Beam Coherence Effects on Coherent X-ray Diffraction Imaging

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EPSRC Engineering and Physical Sciences Research Council
LCN LONDON CENTRE FOR NANOTECHNOLOGY
Argonne NATIONAL LABORATORY

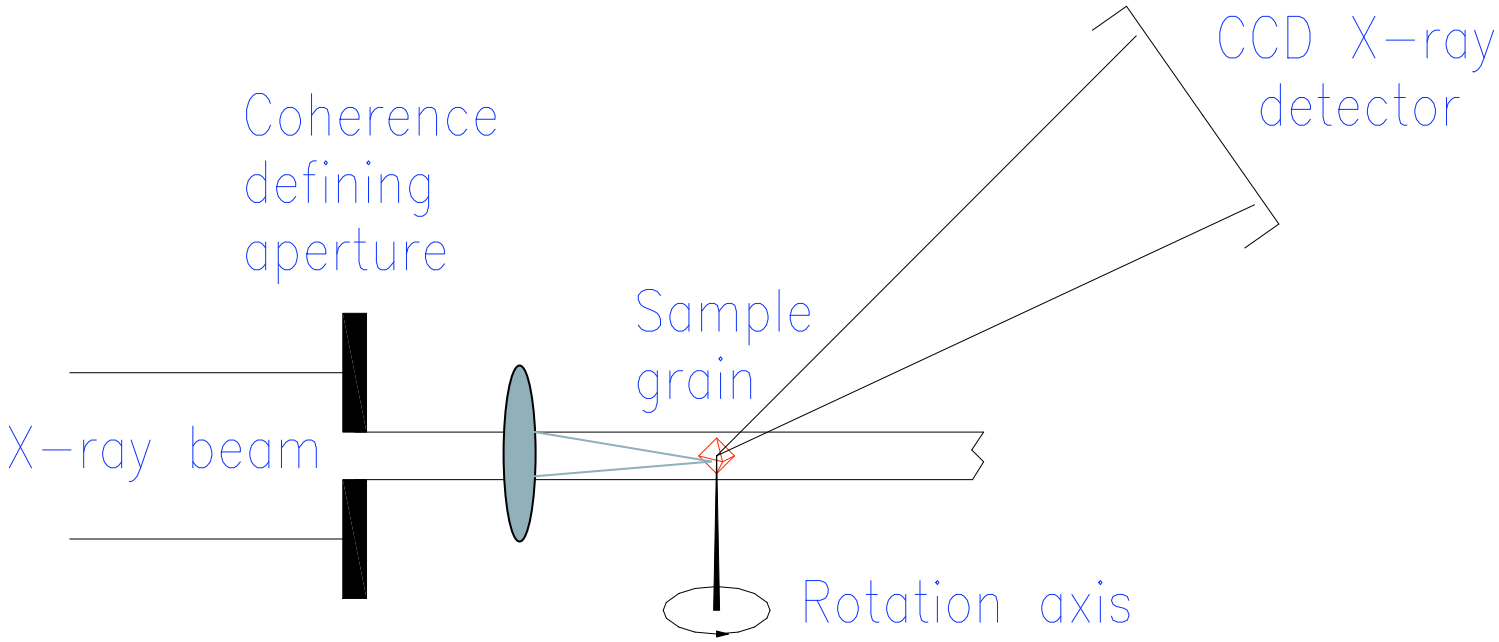
Outline

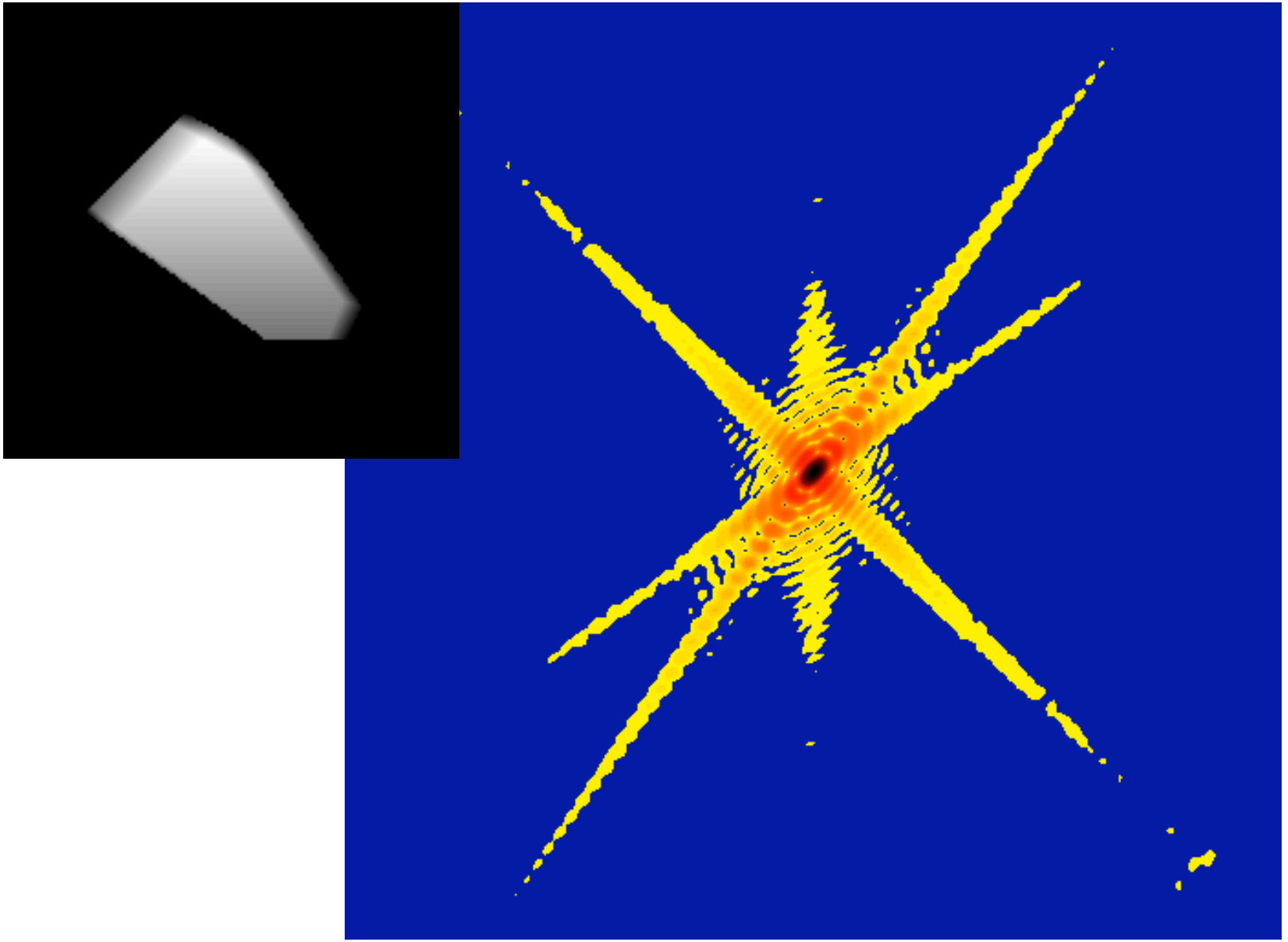
- Overview of CXD technique
- New Sample Preparation method
- Alignment method
- Coherence / Contrast
- Consequences for the reconstructions

Coherent X-ray Diffraction Imaging

APS ξ_{HOR}= 20μm, focus to 1μm

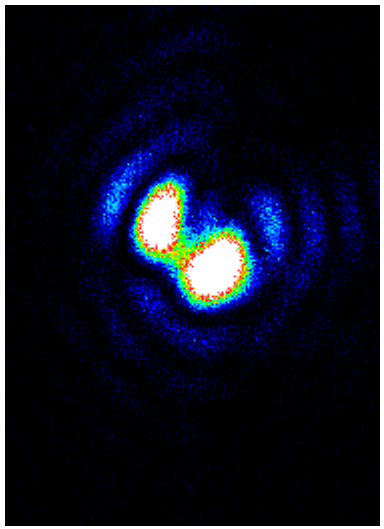
LCLS ξ_{HOR}> 500μm, focus to 0.1μm

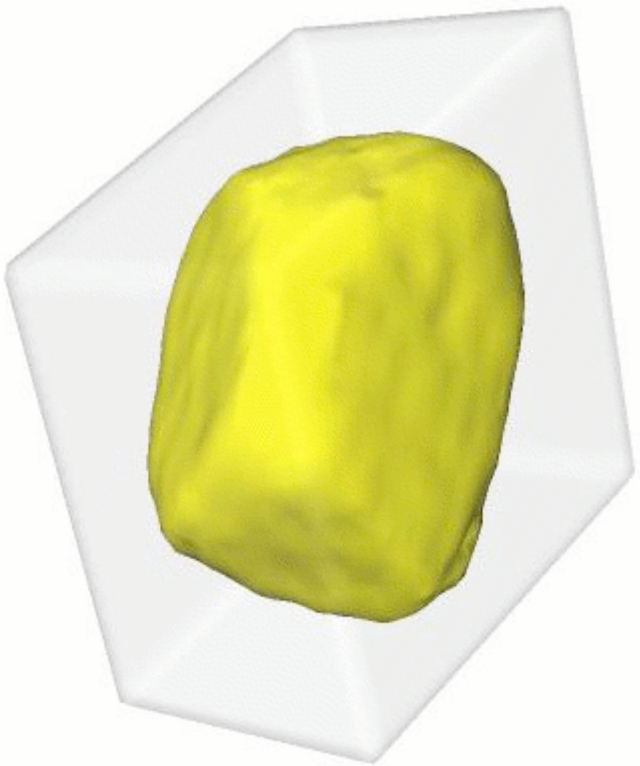


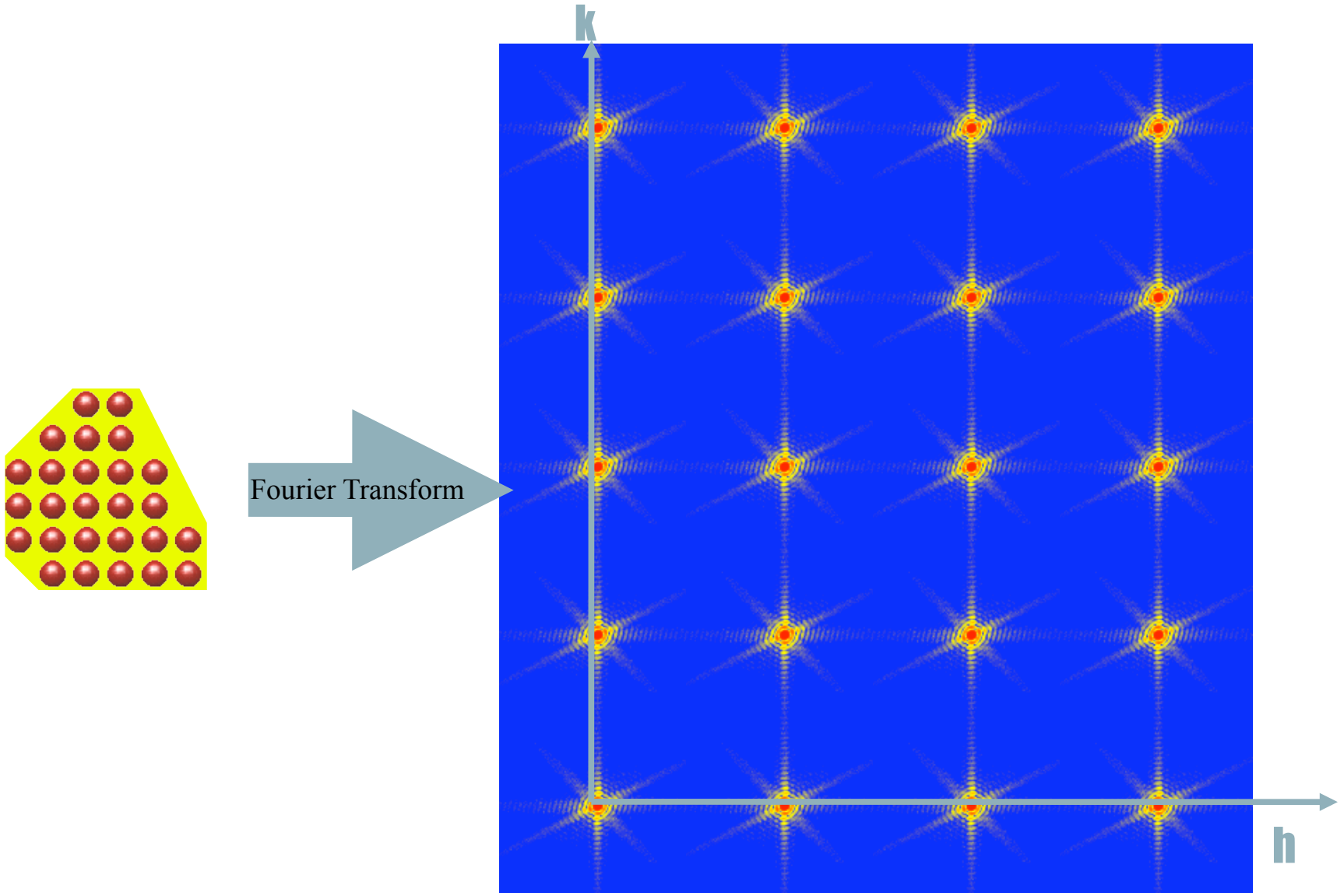


Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER



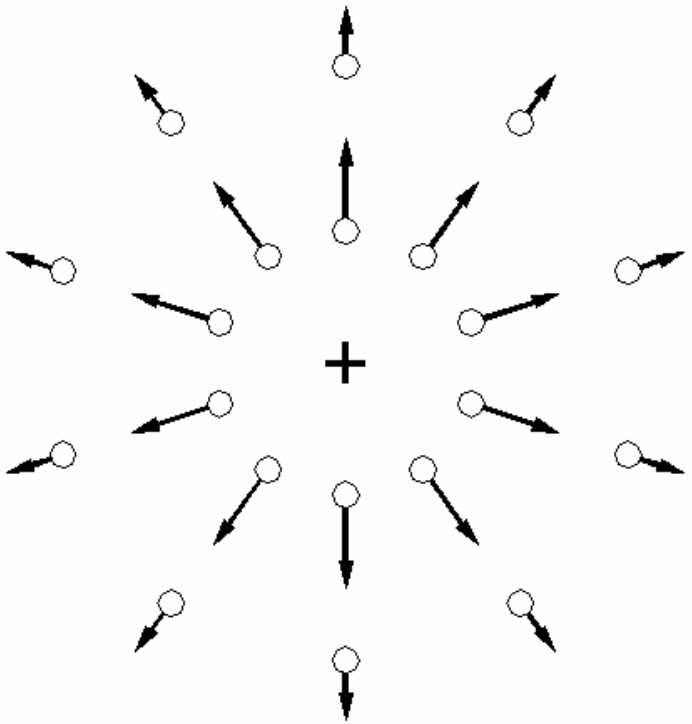


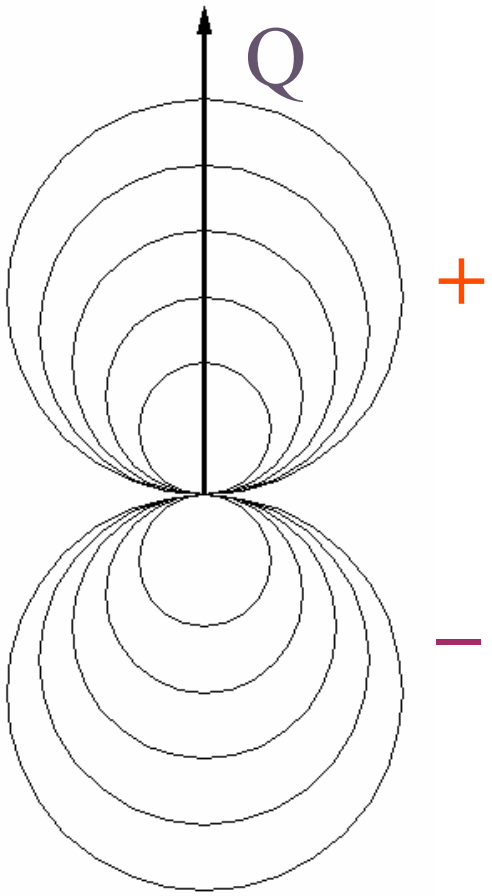

k
Fourier Transform
h

Diffraction by Strain of Point Defect

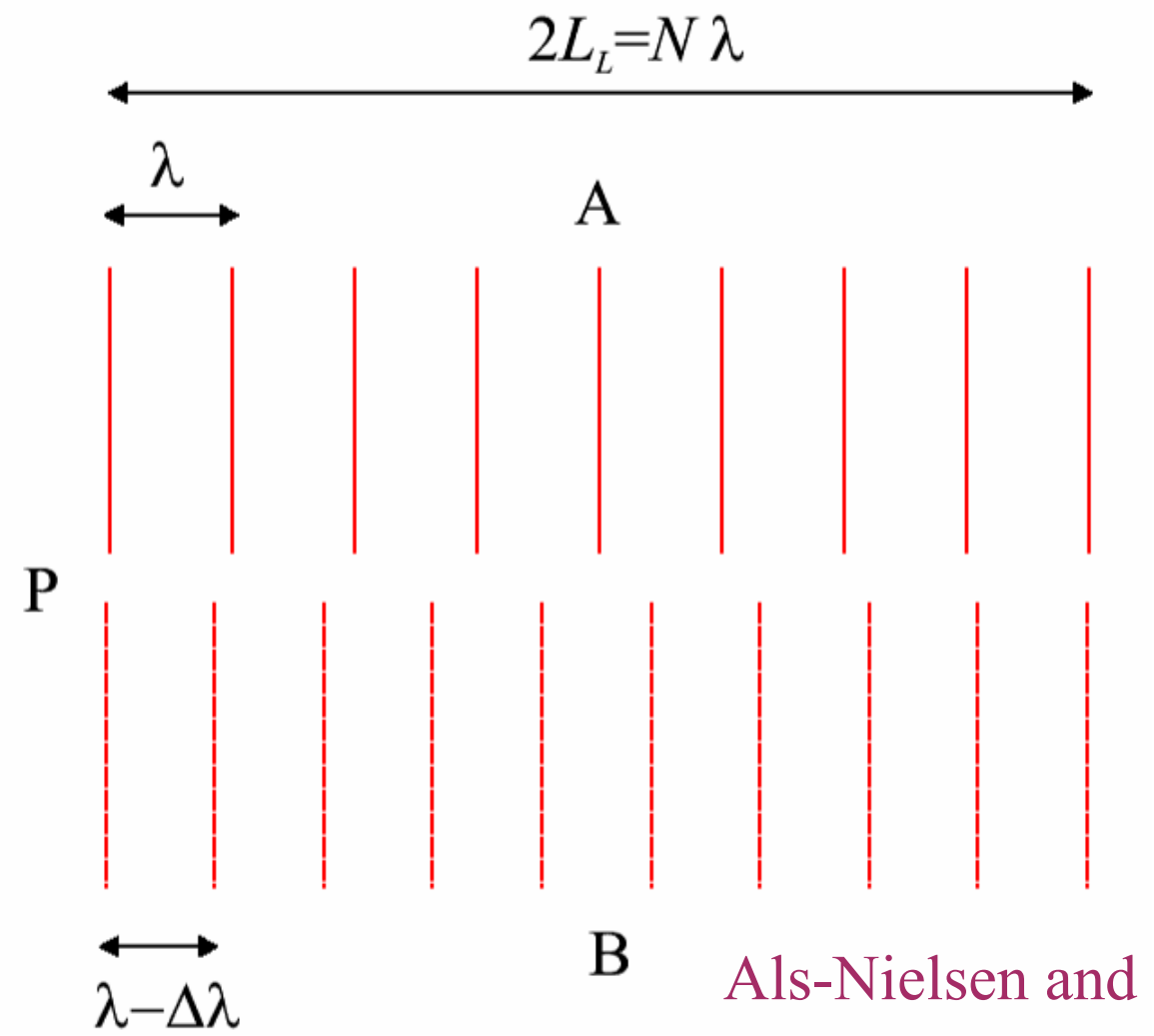
$$A \sim \sum e^{i\mathbf{Q}\cdot(\mathbf{R}_j+\mathbf{u}_j)}$$
$$\approx \sum e^{i\mathbf{Q}\cdot\mathbf{R}_j}\,(1+i\mathbf{Q}\cdot\mathbf{u}_j)$$

Imaginary density





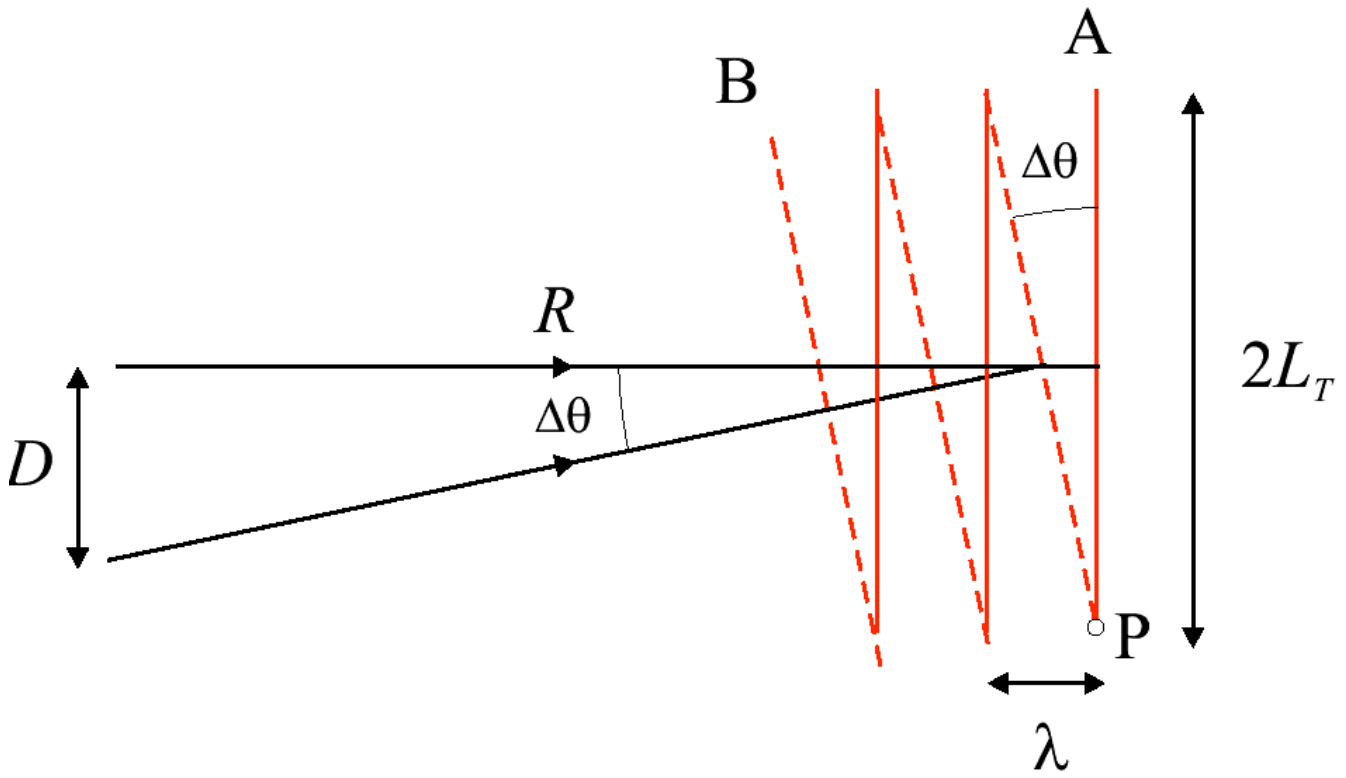
Longitudinal Coherence



$$L_L = \frac{1}{2}\frac{\lambda^2}{\Delta\lambda}$$

Als-Nielsen and McMorrow (2001)

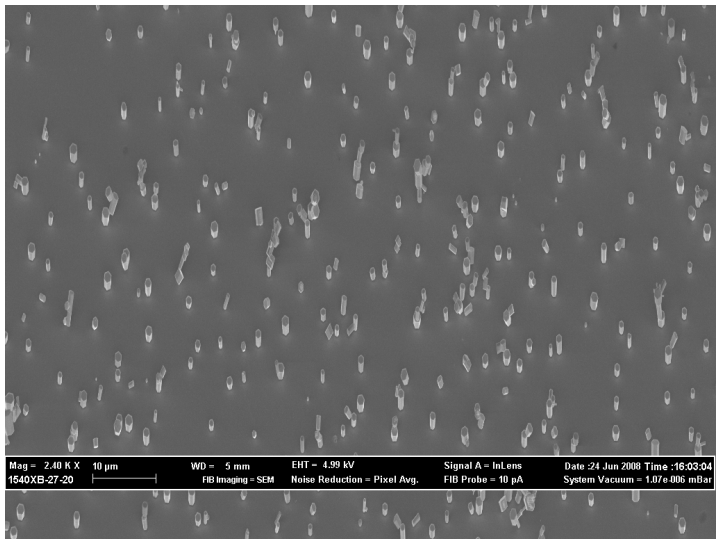
Lateral (Transverse) Coherence

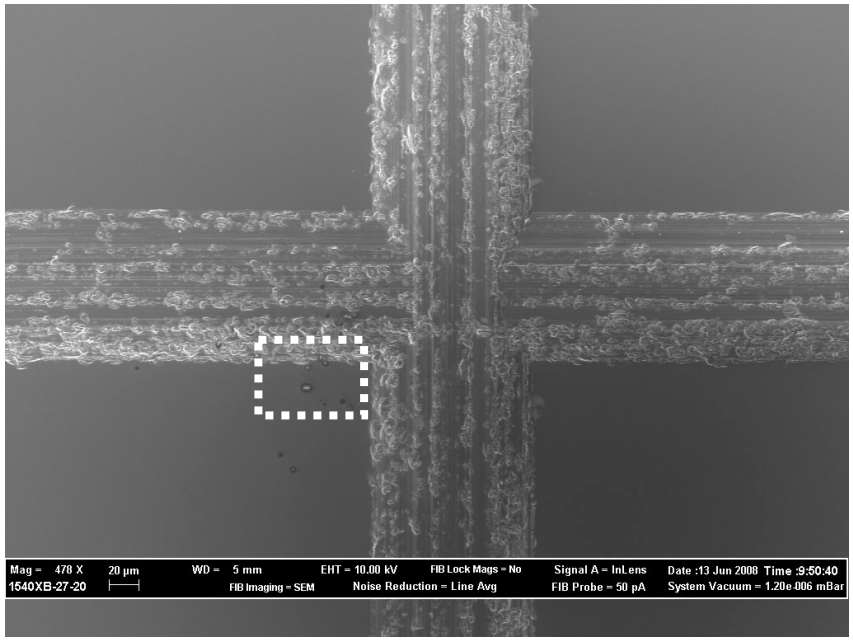


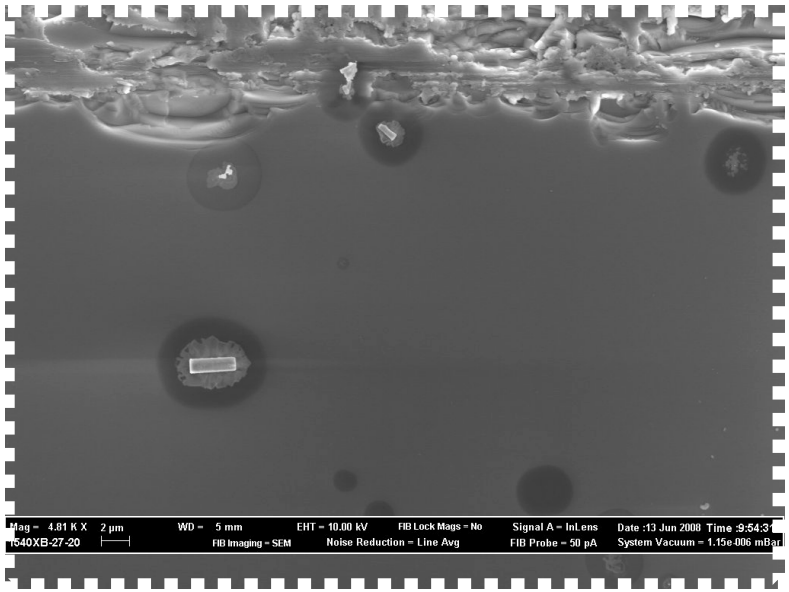
$$L_T = \frac{\lambda}{2}\frac{R}{D}$$

Als-Nielsen and McMorrow (2001)

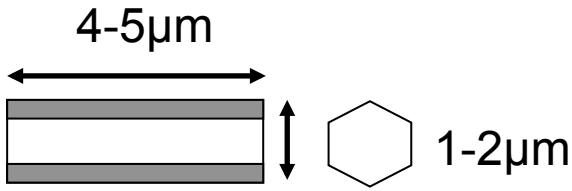
Sample Preparation







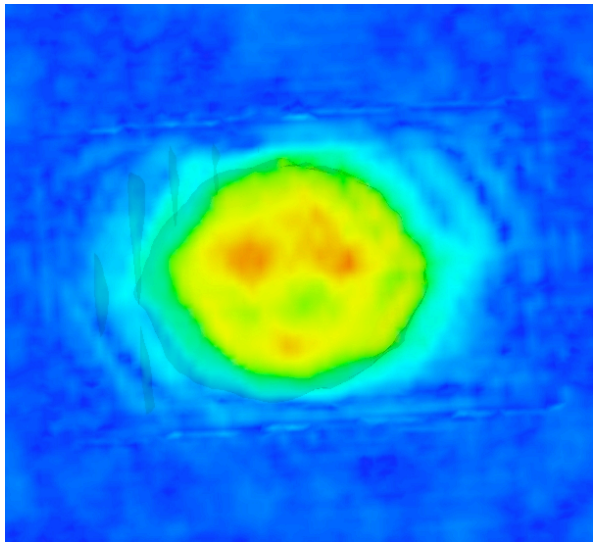
Dimensions:

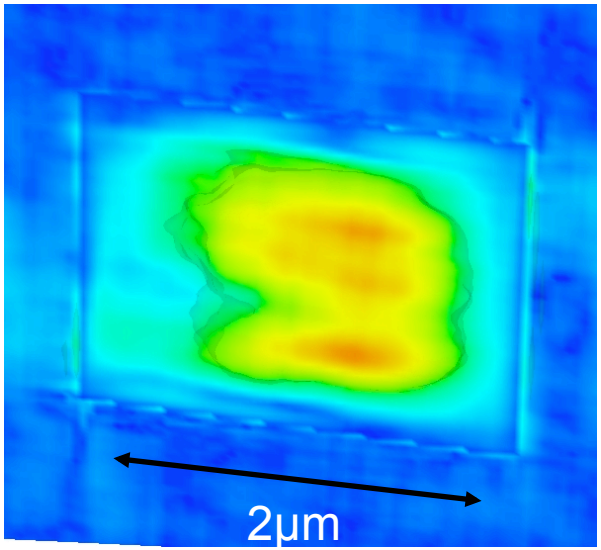


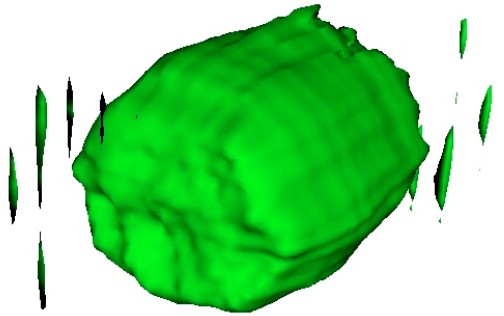
5 Bragg Reflections on the same crystal!

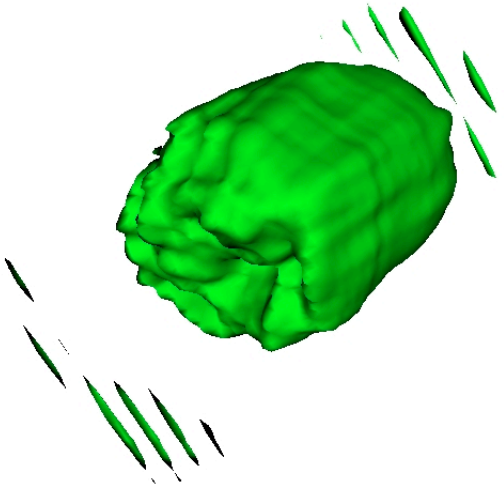
- Align the crystal (the hard part)
  - spec orientation matrix
  - TV alignment system and groove scatter
  - move detector forward/backward
  - Laue orientation matrix (34-ID-E)
  - patience
- Measure 3D diffraction (3hours – each peak)
- Coordinate transform for comparison

Reconstruction 002



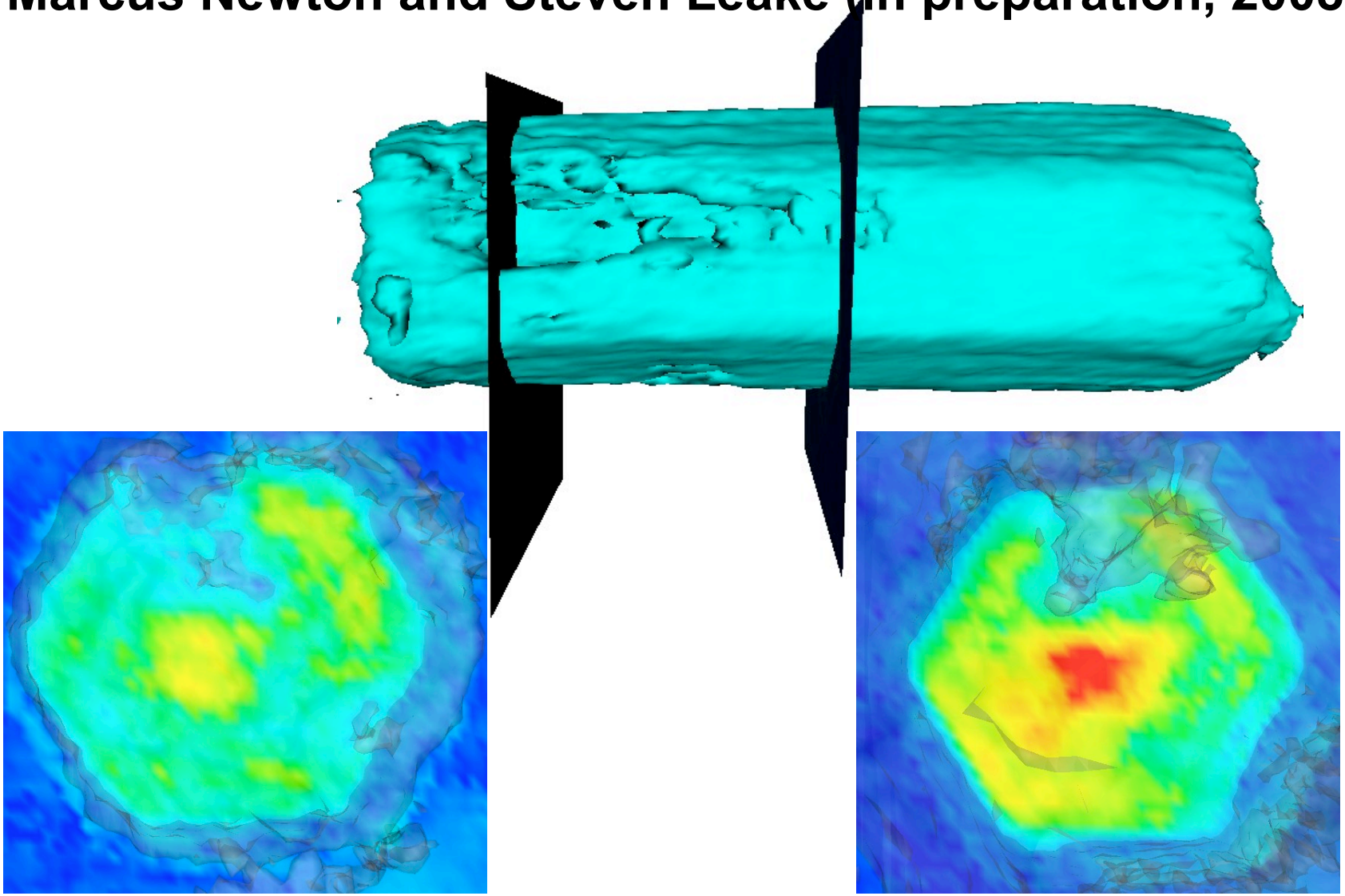






Density sections ZnO-39 (010)

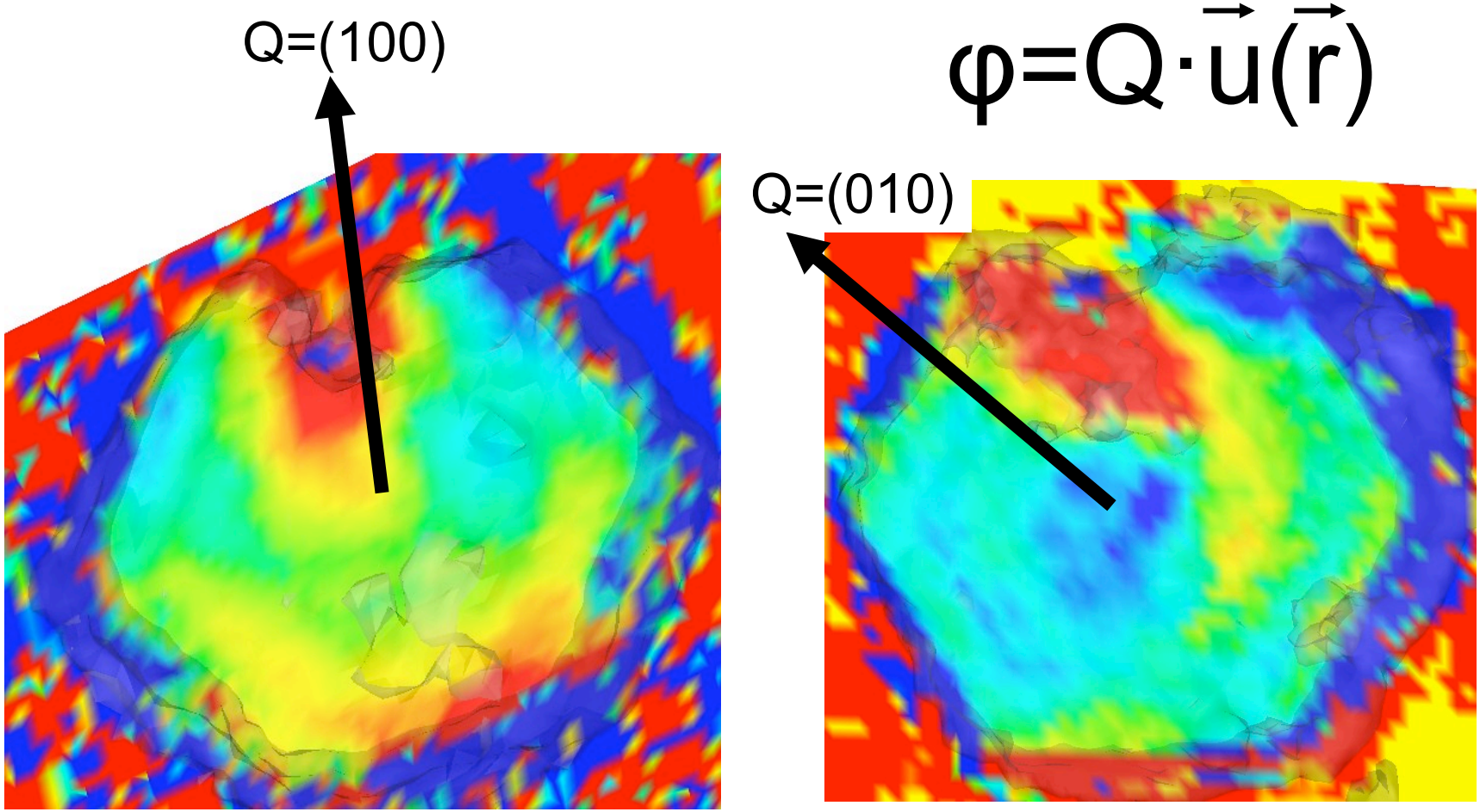
Marcus Newton and Steven Leake (in preparation, 2008)



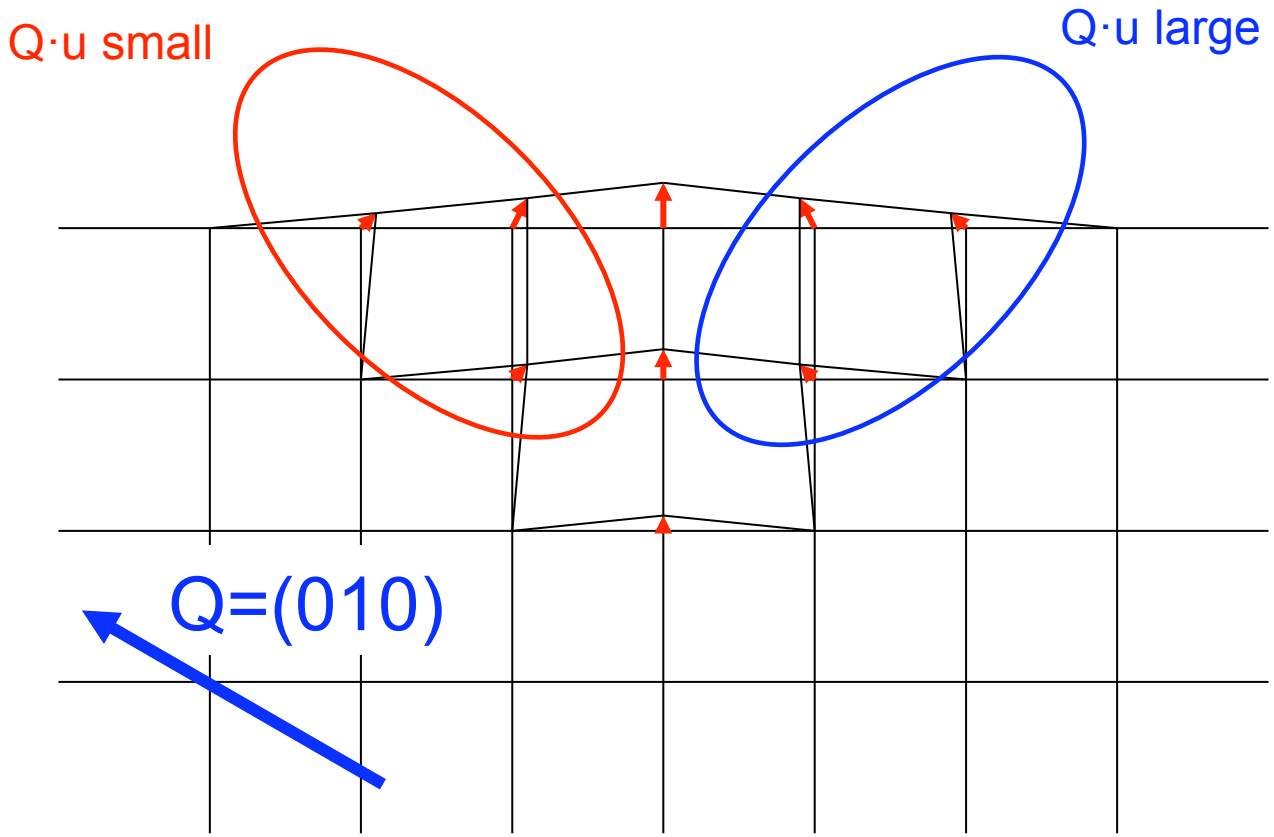
Phase maps from 2 Bragg peaks

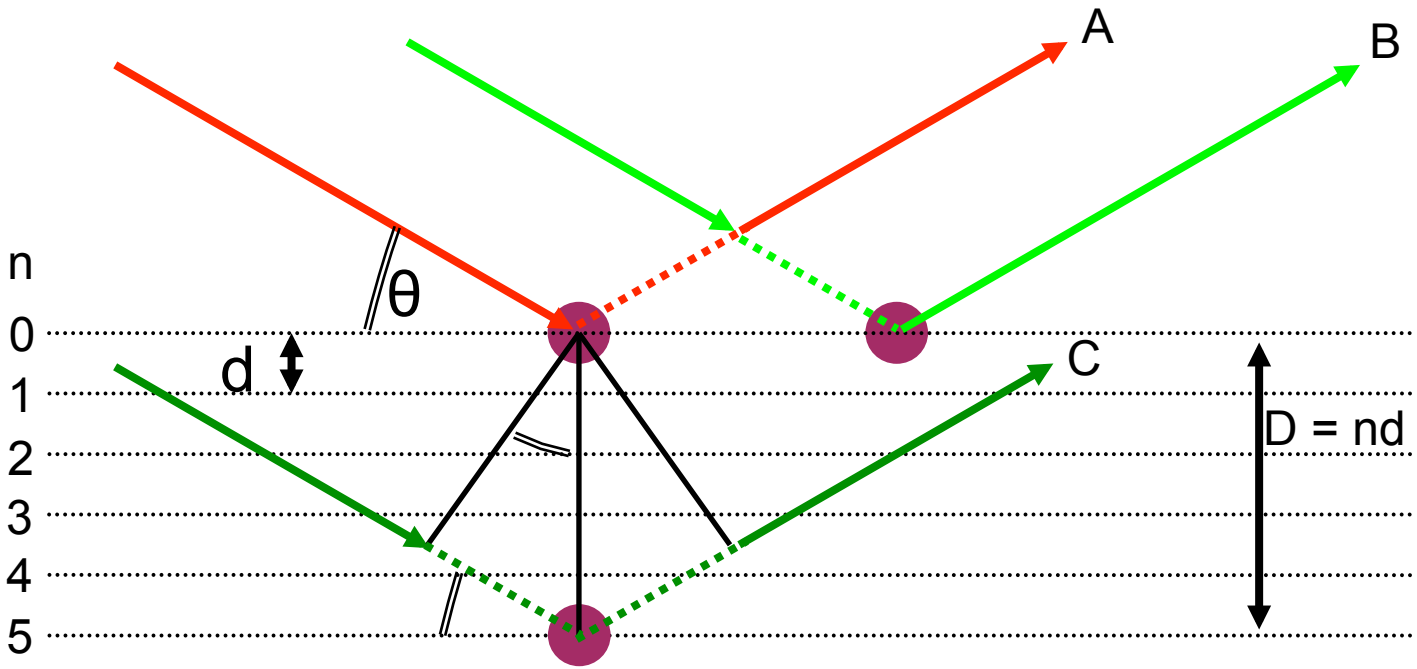
Blue-Red is +2 radians. Slice at -1500nm from centre ZnO-5 -39

$$\varphi = \vec{Q} \cdot \vec{u}(\vec{r})$$



Typical displacement field

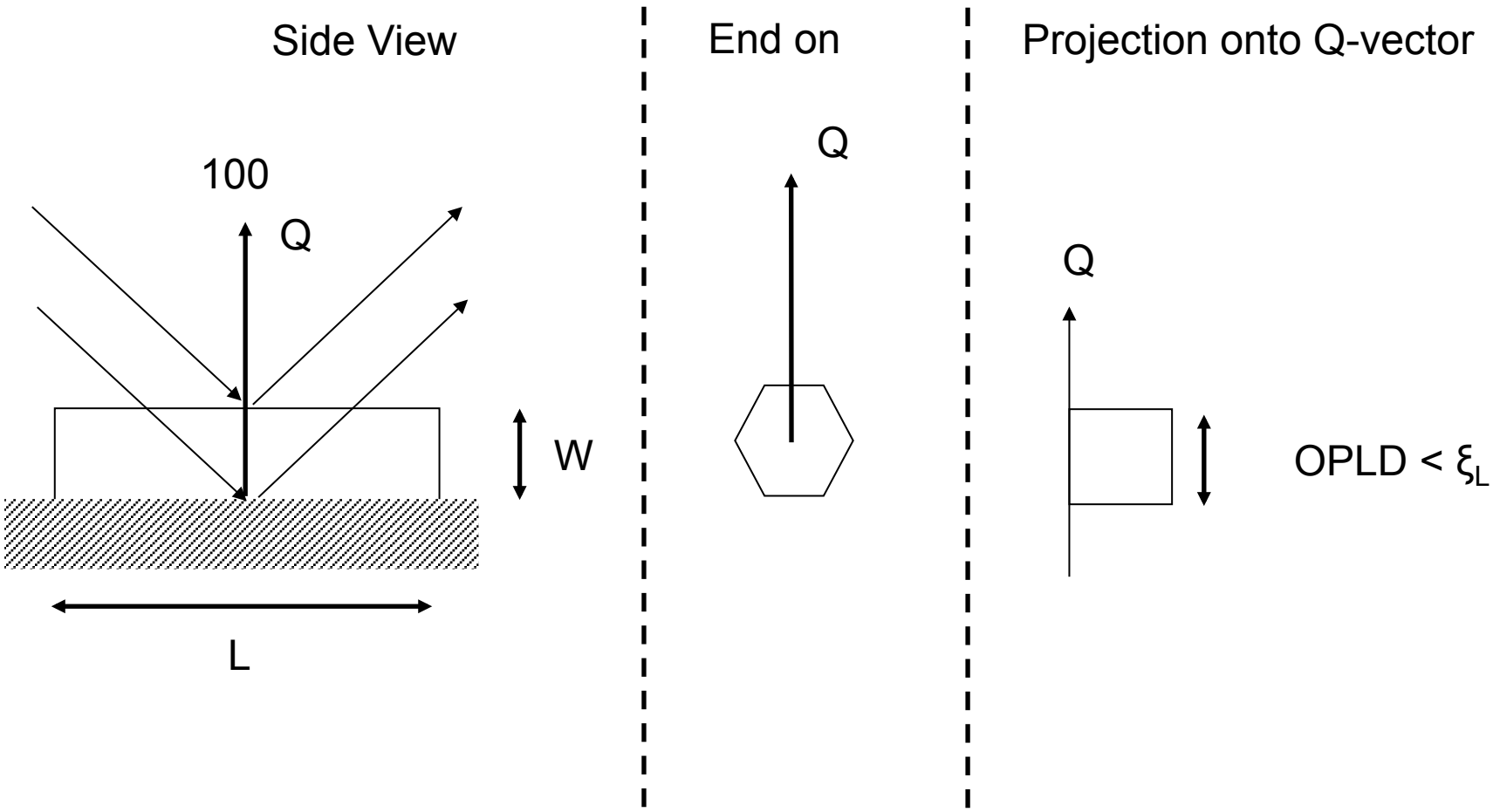




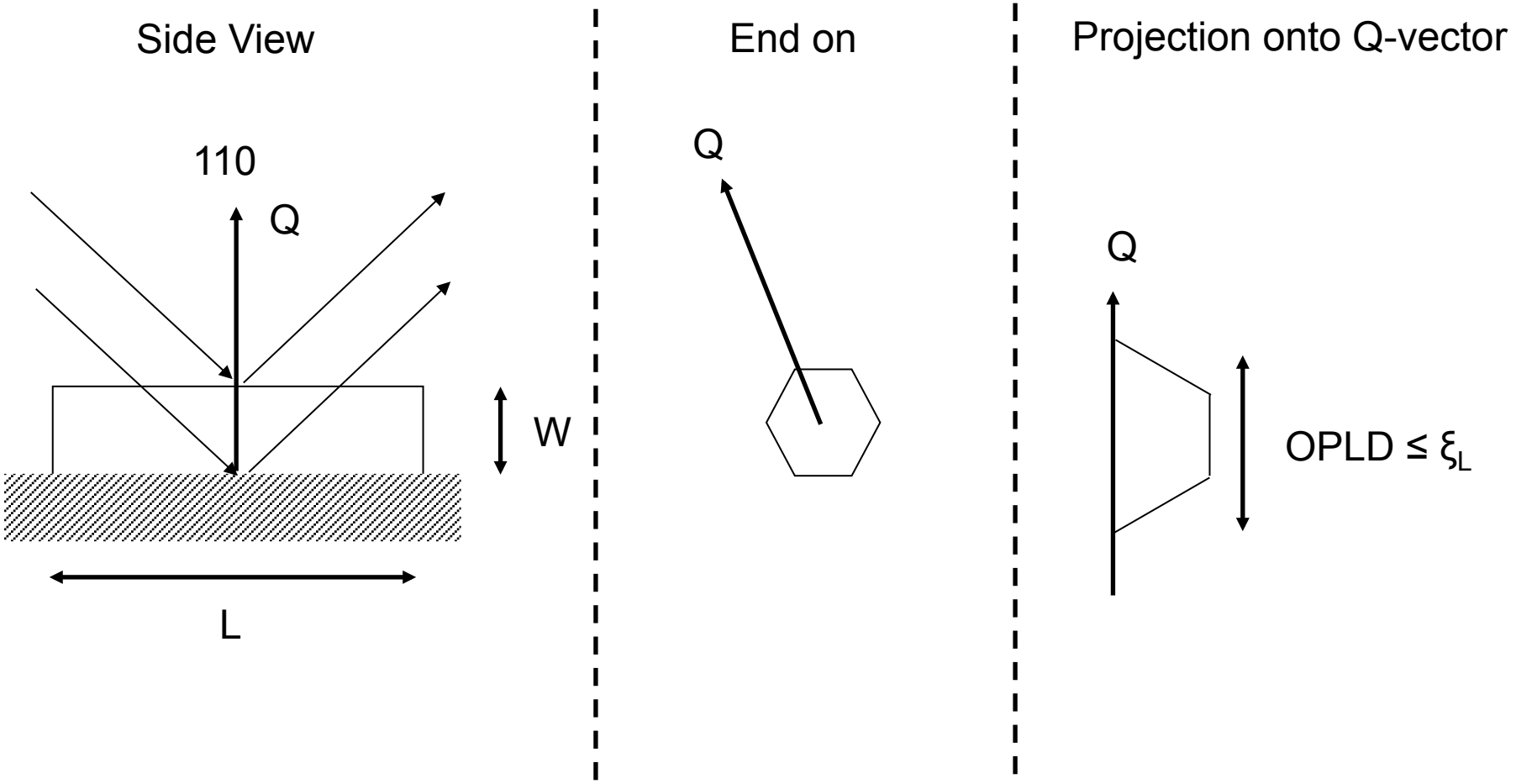
$OPLD_{AB} = 0$

$OPLD_{AC} = 2Dsin\theta$

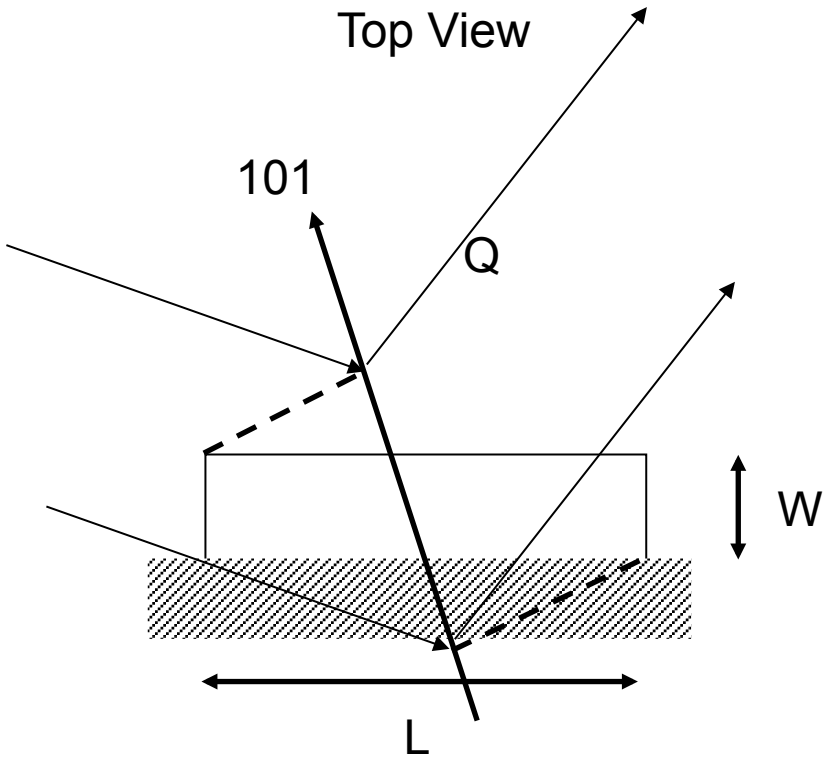
Projection of crystal onto 100 Q-vector

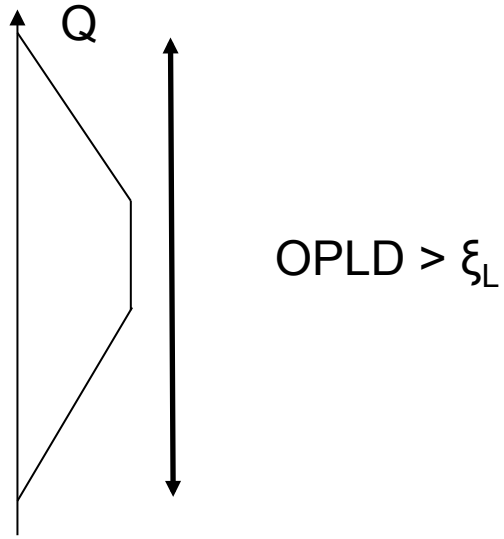


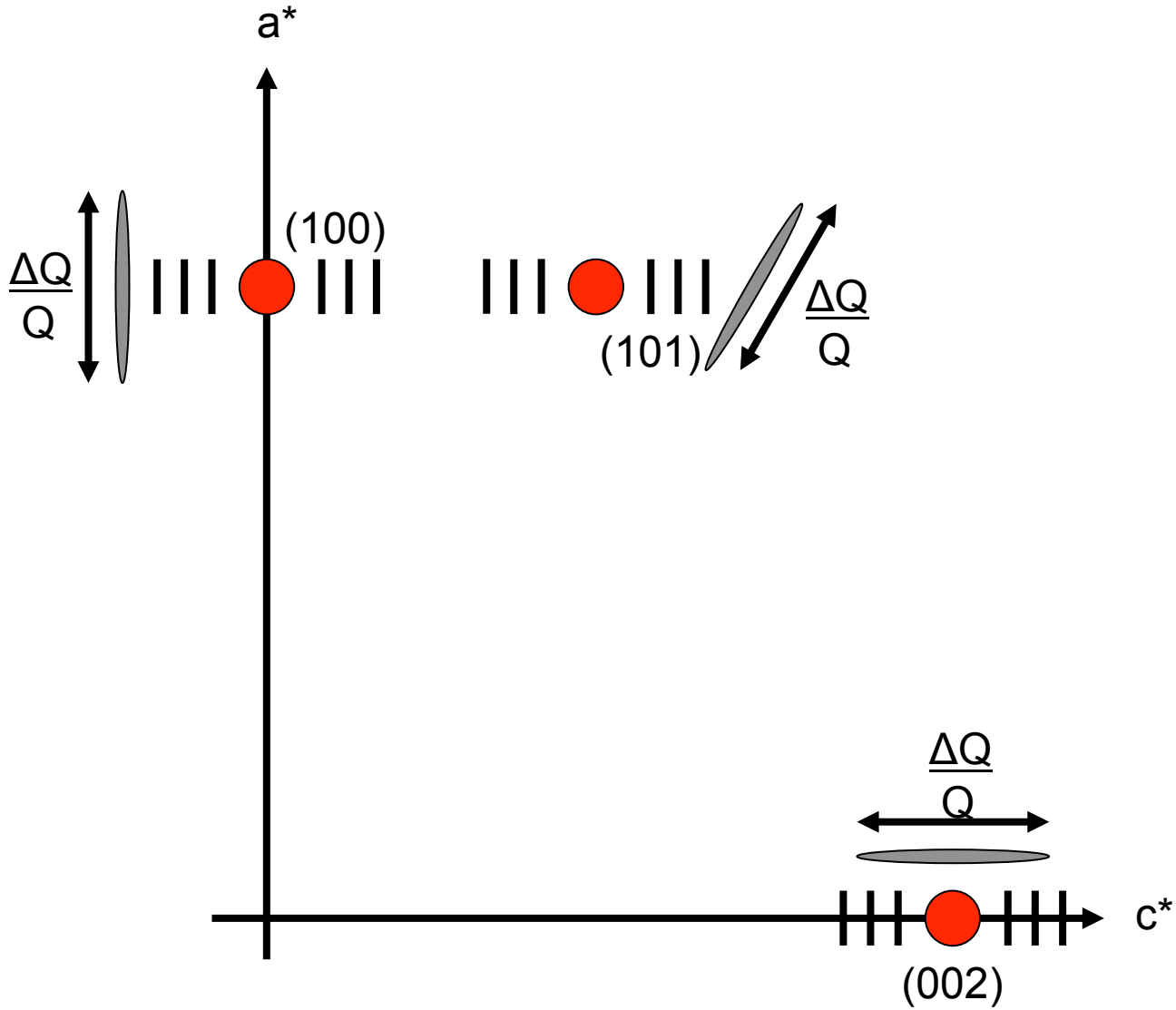
Projection of crystal onto 110 Q-vector



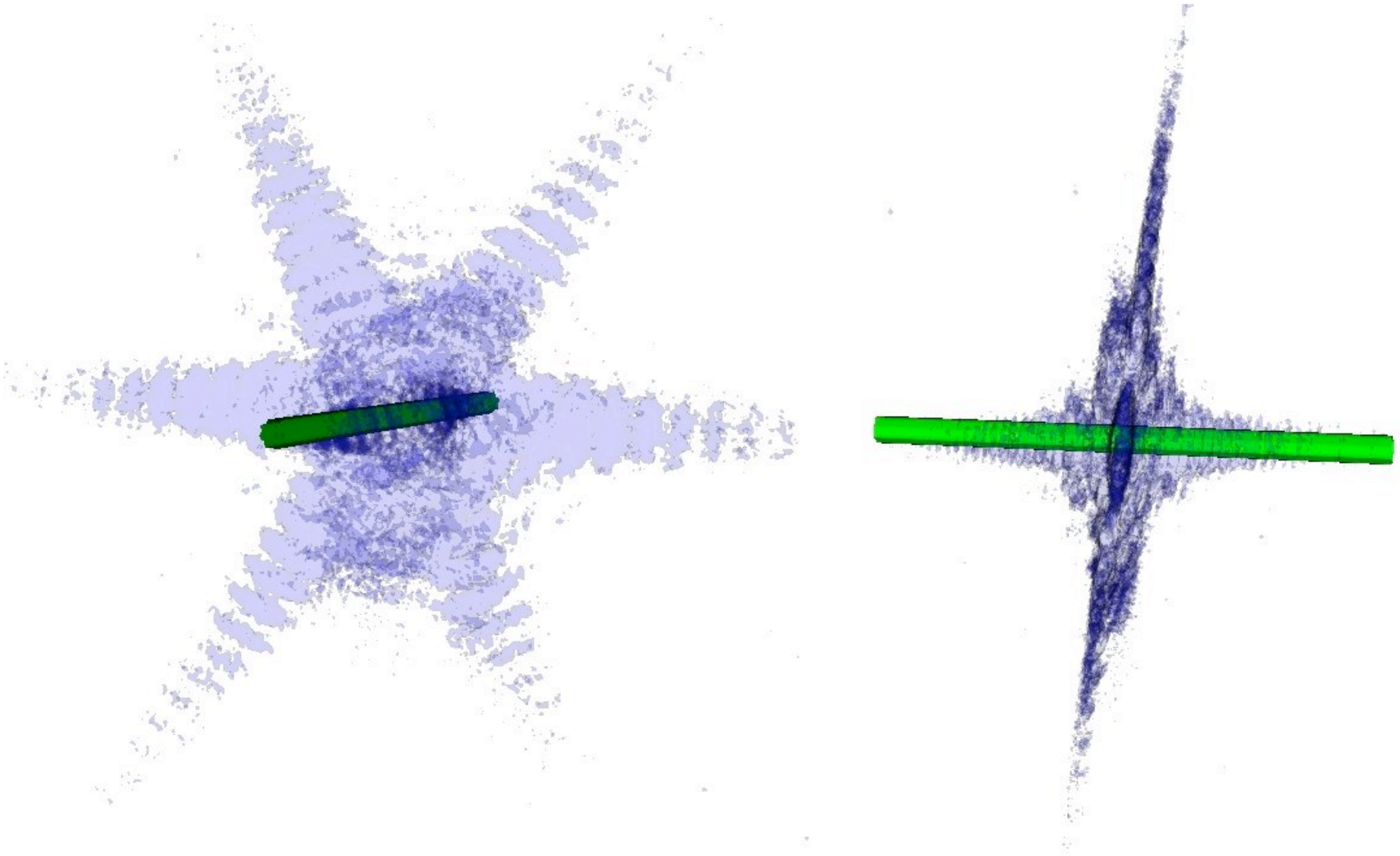
Projection of crystal onto 101 Q-vectors

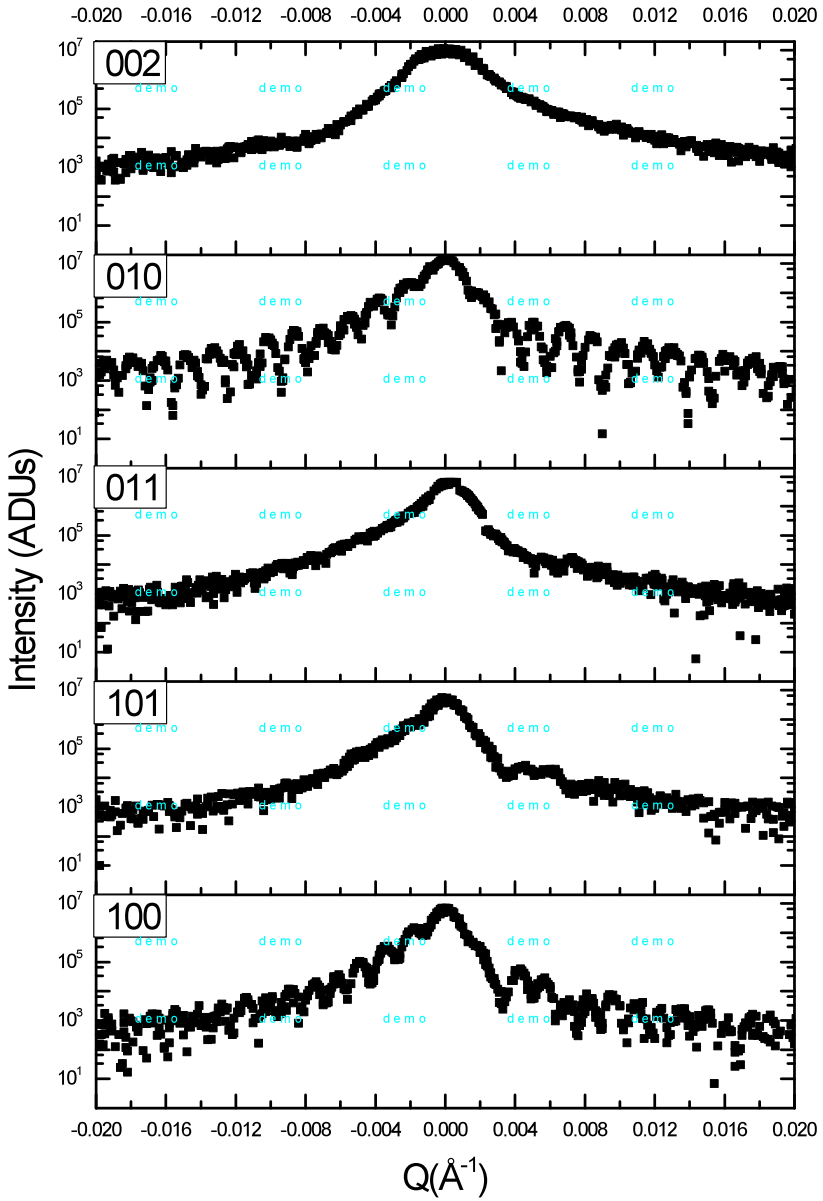





a*
ΔQ
Q
(100)
(101)
ΔQ
Q
ΔQ
Q
c*
(002)

How to extract the data





002 no fringe visibility

010 & 100 good fringe visibility

101 & 011 diminished fringe visibility
but fringes still evident

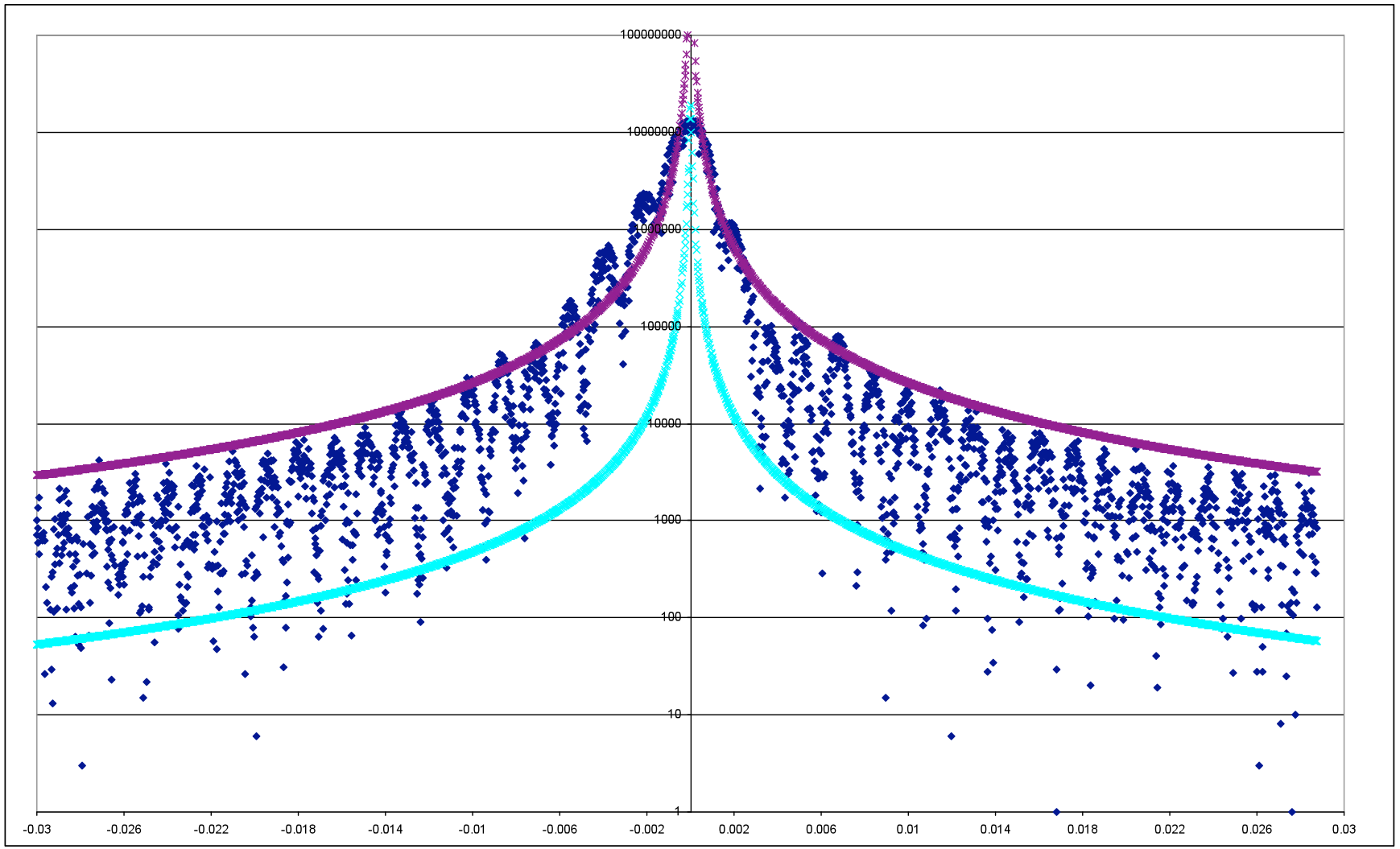
010:011 & 101:100
show complementary fringes
but not between each other

Error in coordinate transform ruled out

010 and 100 reflections fringe spacing
difference ~ 20%

Estimates of Visibility

96±2% 010



Estimates of Visibility

88±6% 100