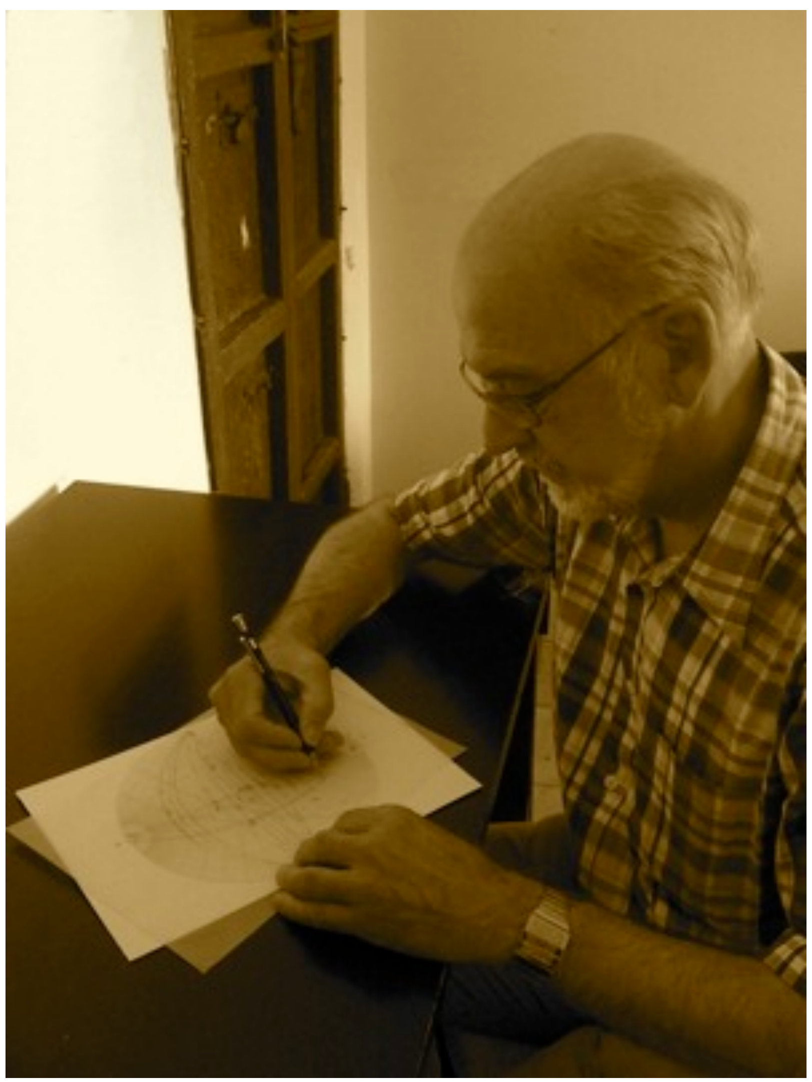

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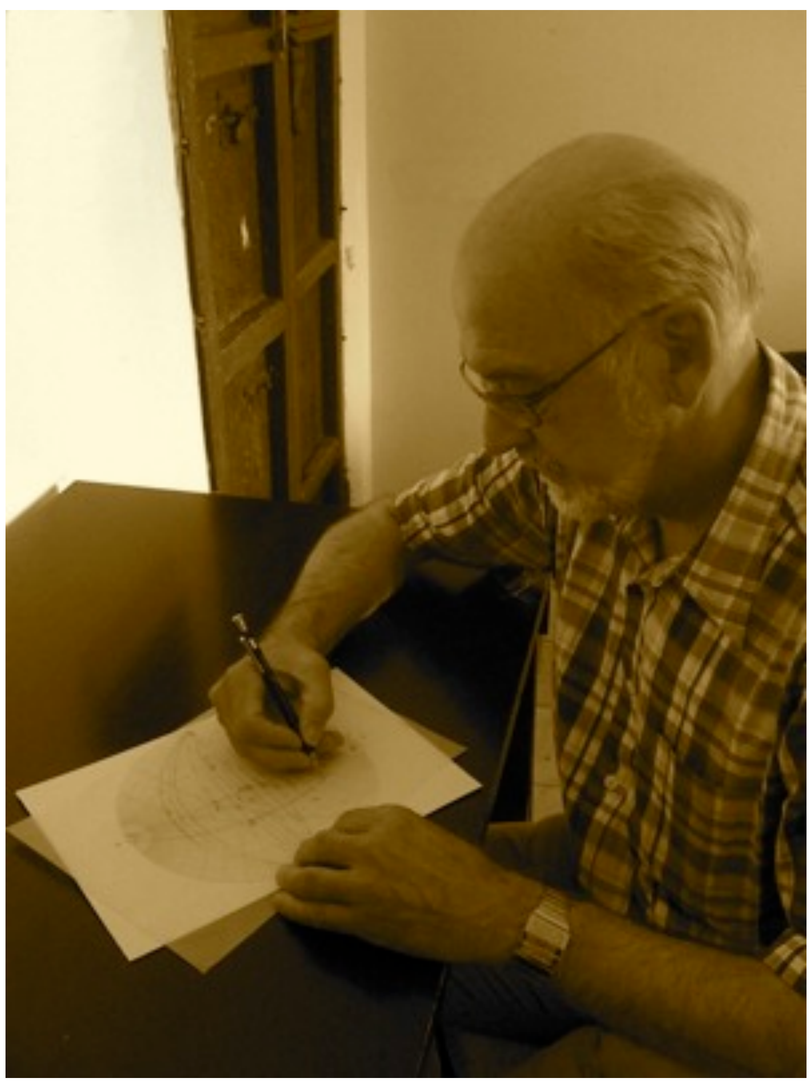

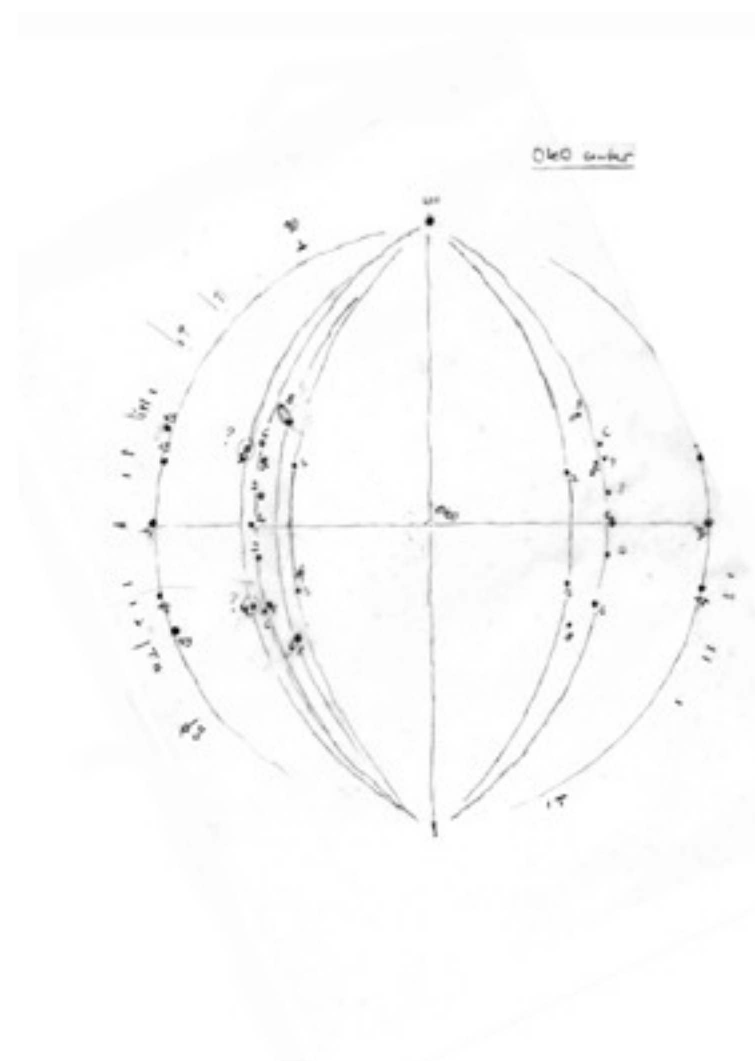

Other benefits from texture data

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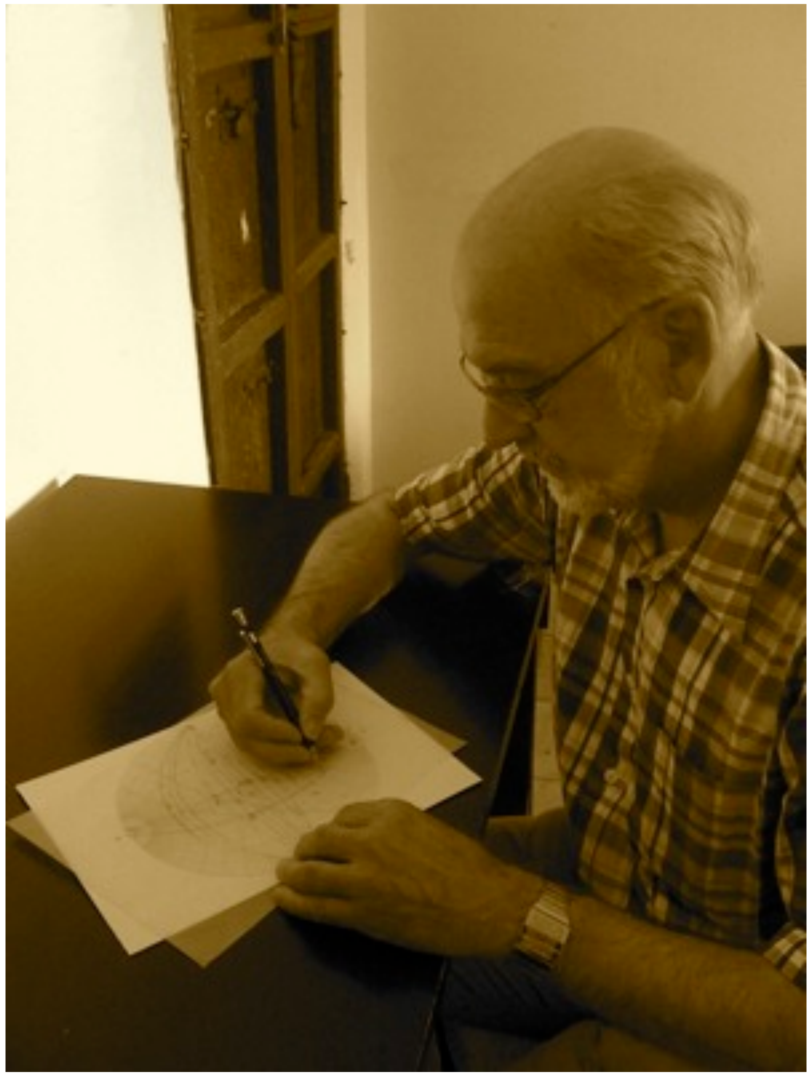
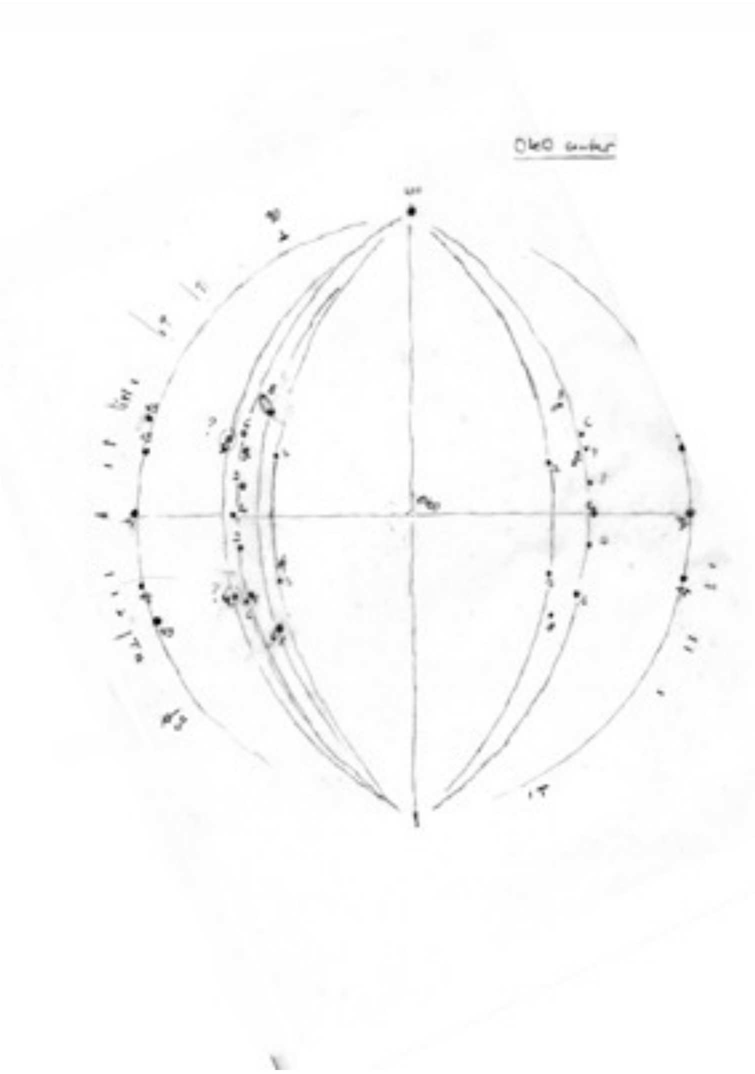
Maxima in pole figures give direction of lattice planes → Normal of corresponding crystal face

d-values of reflections give length of reciprocal lattice vector → reciprocal lattice





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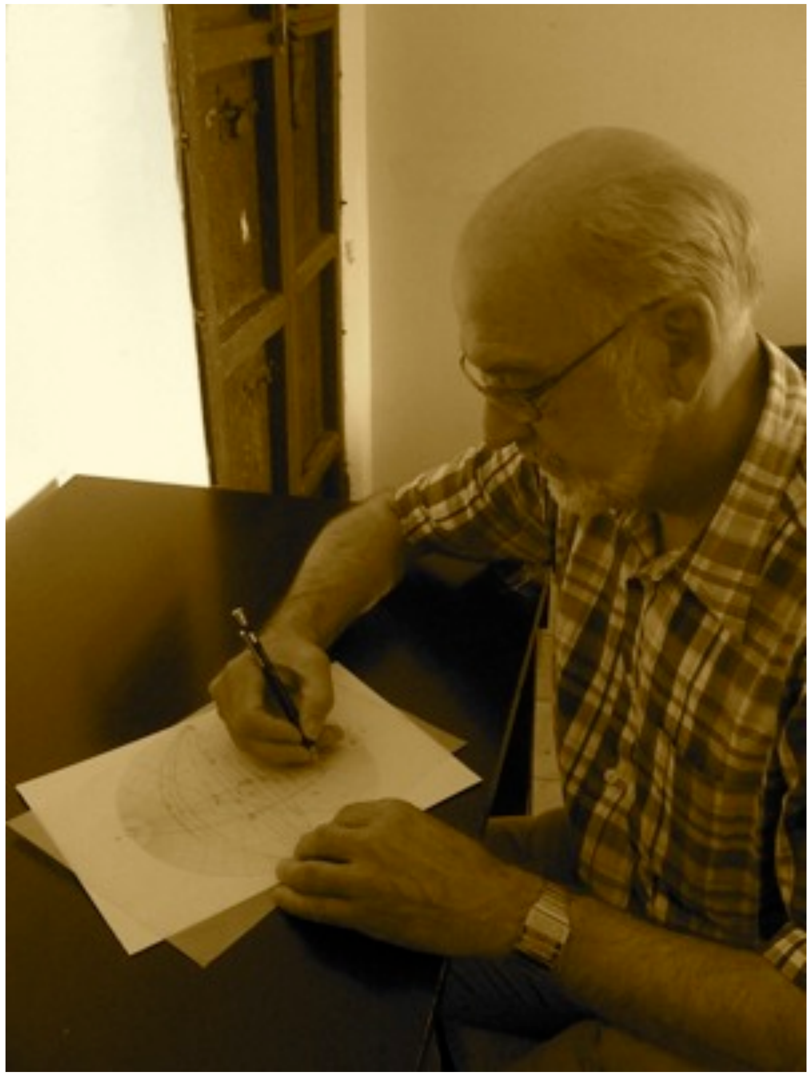

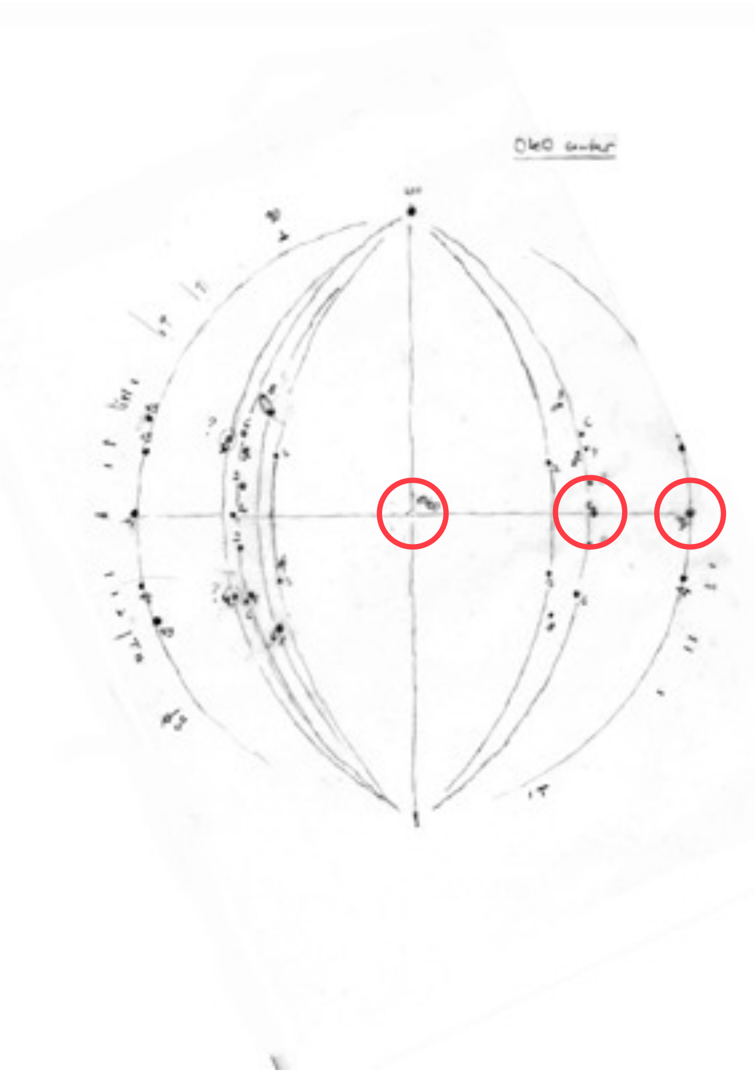

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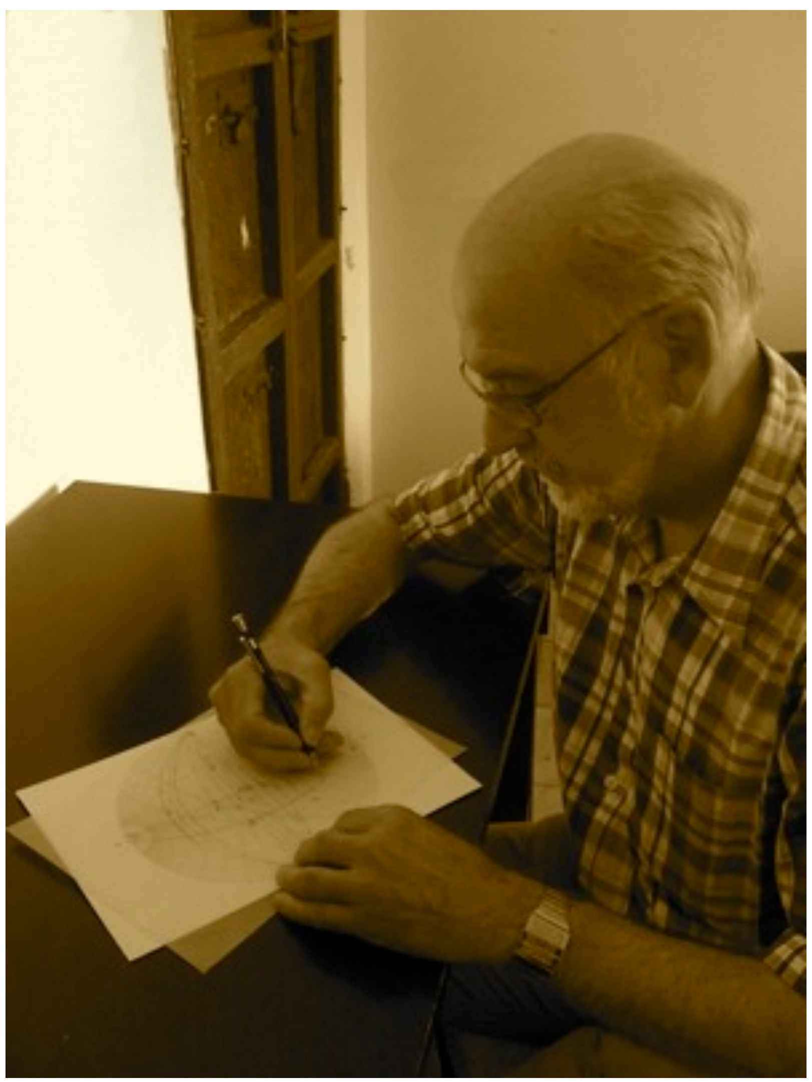

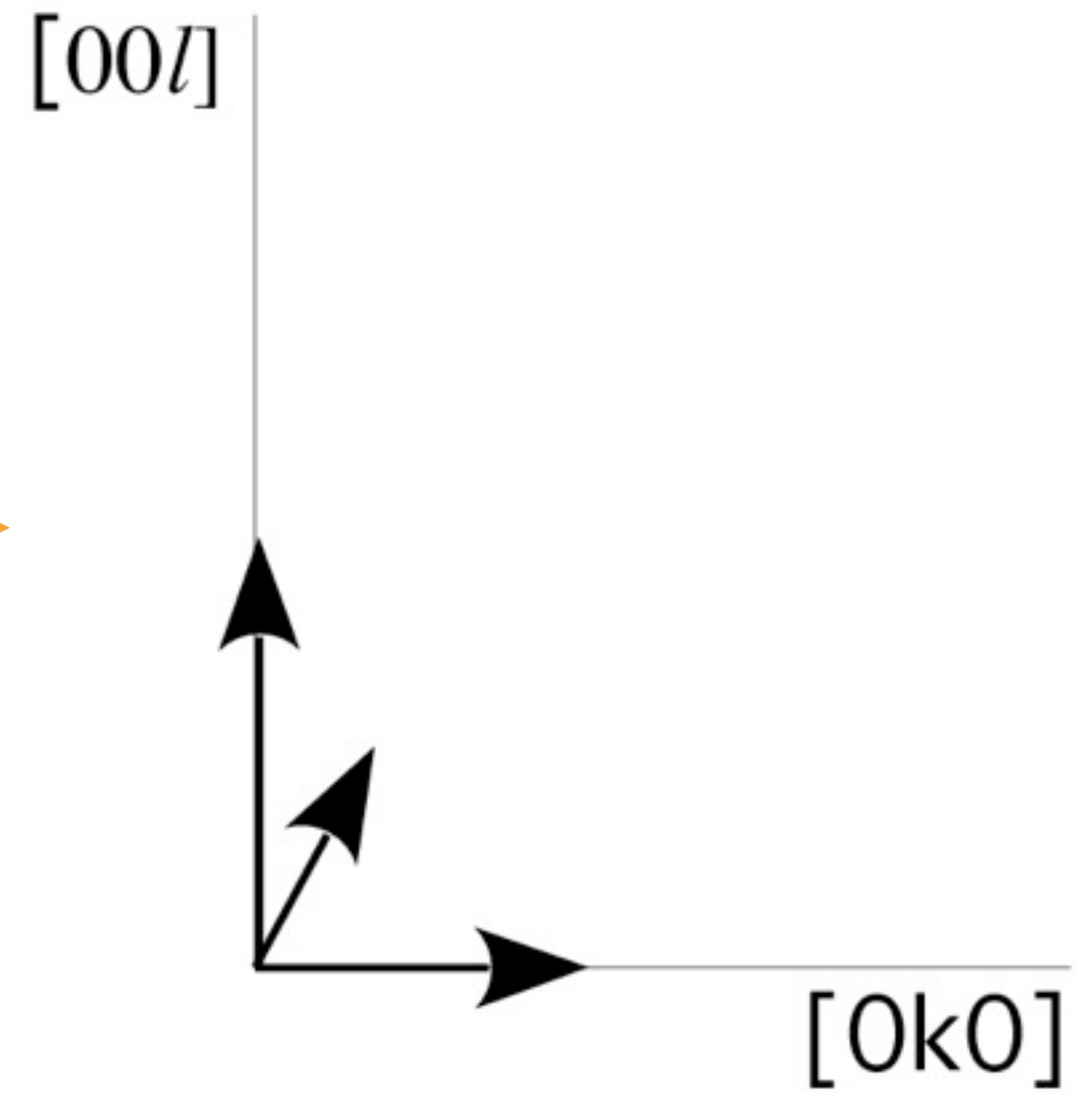

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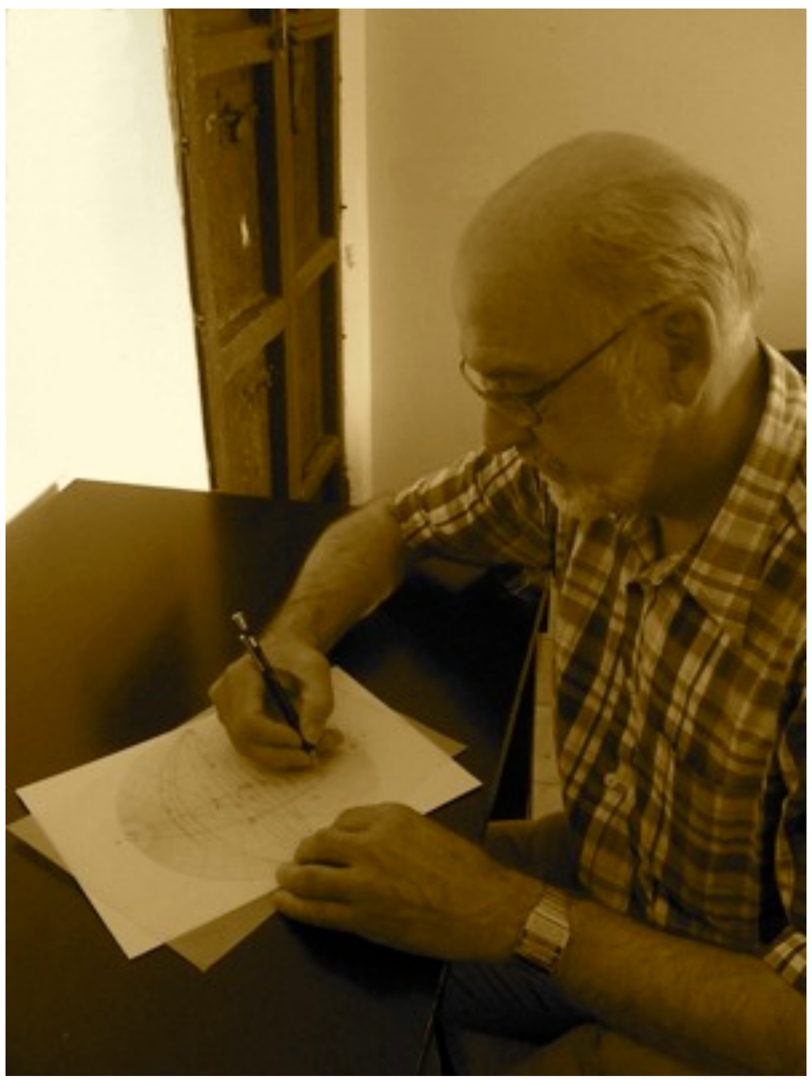

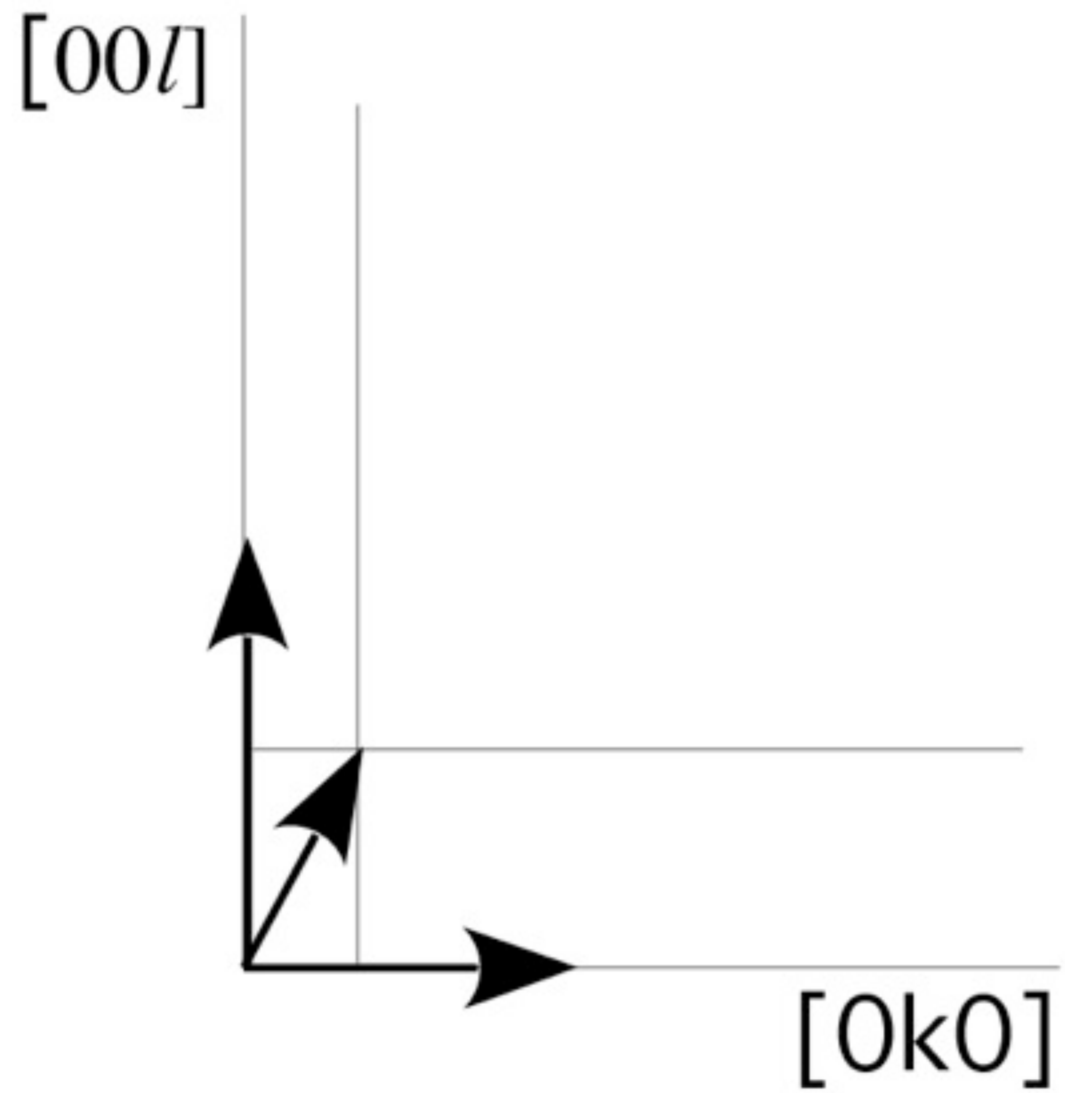

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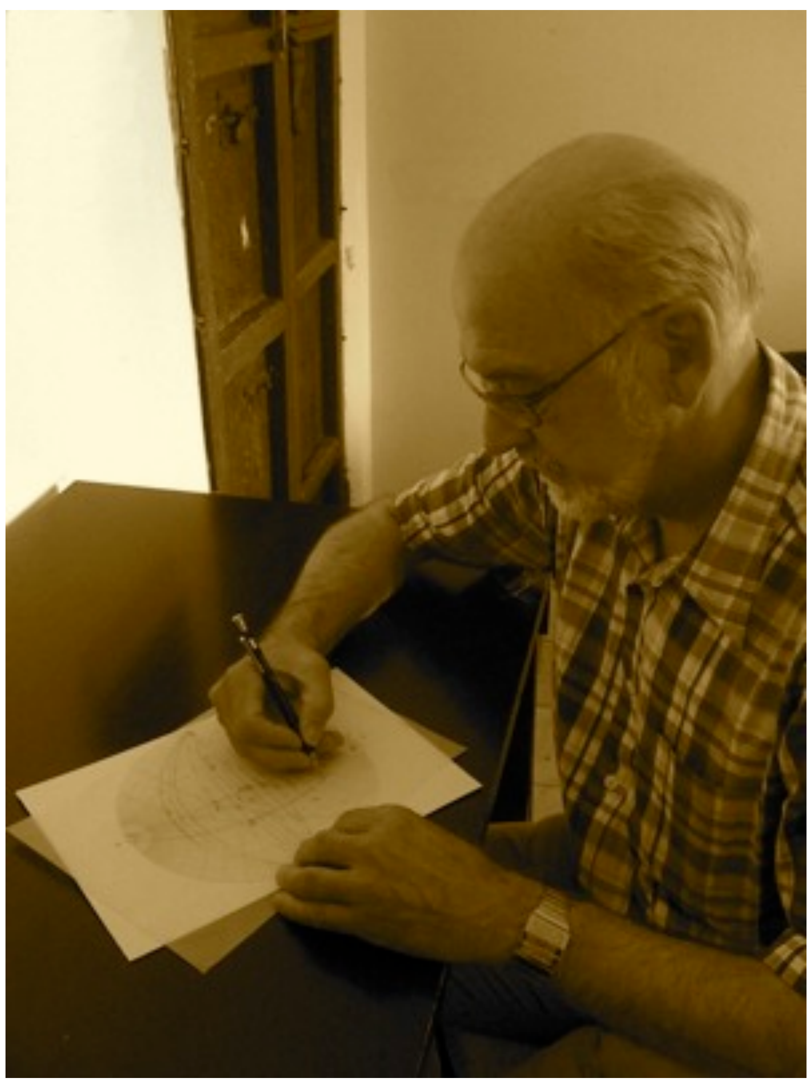

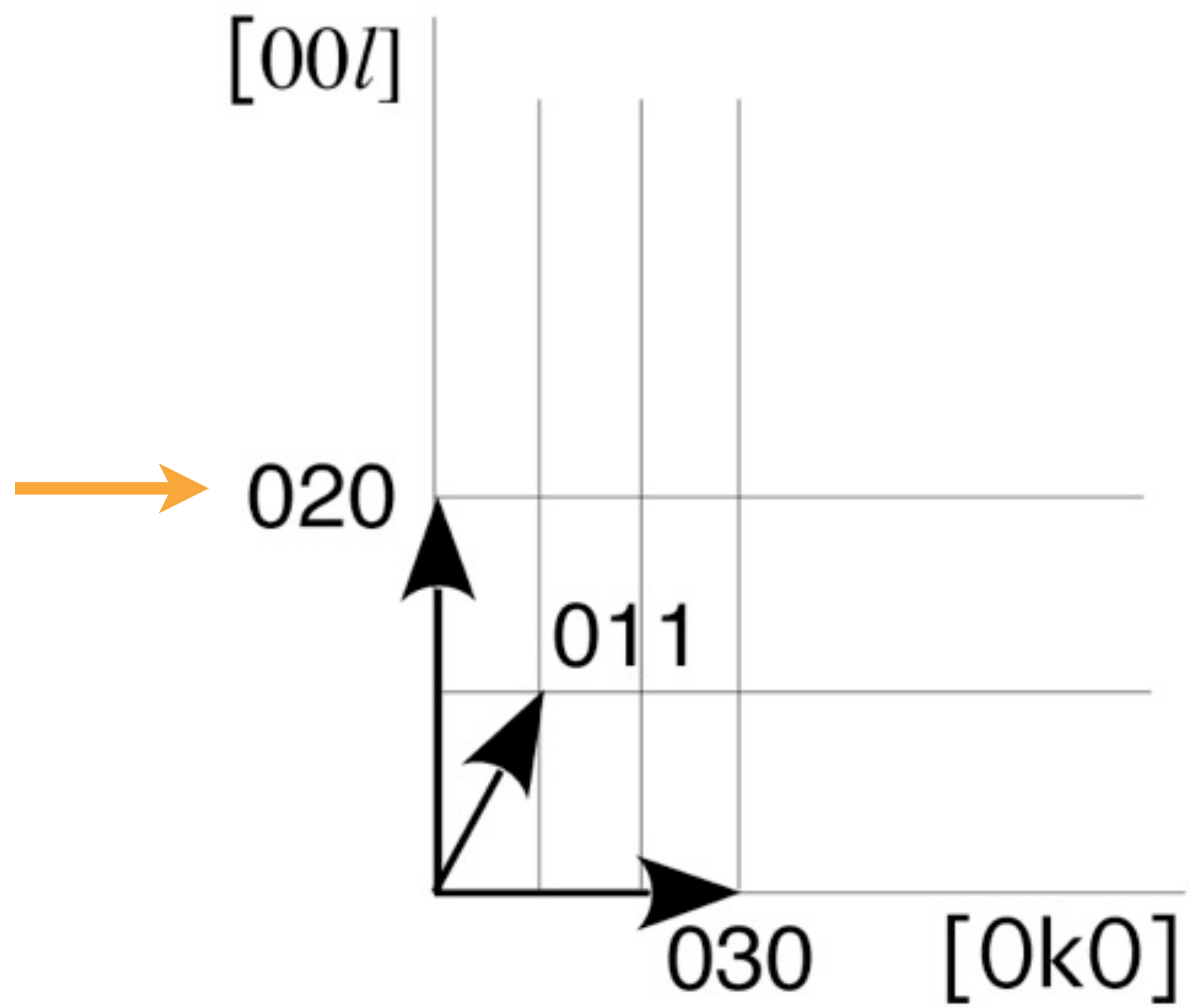

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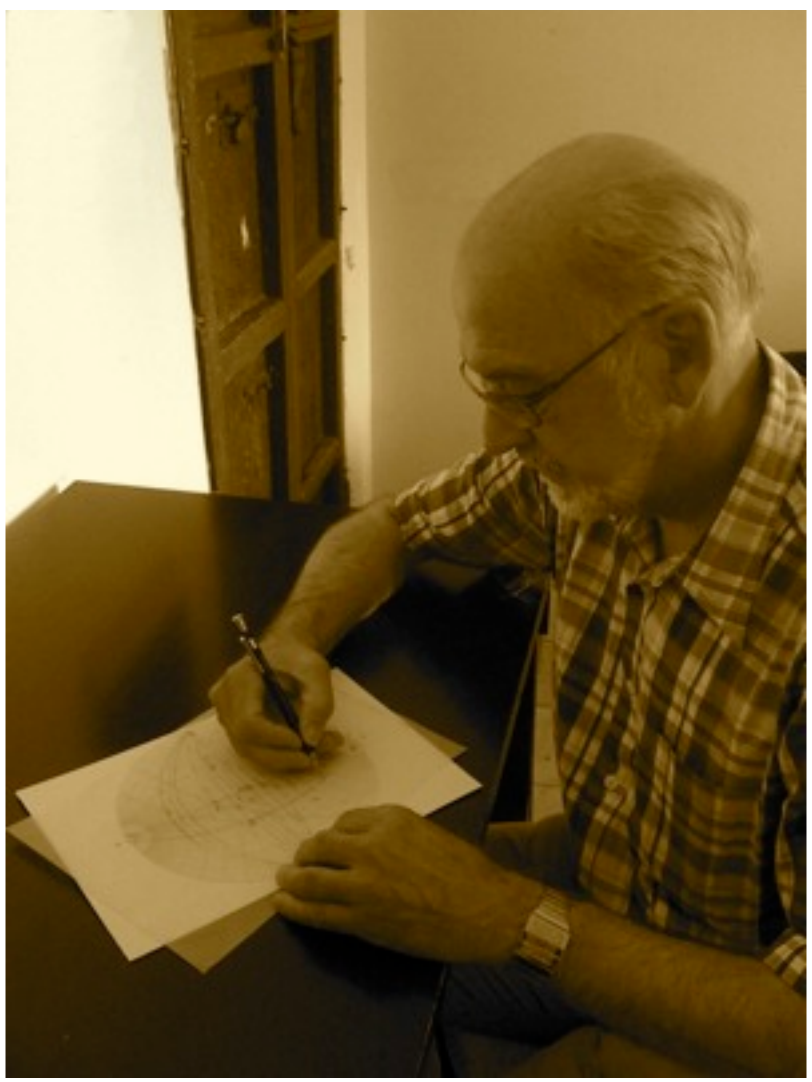

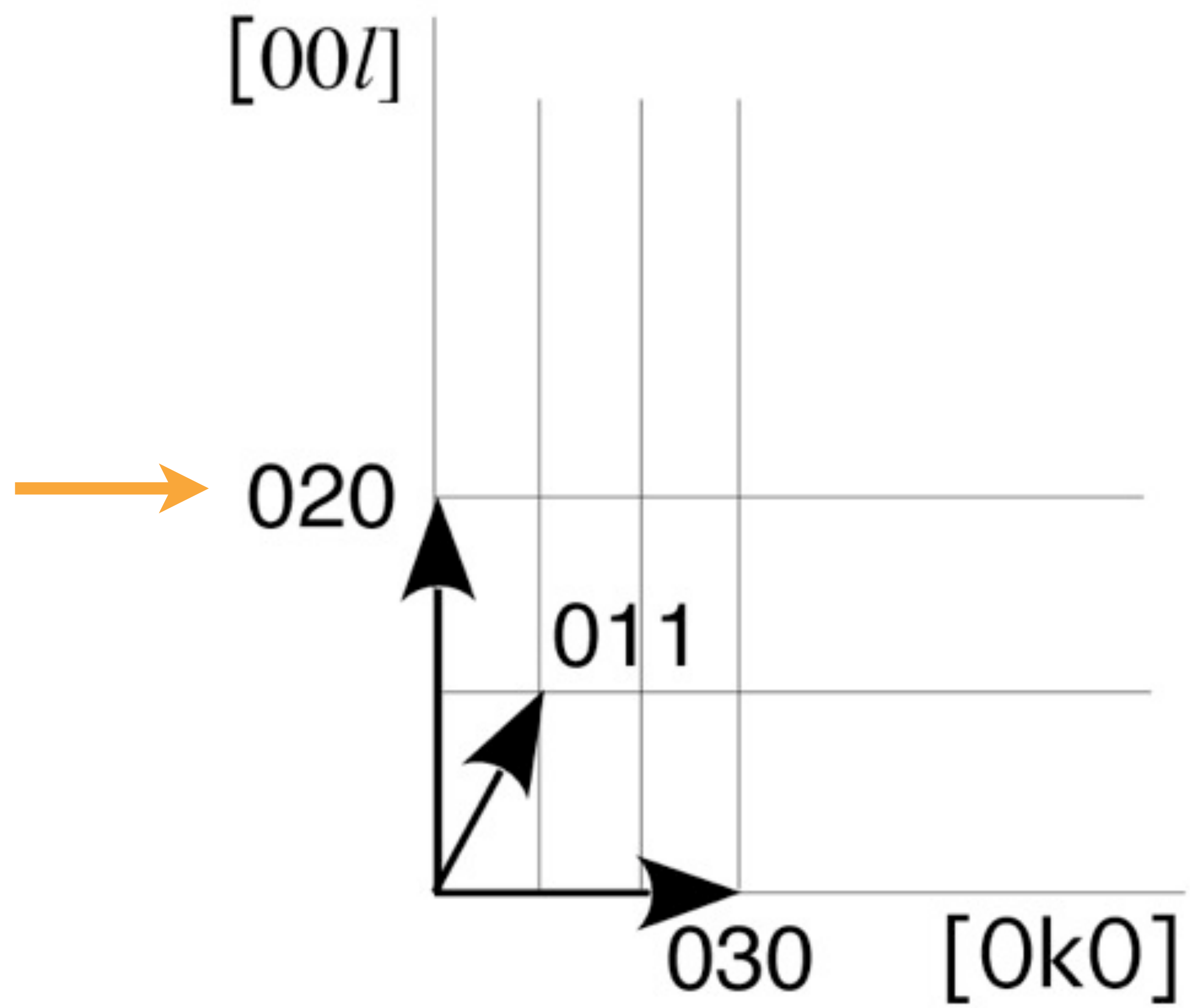

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Pole figures can help in determining the space group and indexing the powder pattern.

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

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Lynne McCusker