

Phase Structure due to Refraction in Coherent X-ray Diffraction

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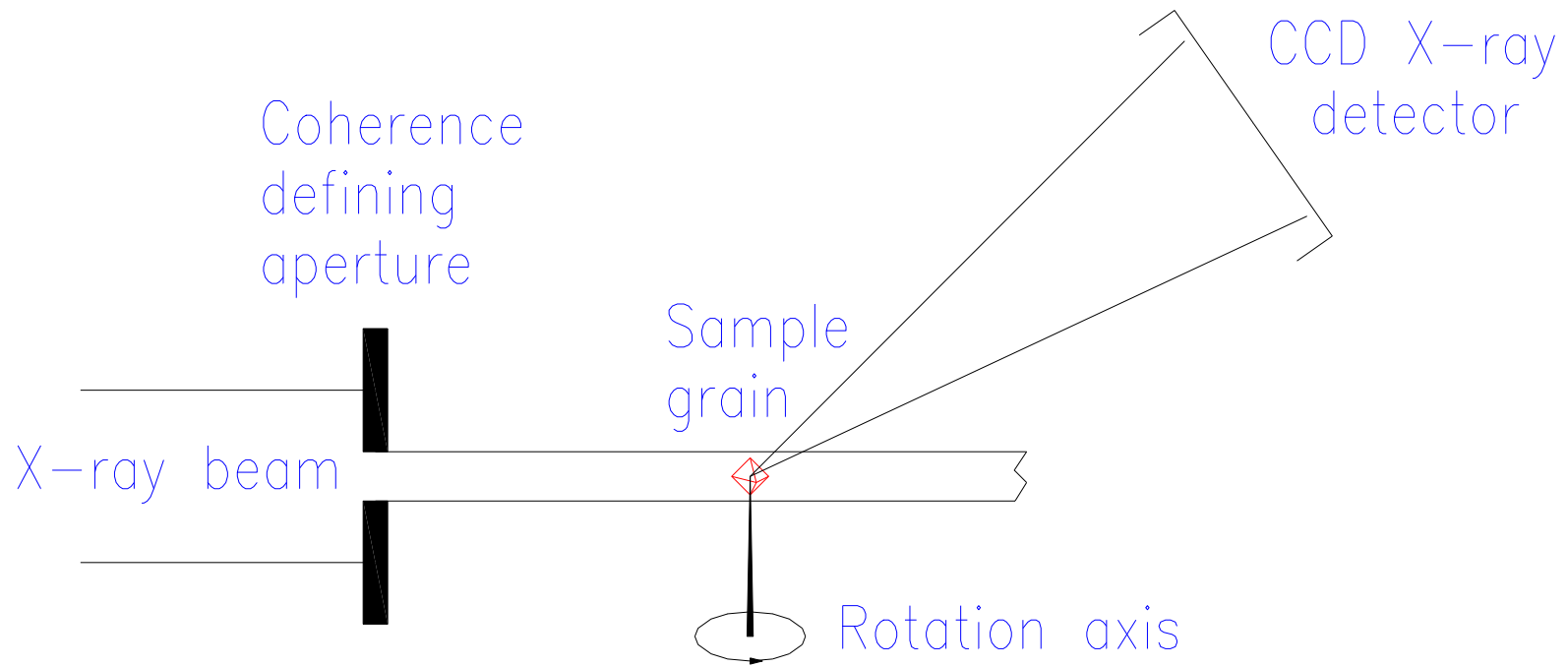
Garth Williams

University of Melbourne

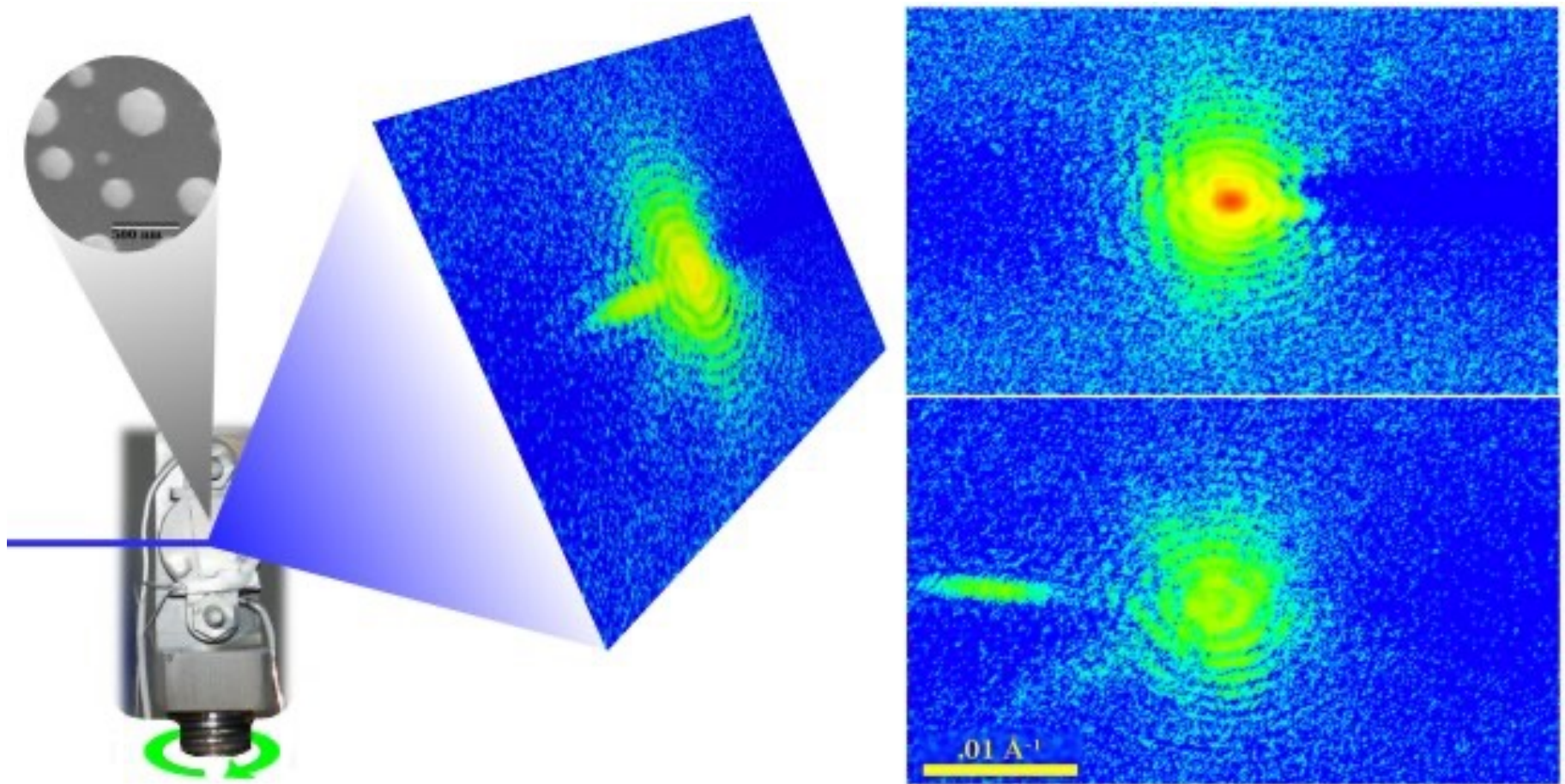
Mark Pfeifer

LaTrobe University

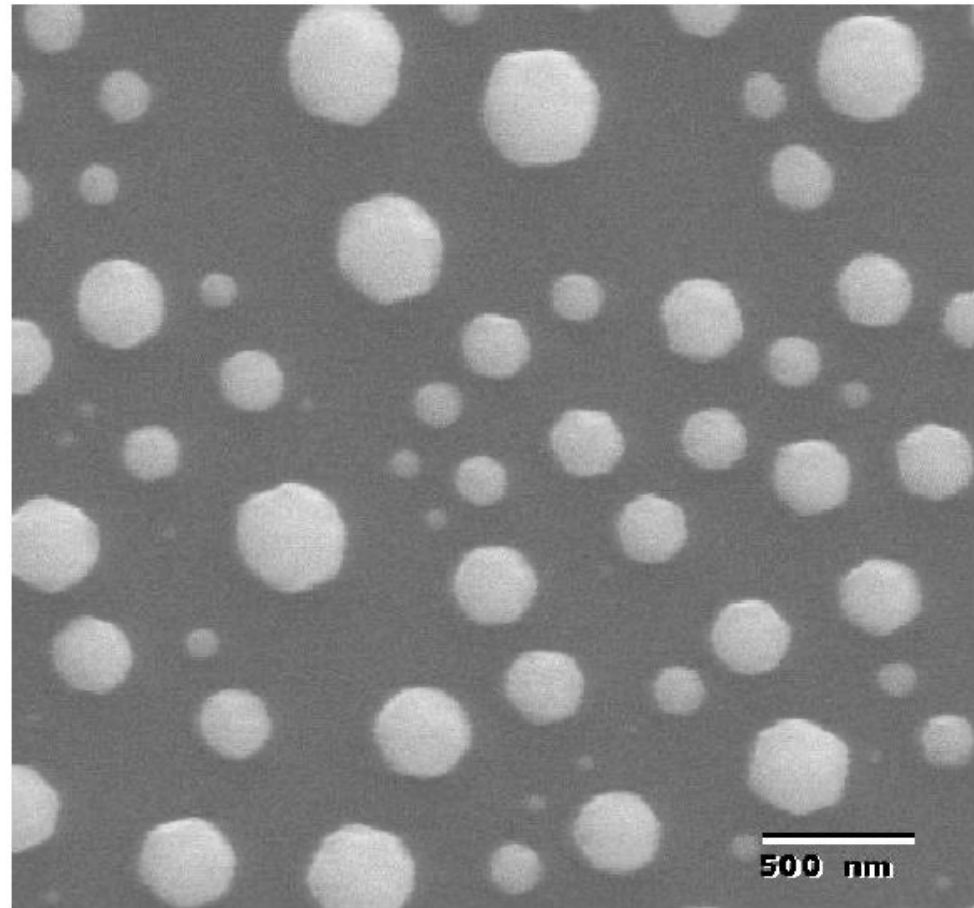
Lensless X-ray Microscope



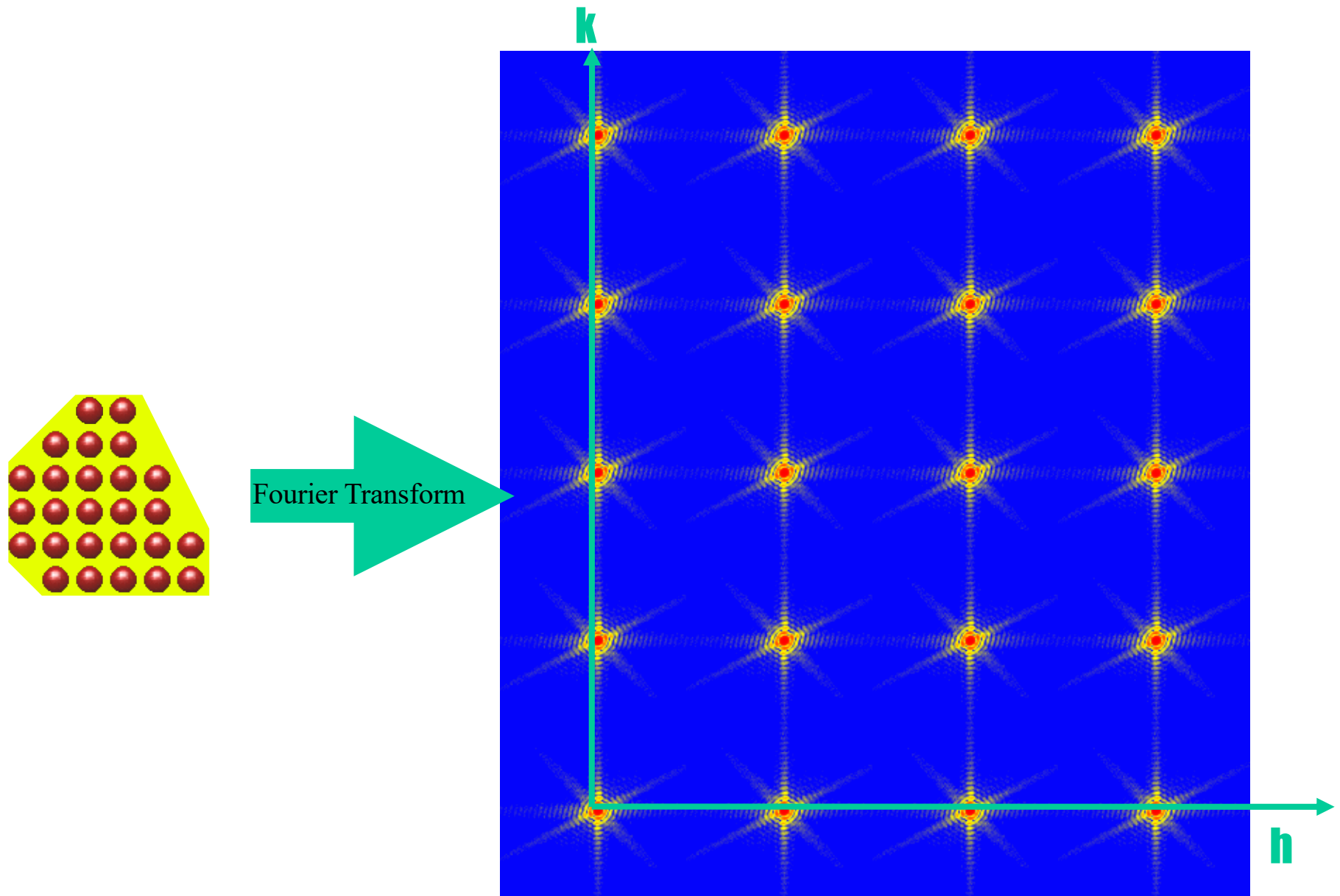
Lensless Imaging setup in UHV



In situ growth of Pb crystals



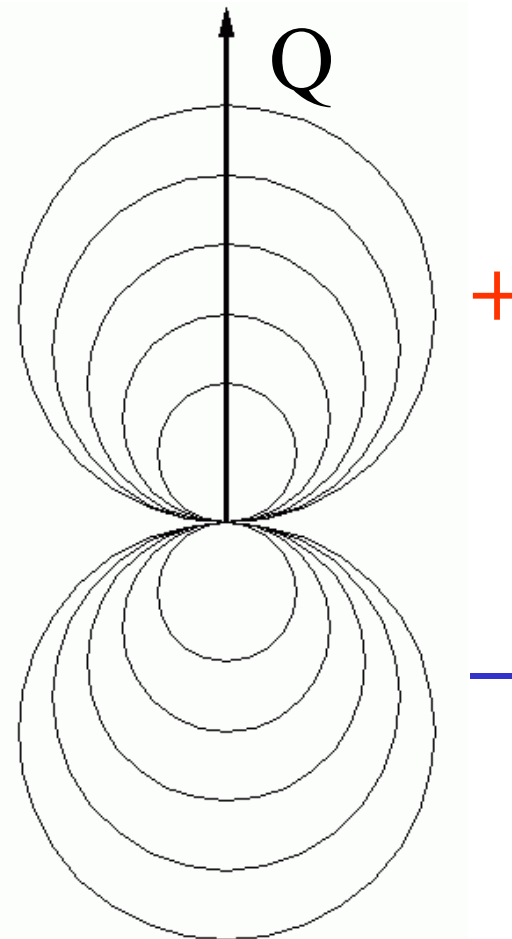
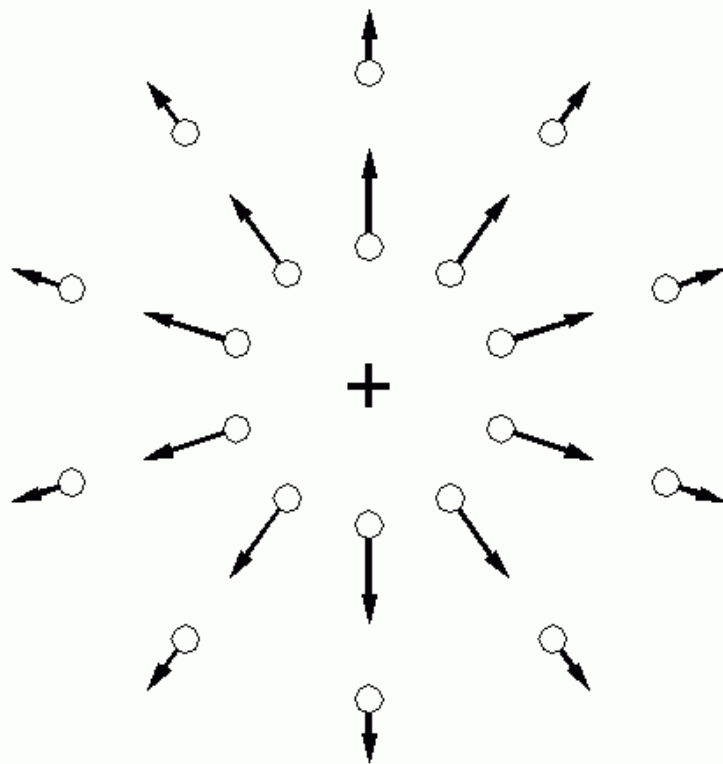
Coherent Diffraction from Crystals



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



Good statistics, 3D diffraction data

Mark Pfeifer, Garth Williams, Ivan Vartanians, Ross Harder

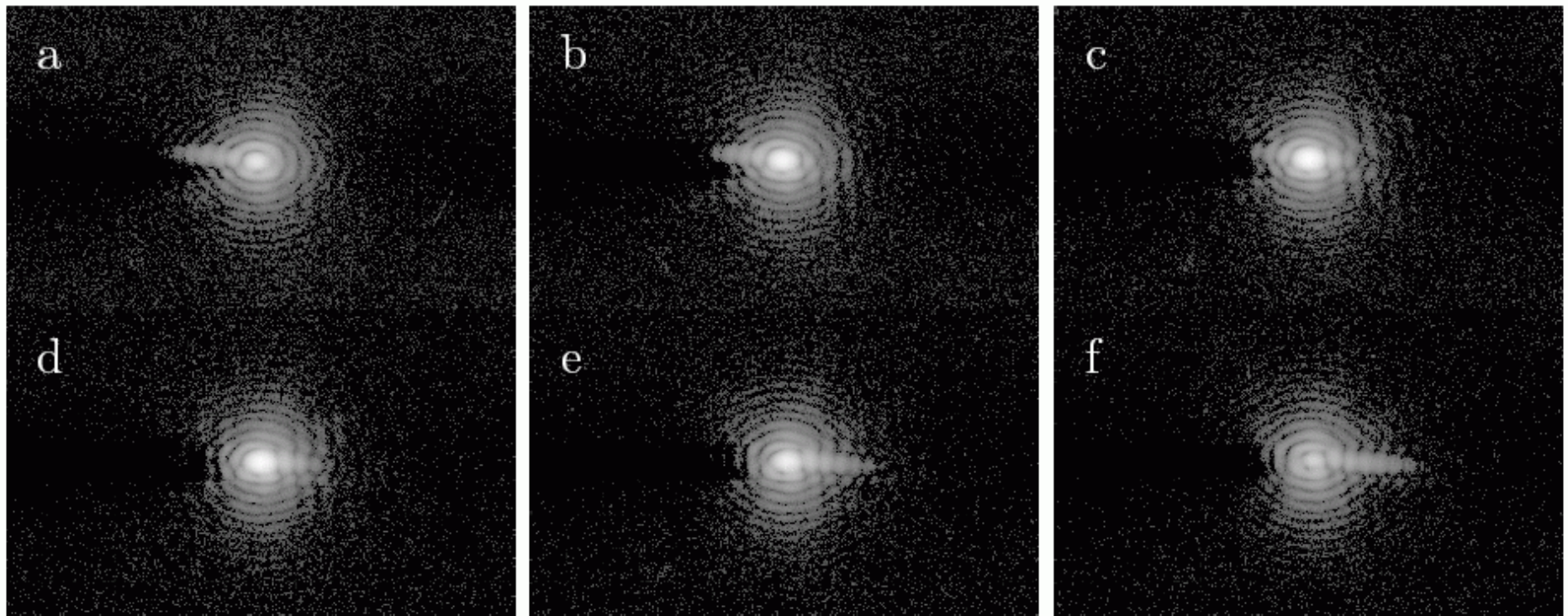
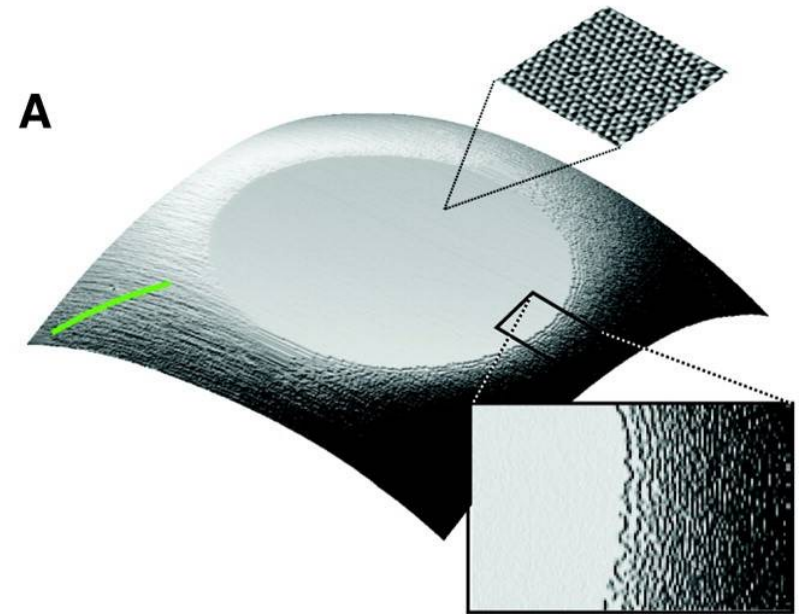
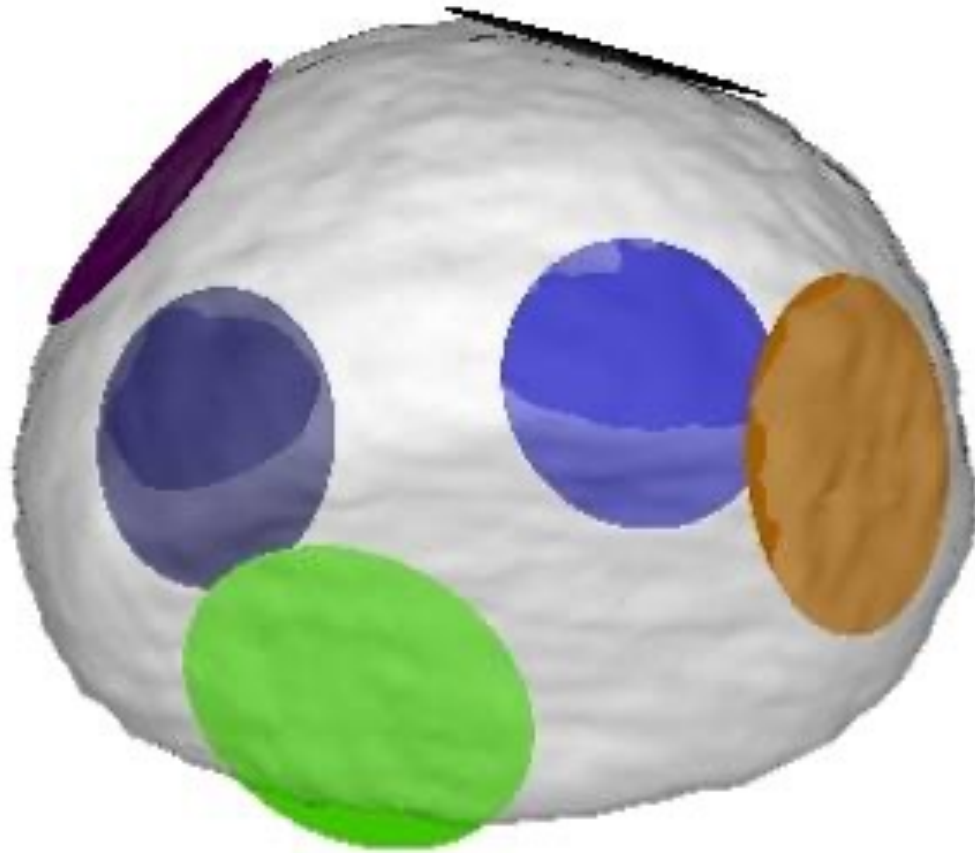


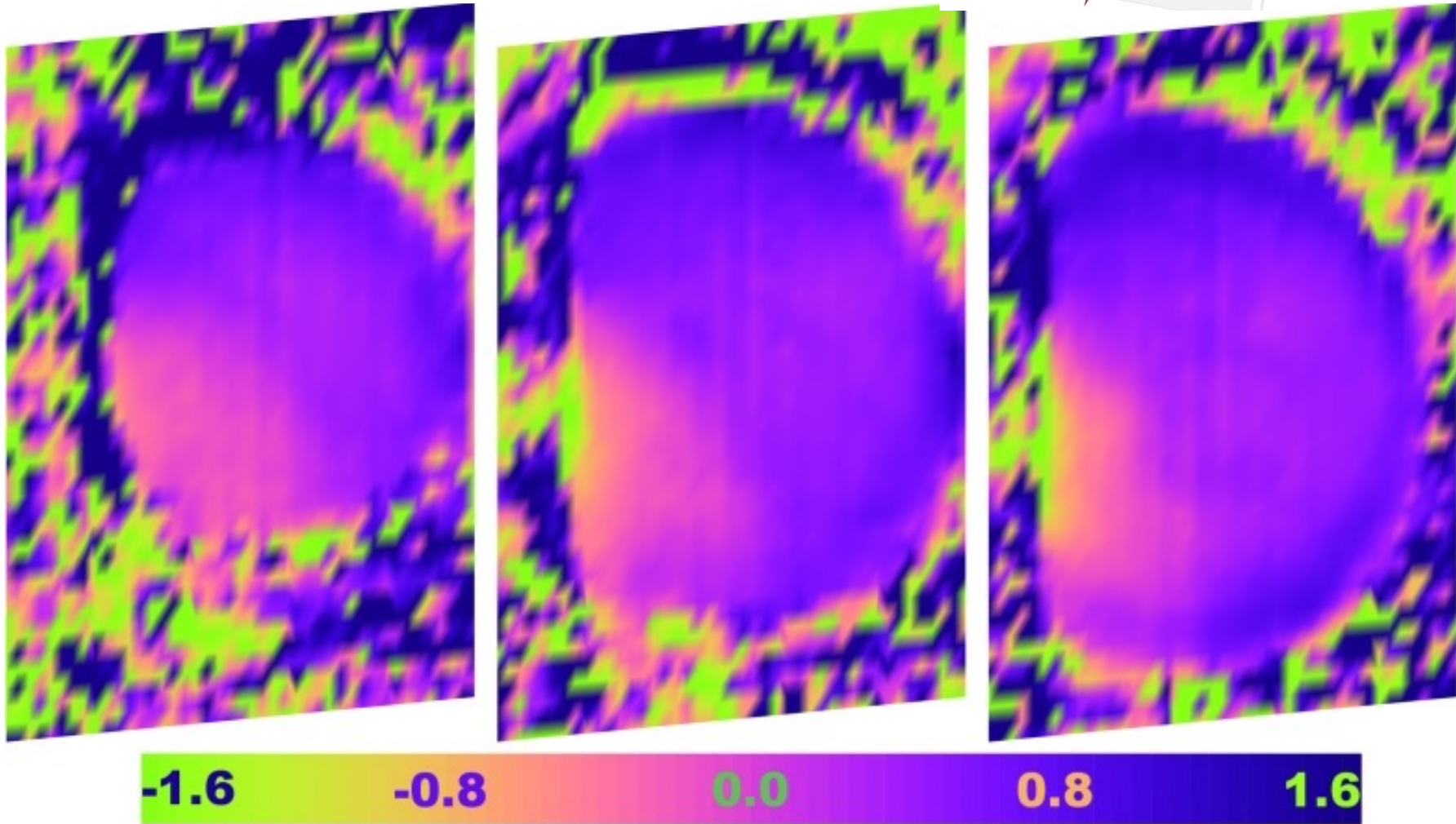
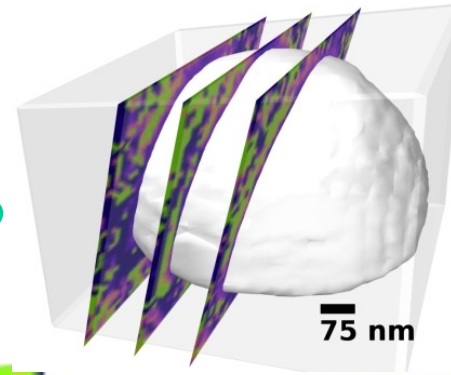
Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

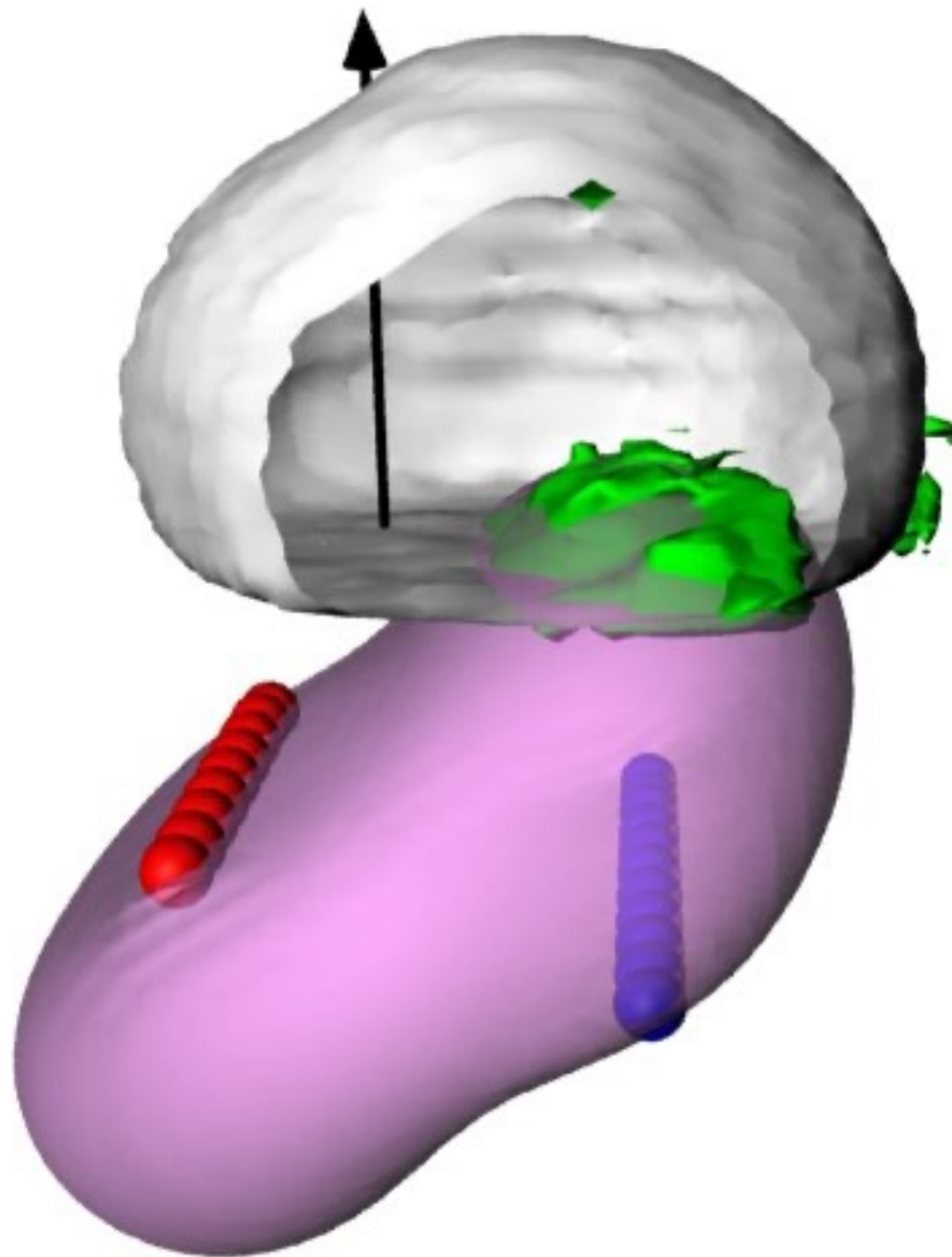
Facets of Equilibrium Crystal Shape



Thurmer K, Williams E, Reutt-Robey J
Science 297 2033 (2002)

3D phase map sections

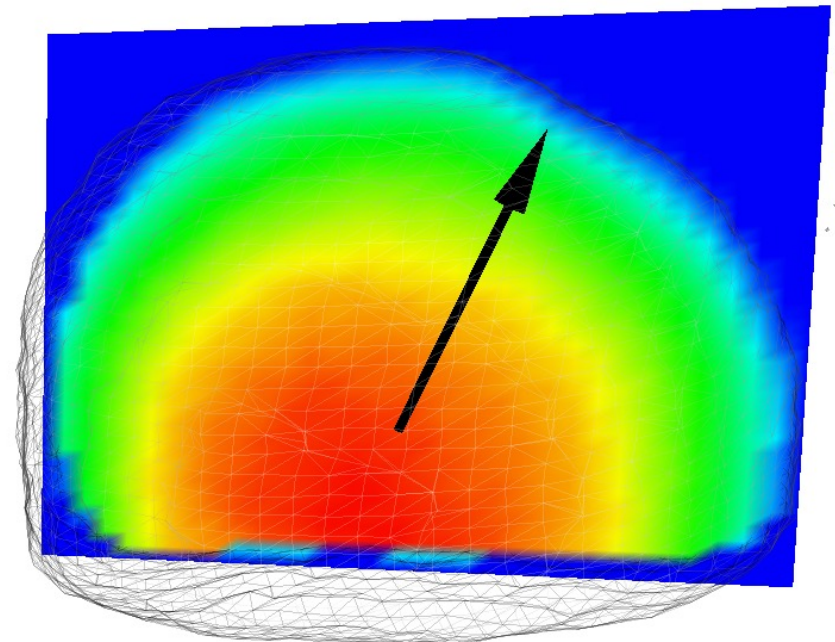
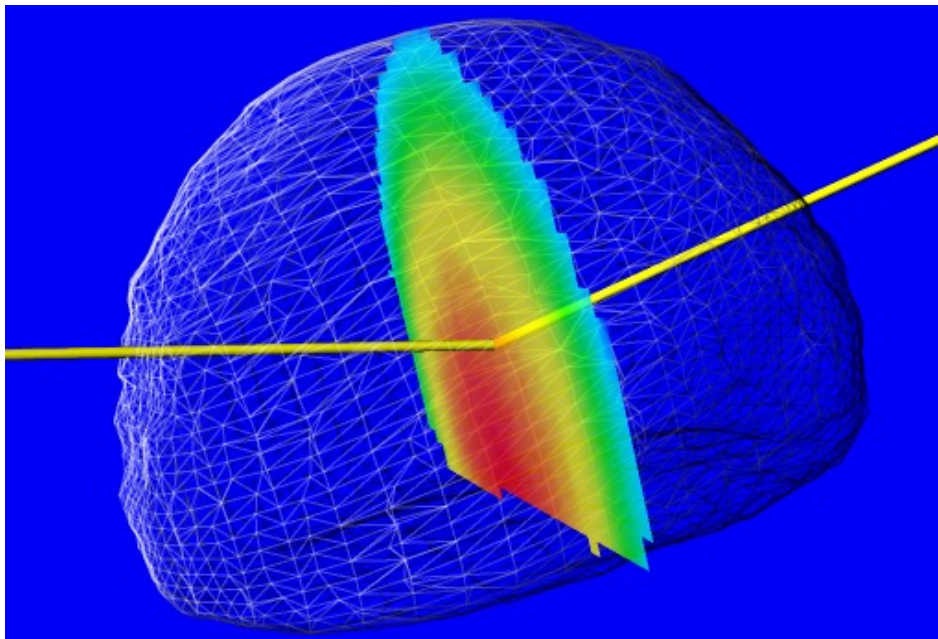




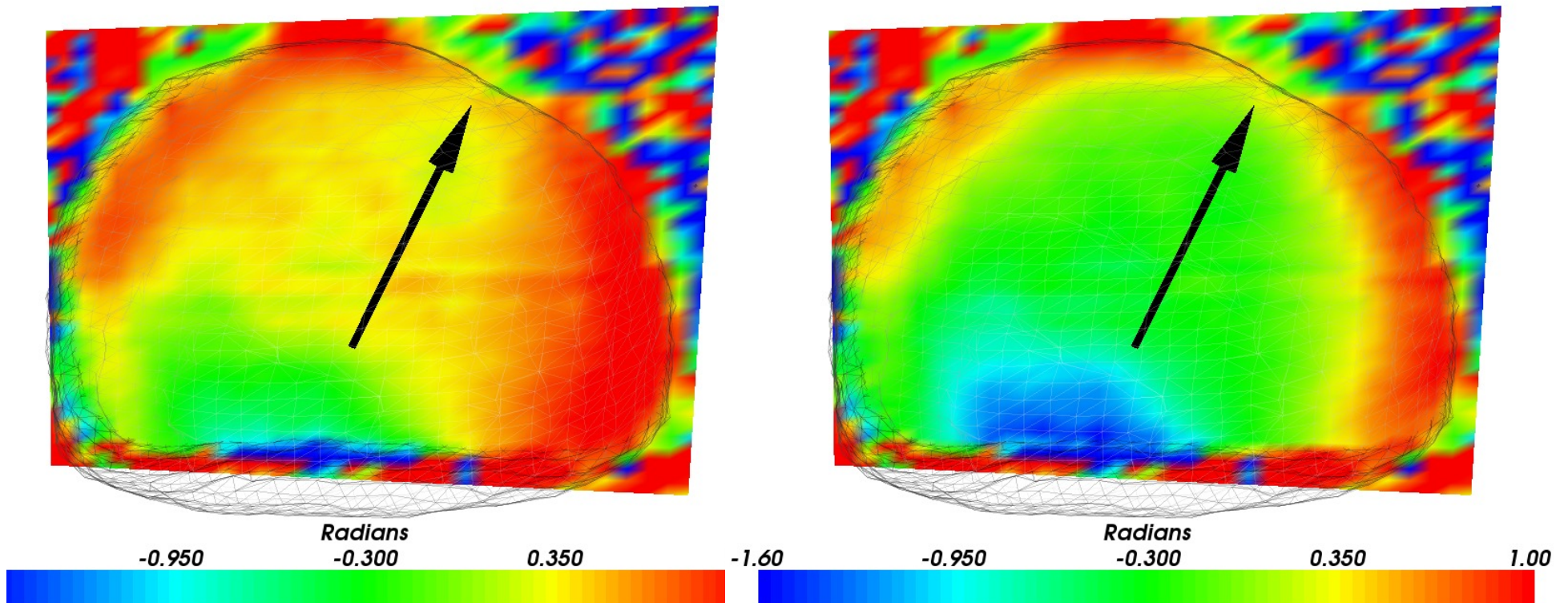
Refraction effects in Lead at 8.9keV

Phase accumulation due to refraction along scattering path
 $d=750\text{nm}$: $kd\delta = 0.76\text{rad}$
 $kd\beta = 0.07$

$$\delta = 2.23 \times 10^{-5}$$
$$\beta = 2.19 \times 10^{-6}$$

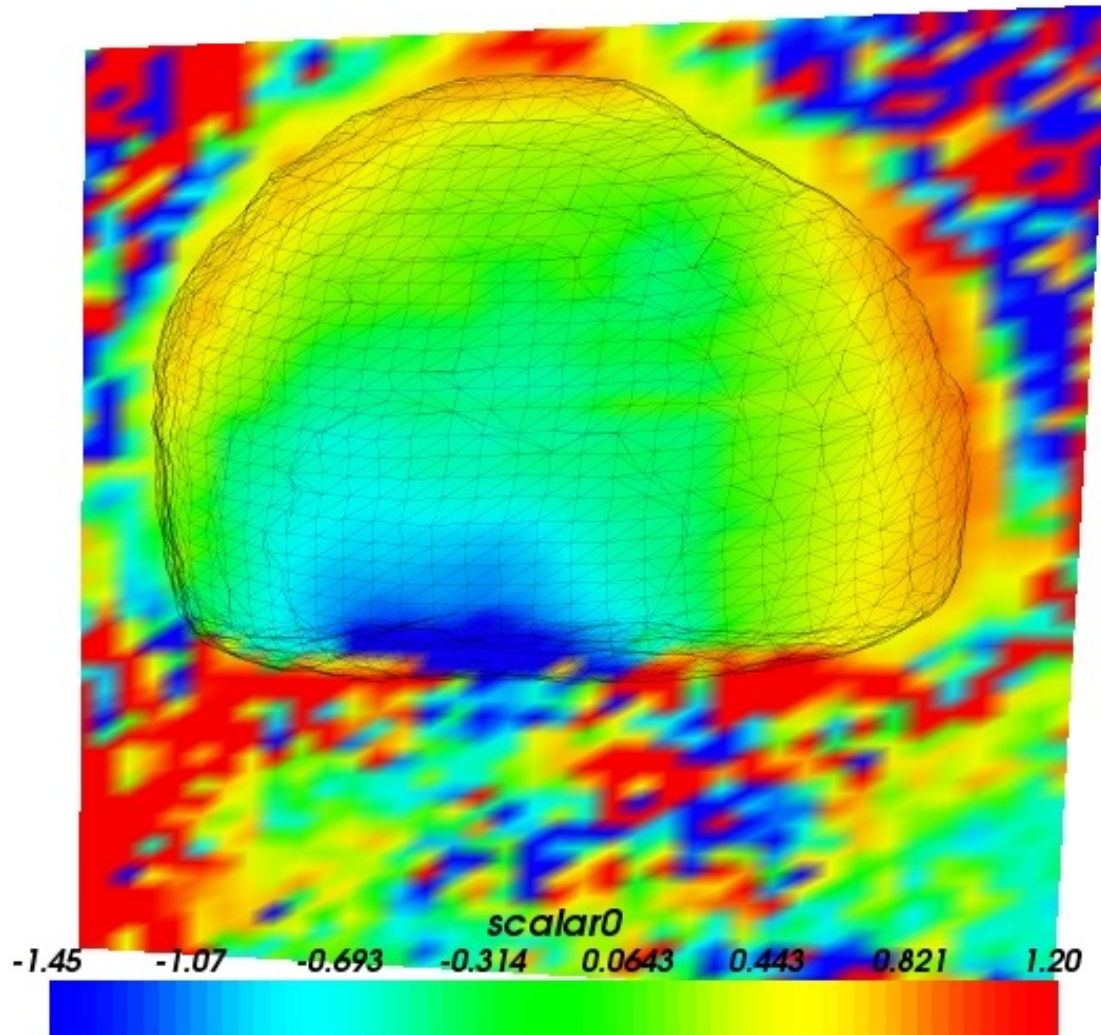


Phase Maps before and after Correction



Positive Phase is Surface Expansion

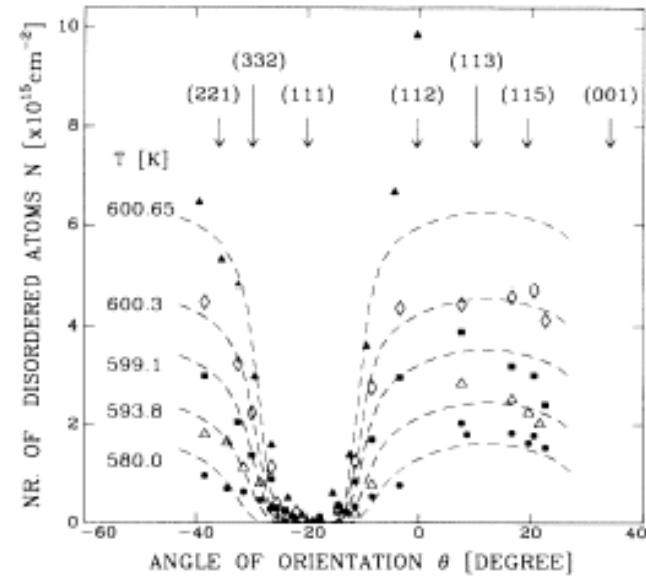
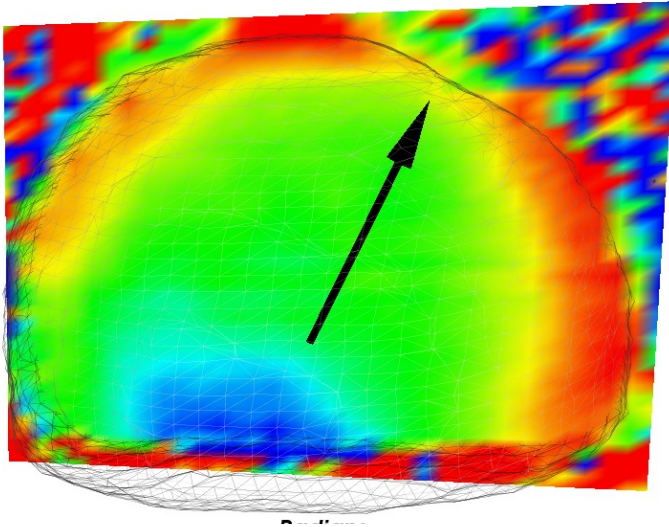
including correction for refraction by crystal



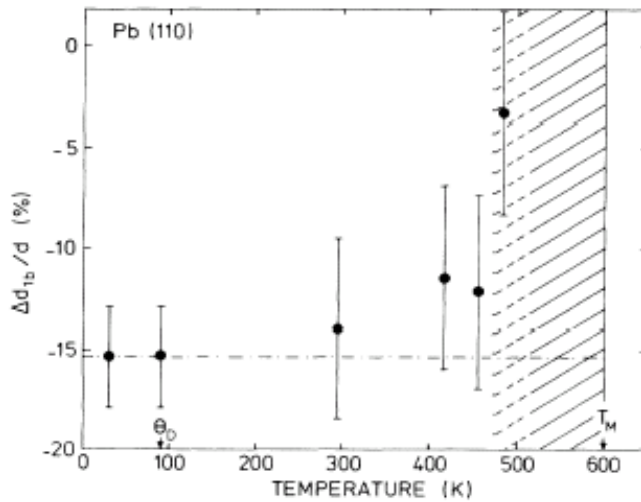
Max phase = 1.15rad
= 0.052nm

Phase on (111) facet:
= 0.47 rad
= 0.02nm

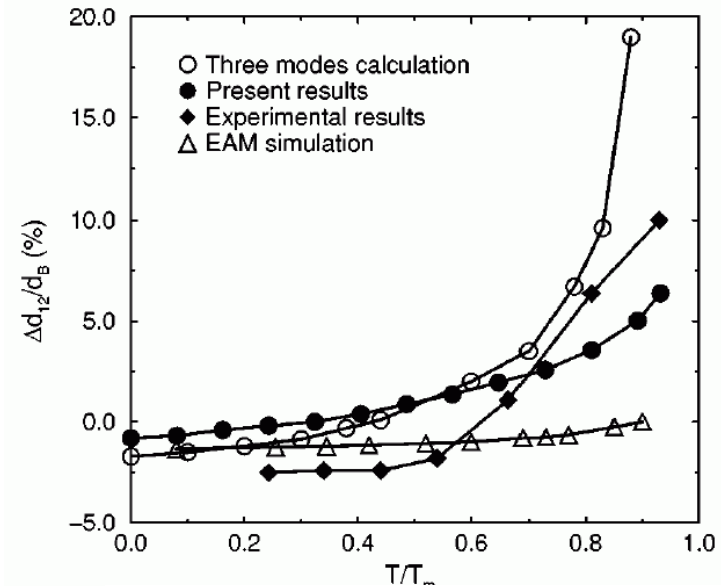
Surface Thermal Expansion: ion channeling + theory



Pluis, van der Gon, Frenken, van der Veen
PRL 59 401(1987)



Frenken, Huusen, van der Veen
PRL 58 (1987)

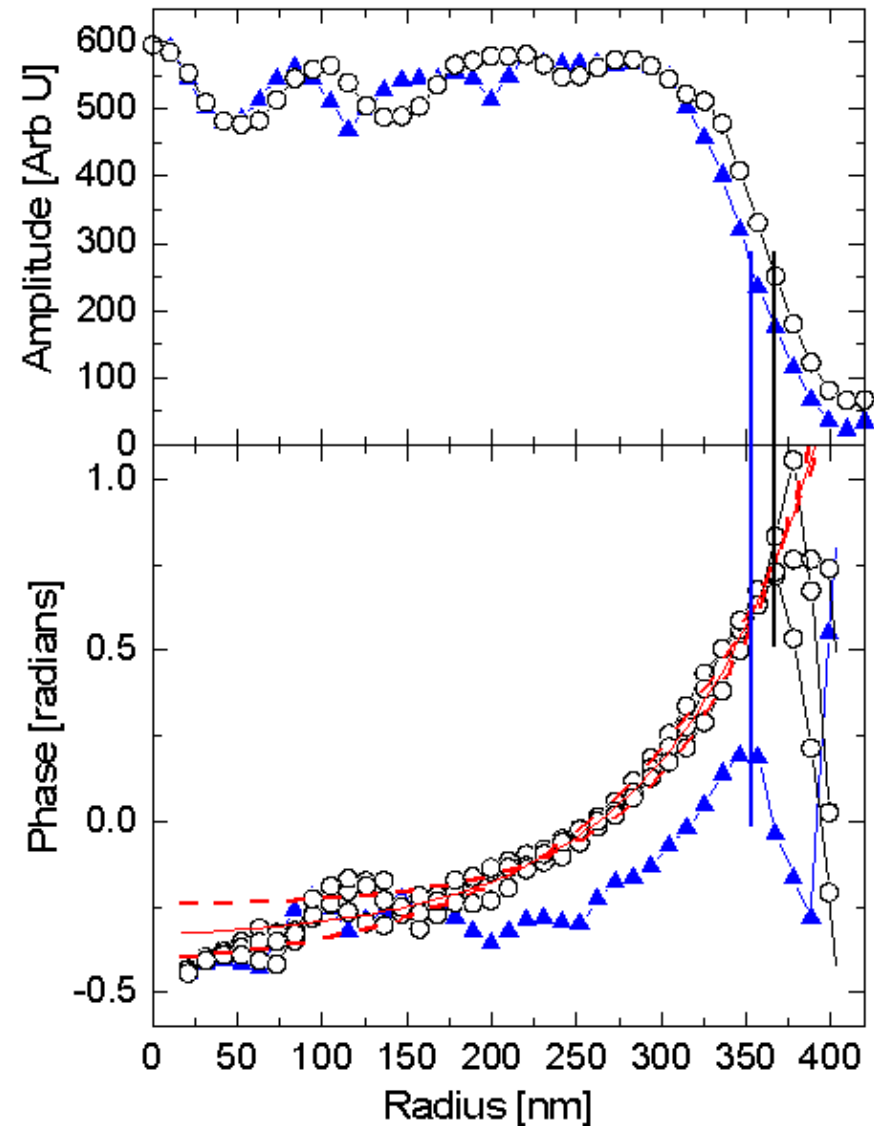
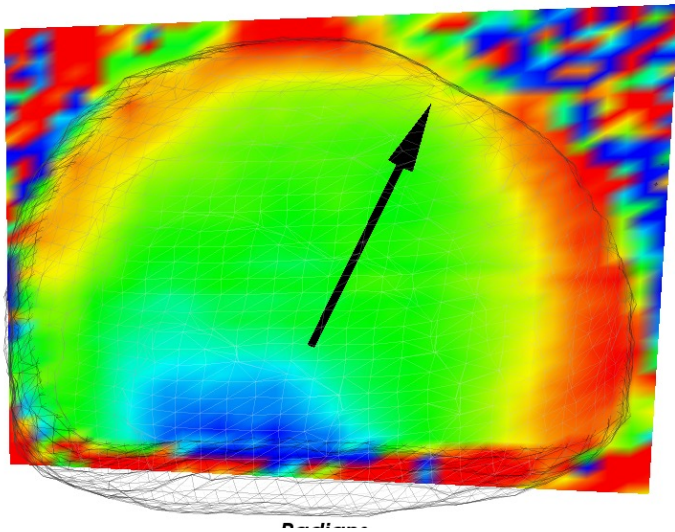


Ag(111) theory J. Xie (Scheffler group)
I. K. Robinson, Coherence PRB 59 970 (1999)

Depth Variation of Distortion

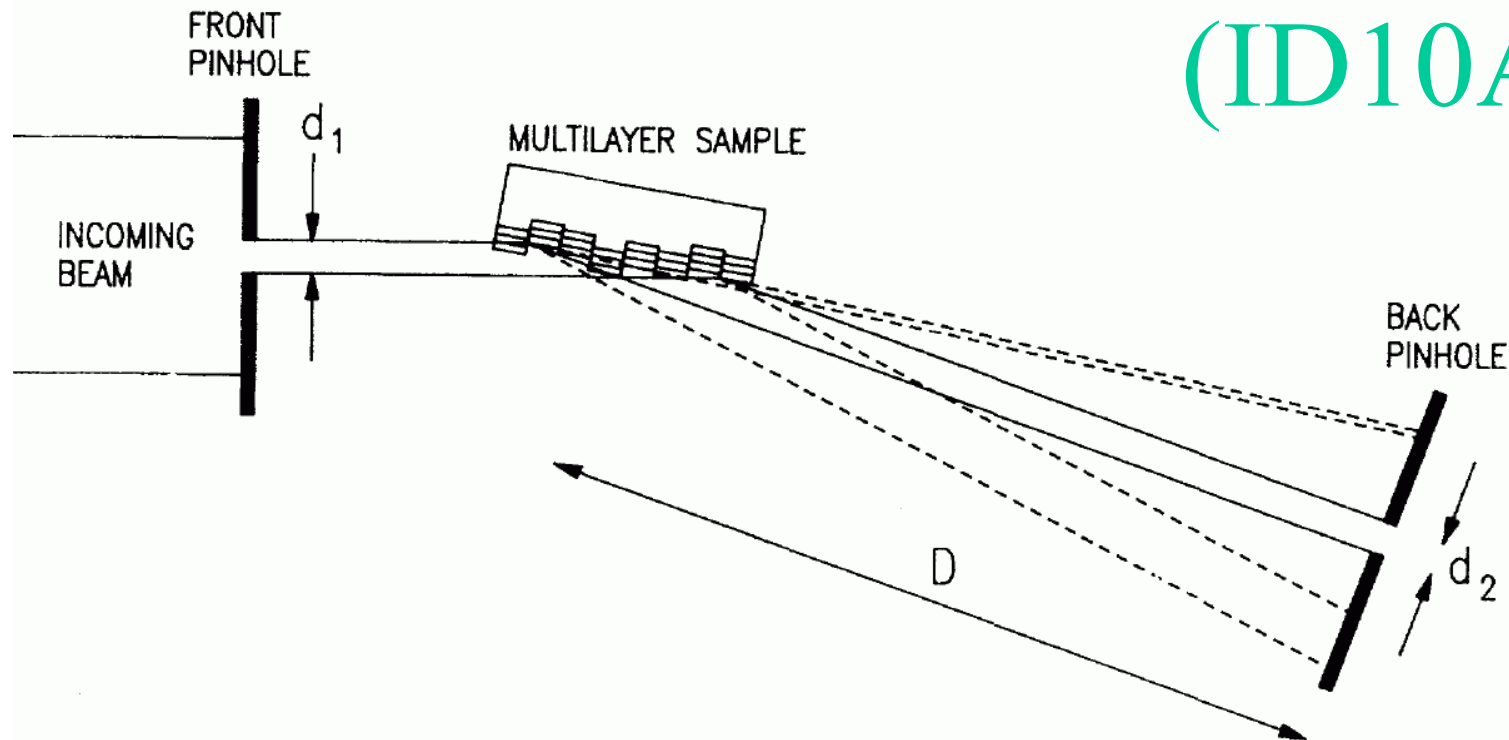
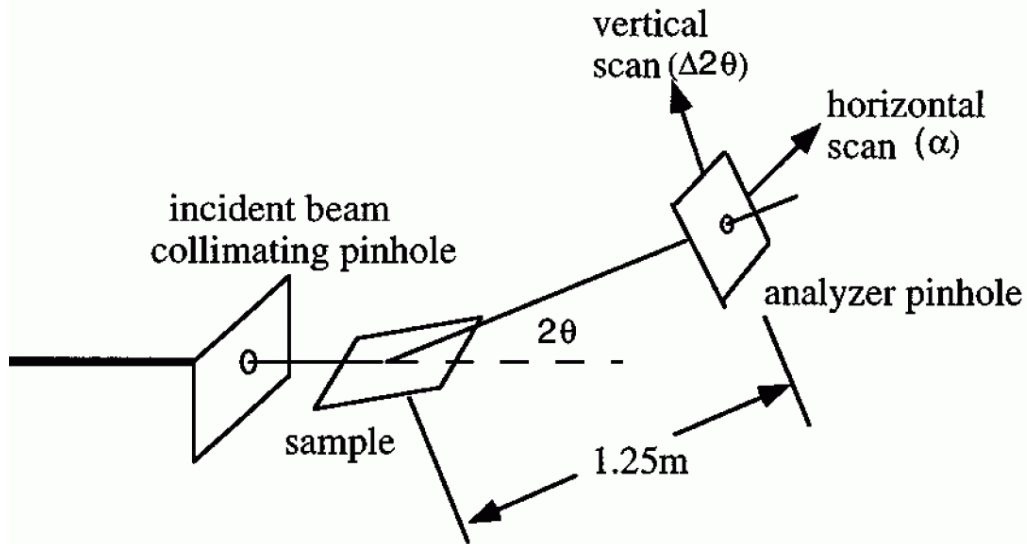
Facets subtend $18.6 \pm 2.6^\circ$
ECS predicts 14°

Depth measured $90 \pm 20\text{nm}$
Theory says 75nm

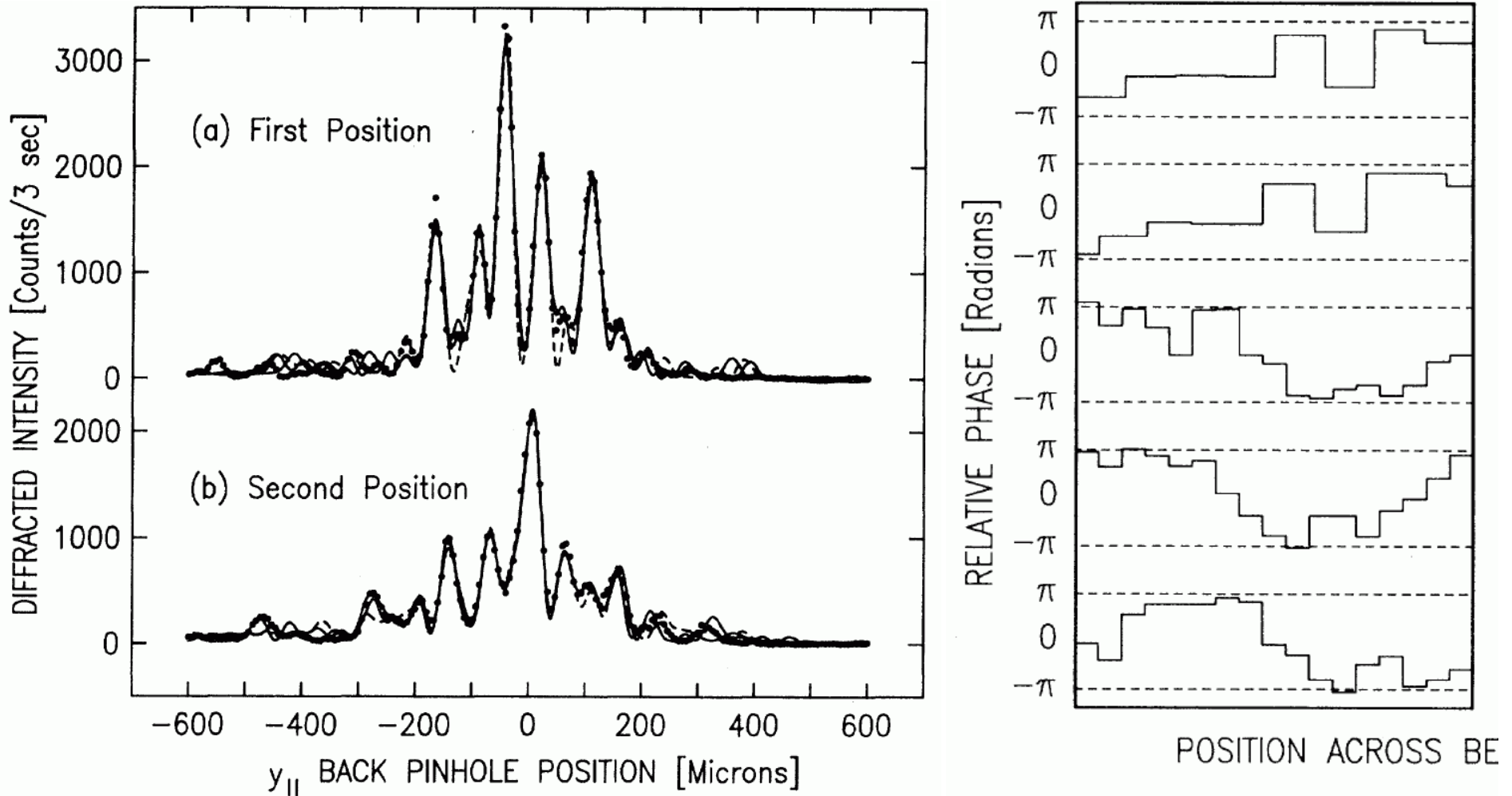


I. K. Robinso

Pinhole Speckle Experiments at “Troika” (ID10A)

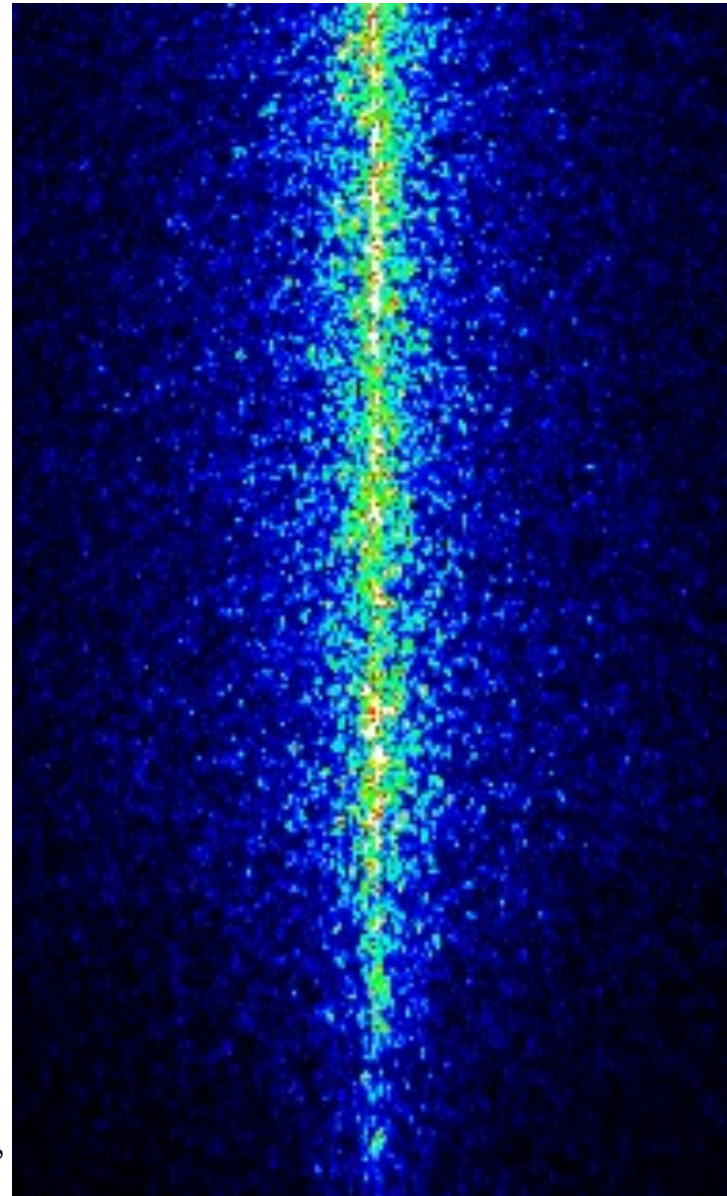
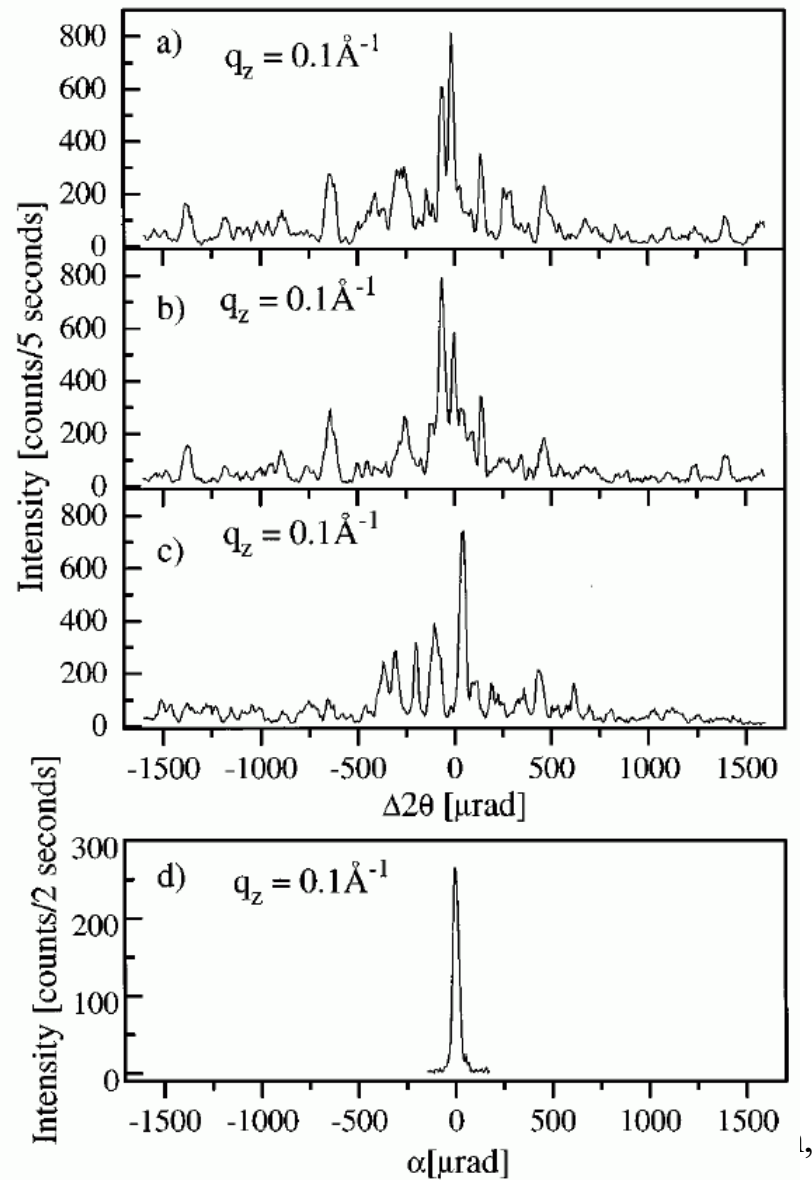


Fitting of speckle with block phase model



Speckle in Reflectivity from Si

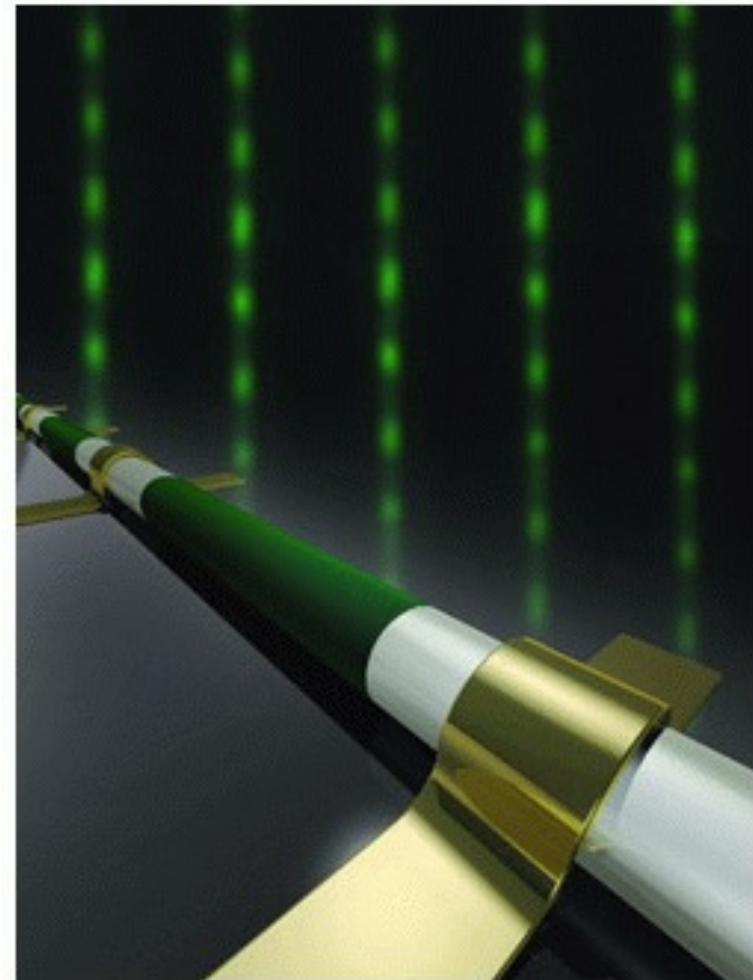
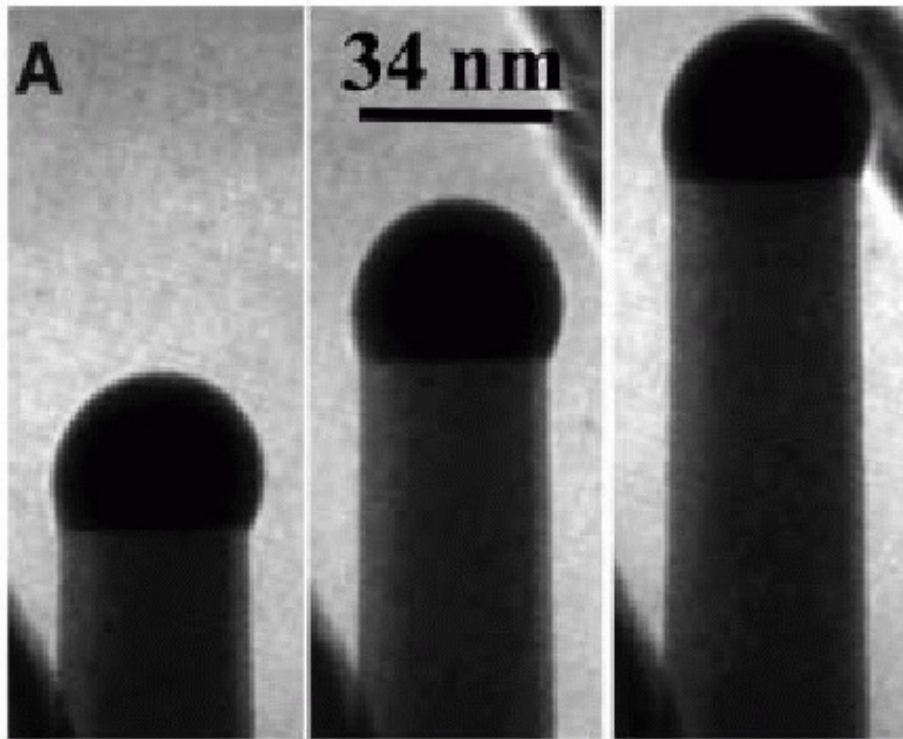
J. L. Libbert et al Phys. Rev. B 56 6454 (1997)



fe1103-24.spe 1x1 20 micron 20s x 31acc

VLS growth of nanowires

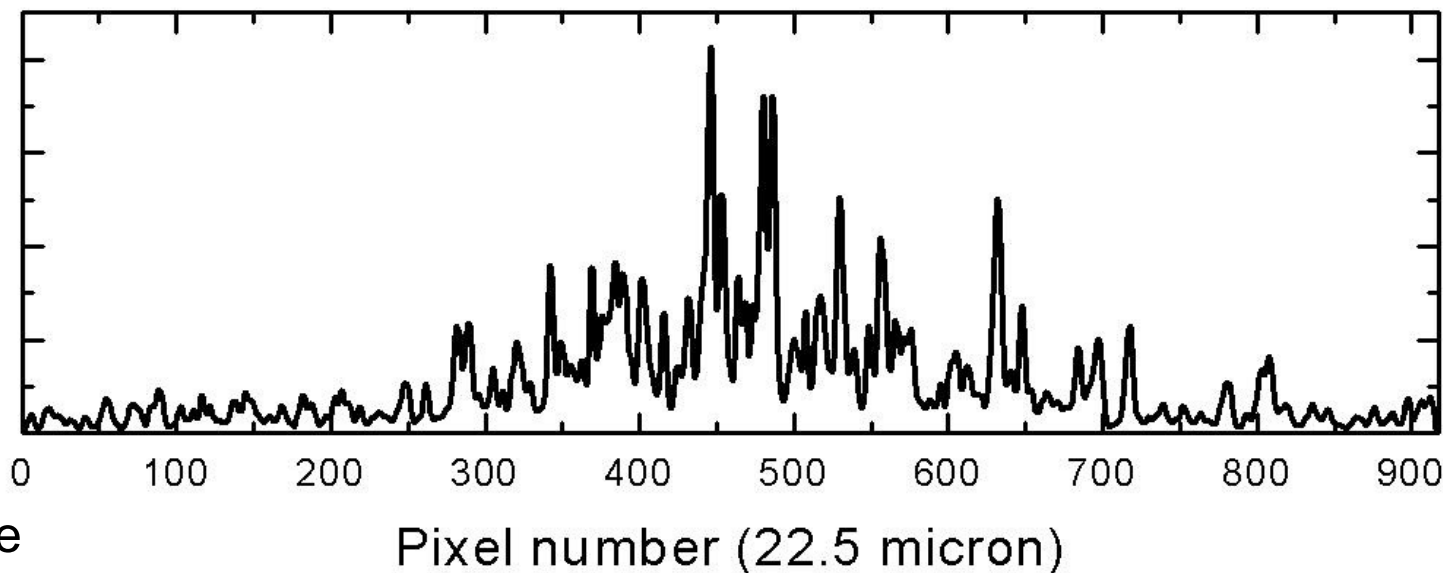
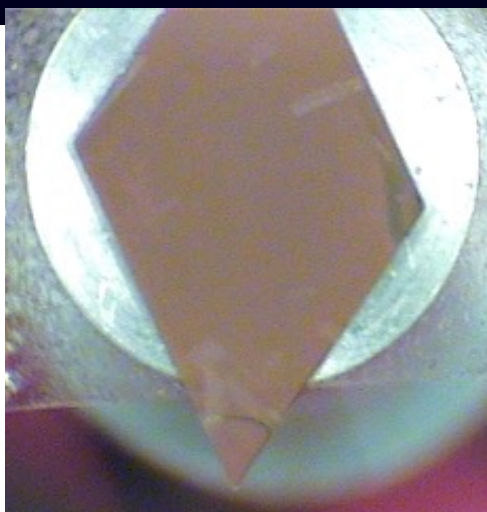
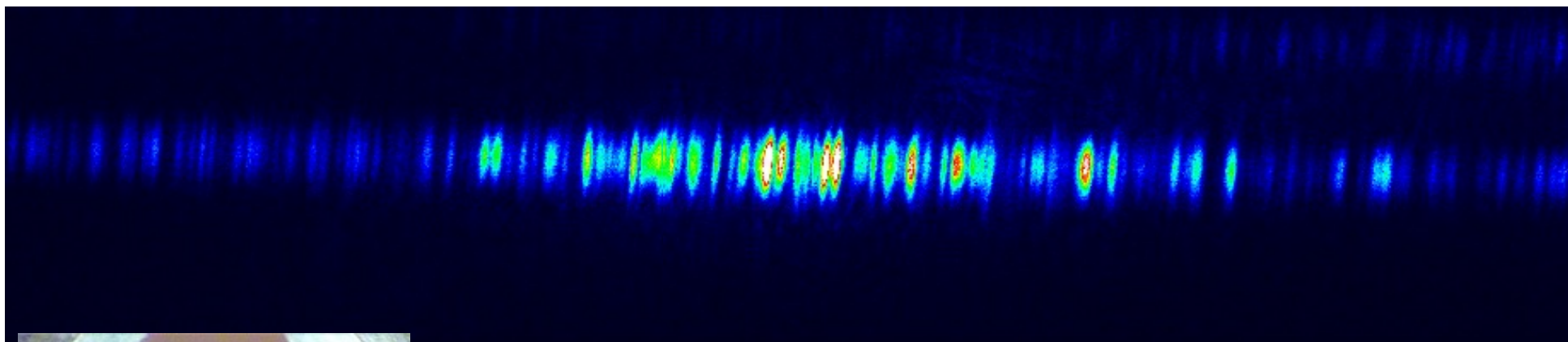
S. Kodambaka et al., *Science* 316 729 (2007)



I. K. Robinson, *Cohere* NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

GaAs Nanowire “Barcode”

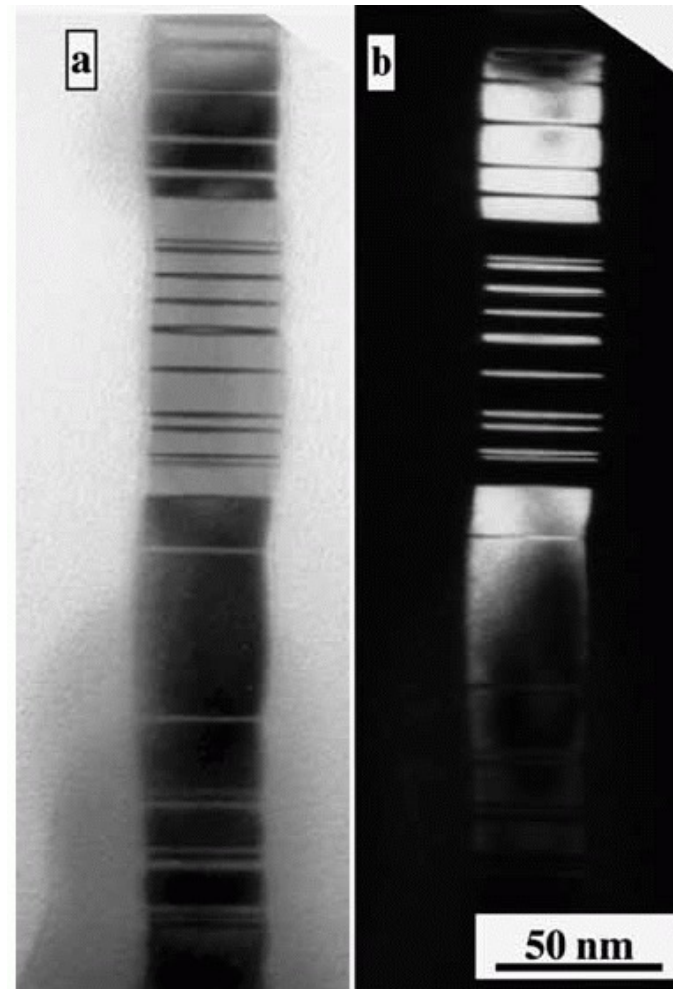
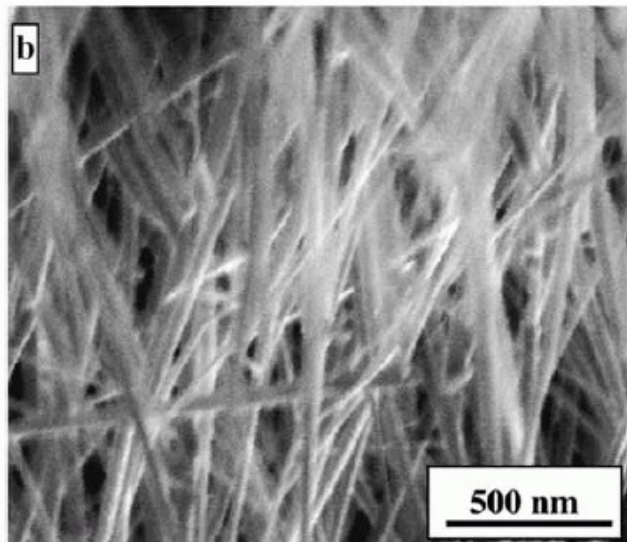
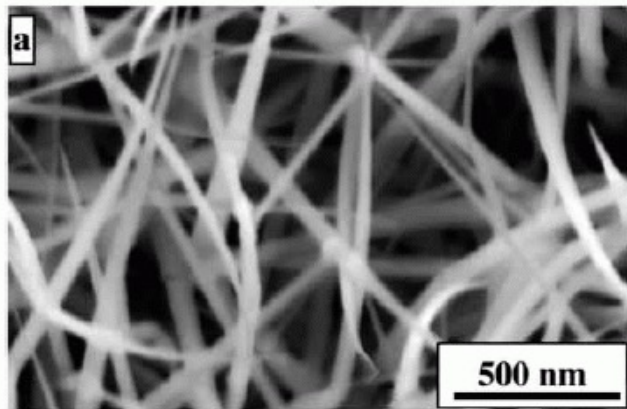
Vincent Favre-Nicolin, Joel Eymery (CEA),
Rienk Algra (Philips), Ross Harder



GaAsNW1106-22.spe
B9348 from Philips

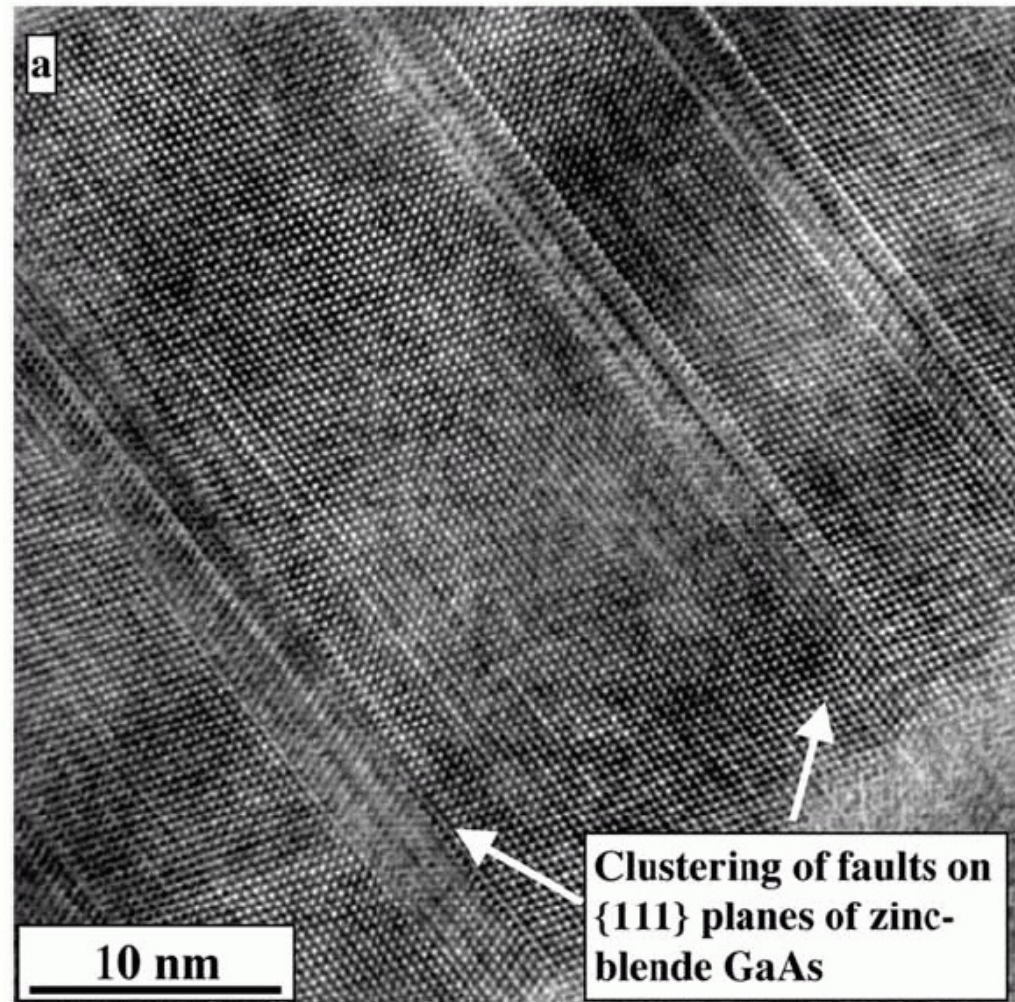
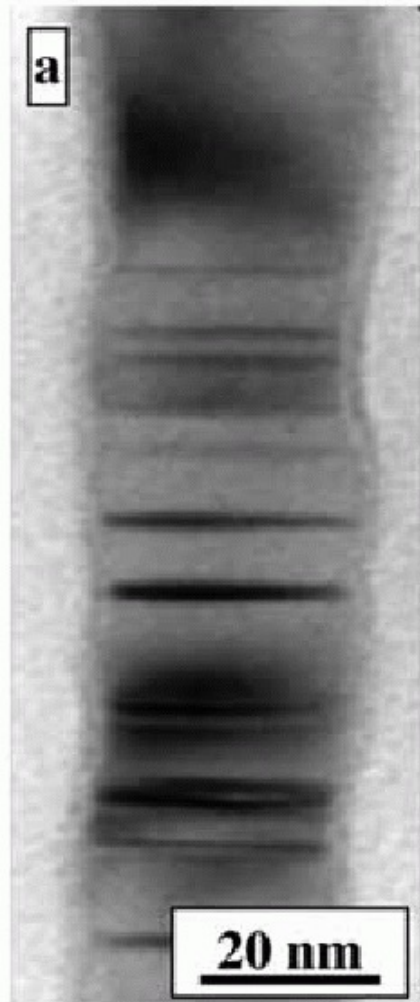
Dark Field TEM of GaAs Nanowires

R. Banerjee et al, Phil. Mag. Lett. 86 807 (2006)



Dark Field TEM of GaAs Nanowires

R. Banerjee et al, Phil. Mag. Lett. 86 807 (2006)

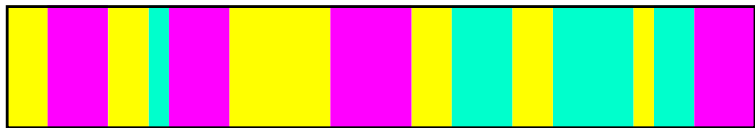


Models of Barcode Diffraction

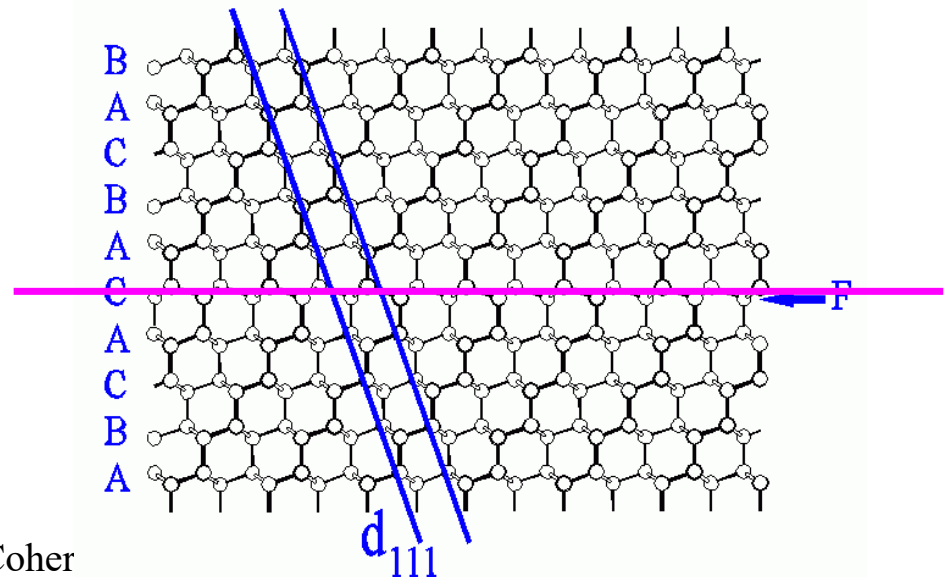
(111) wires at (11-1) reflection



- Twinned stacking sequence

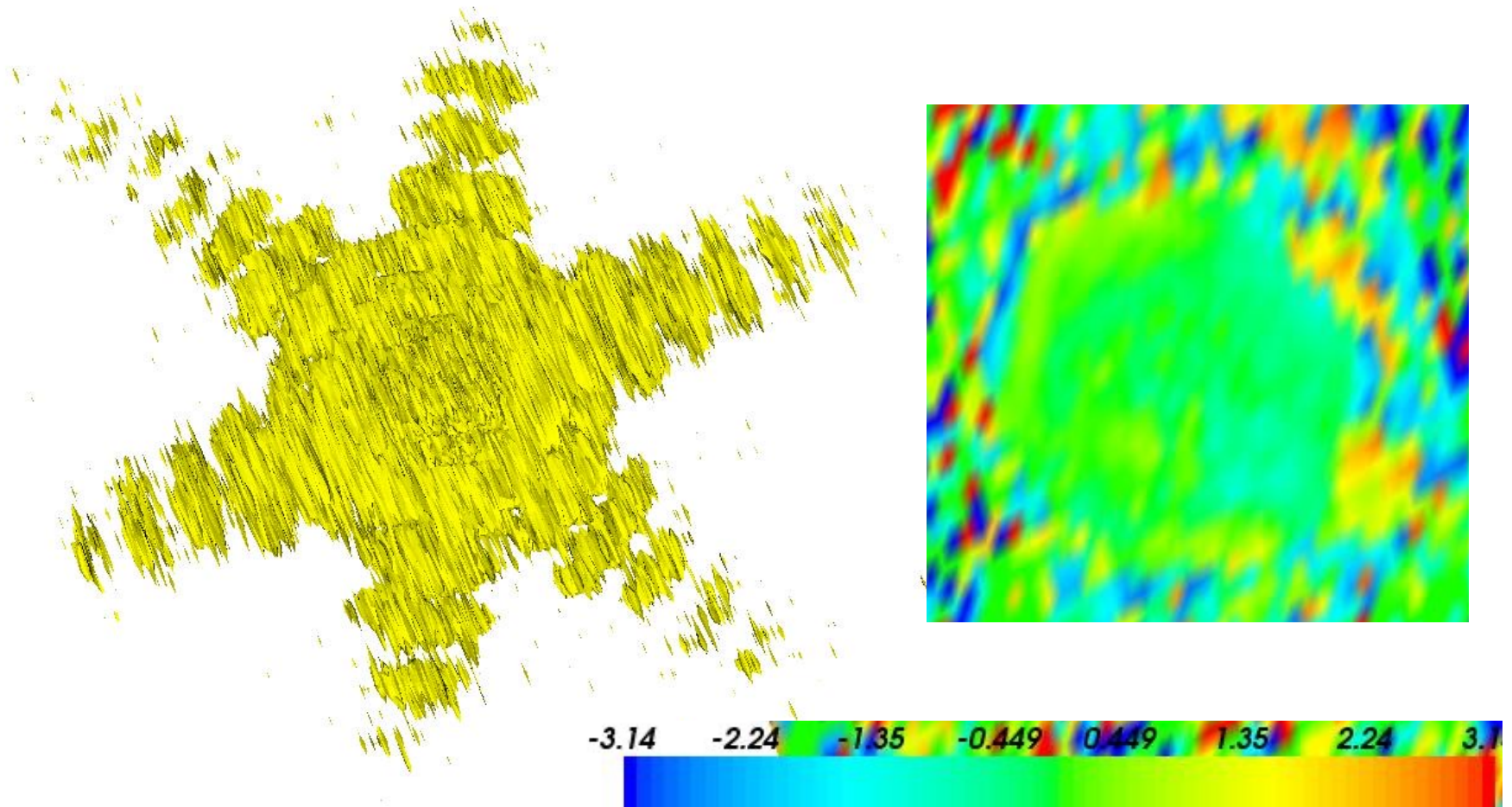


- Deformation faults



ZnO Nanowire Reconstruction

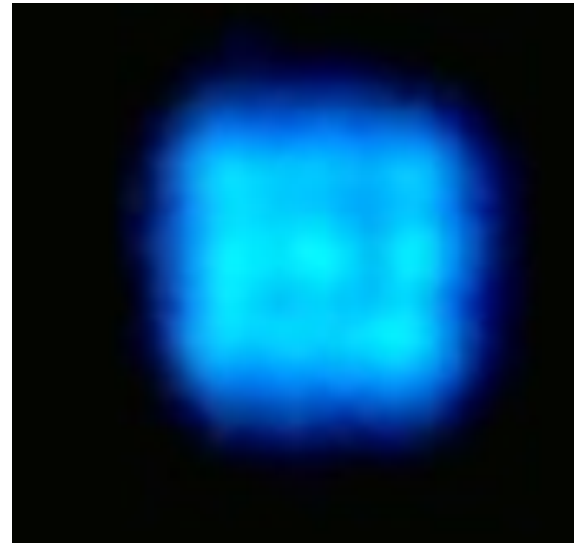
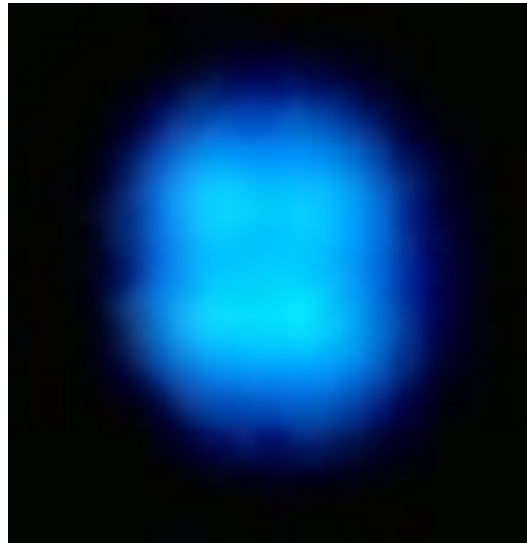
Ross Harder, Steven Leake, PhD project at UCL



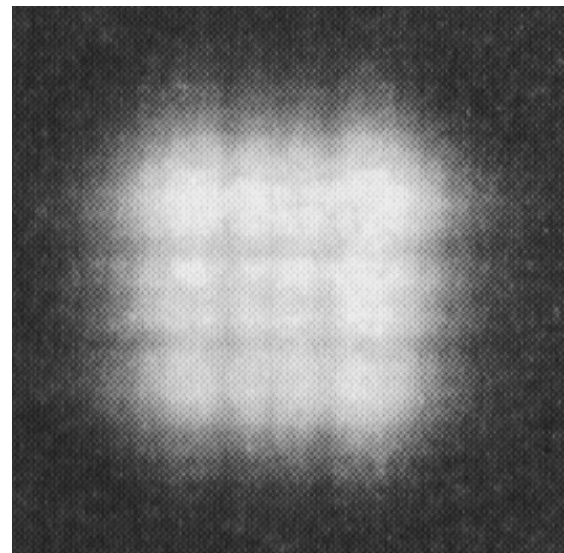
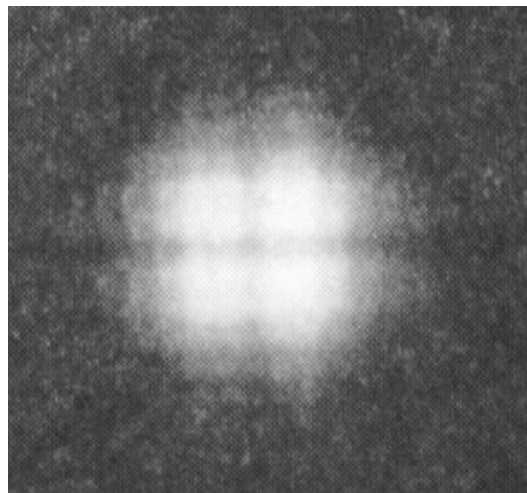
Phase Images using CXD

- Strain, displacements along **Q**-vector
- Chemical contrast (especially at resonance)
- Lattice shifts due to stacking faults
- Height of a reflecting surface
- Antiphase domain structures
- **Refraction** along path through object
- Illuminating wavefront, resulting from slits, focussing optics

Fresnel Diffraction when $d^2 \sim \lambda D$



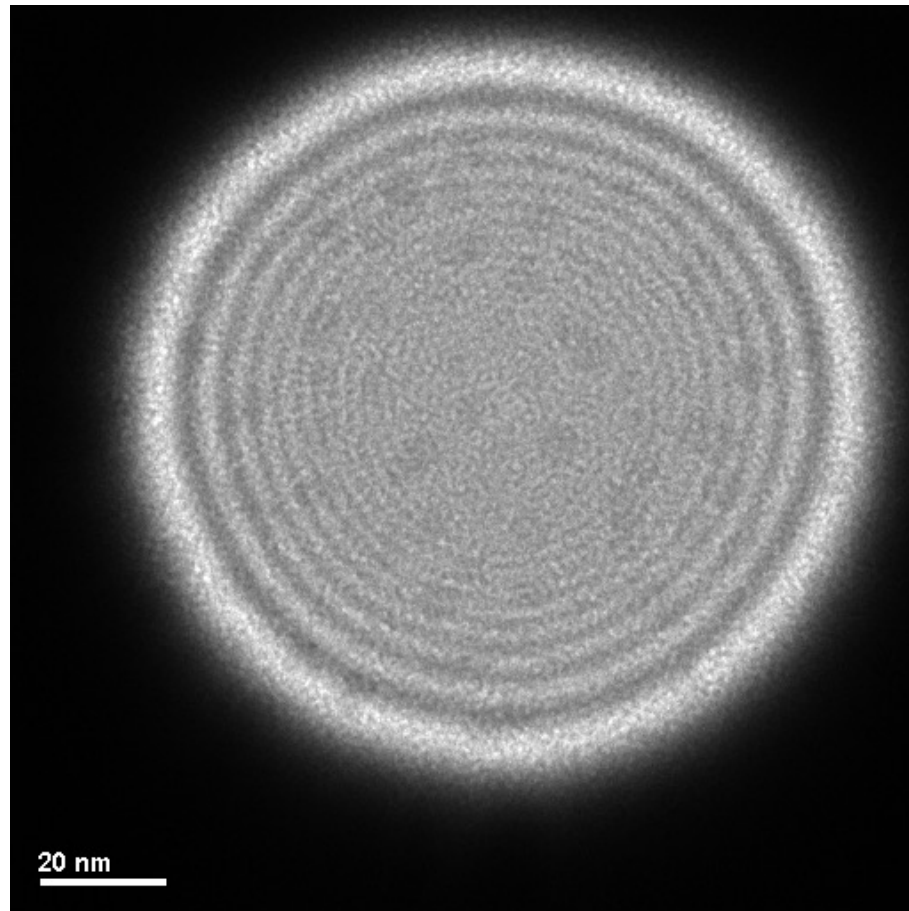
X-ray
beam
defined
by RB
slits 5 μ m



Visible
Fresnel
diffraction
from
Hecht
“Optics”

I. K. Robinson,

100nm Electron Microscope probe



FeAl antiphase domains (001)

Lorenz Stadler, PhD dissertation, TU Wien (2005)

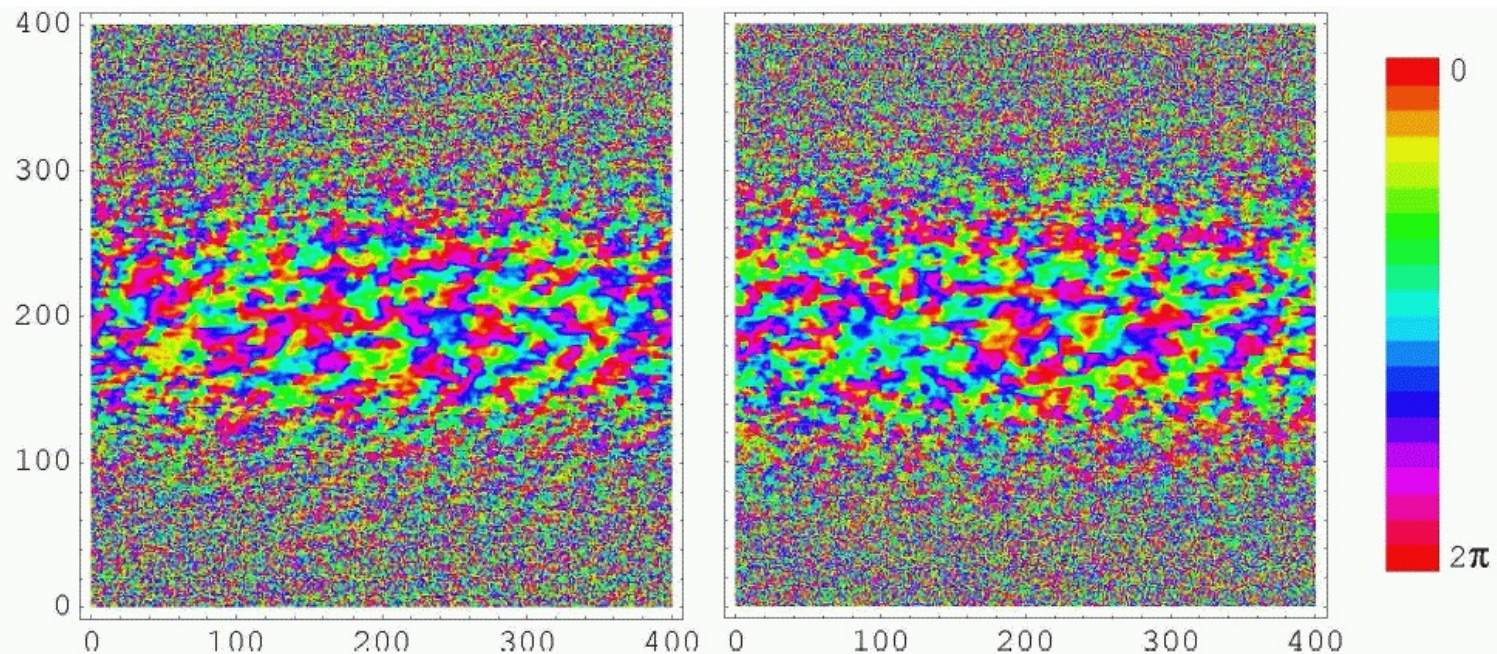
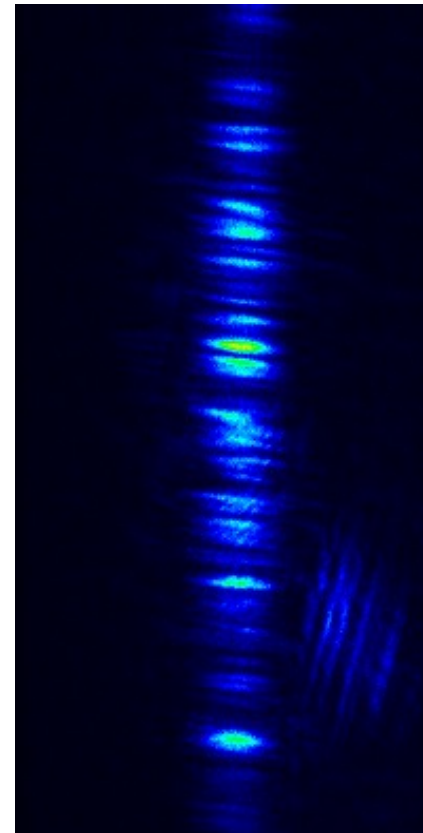
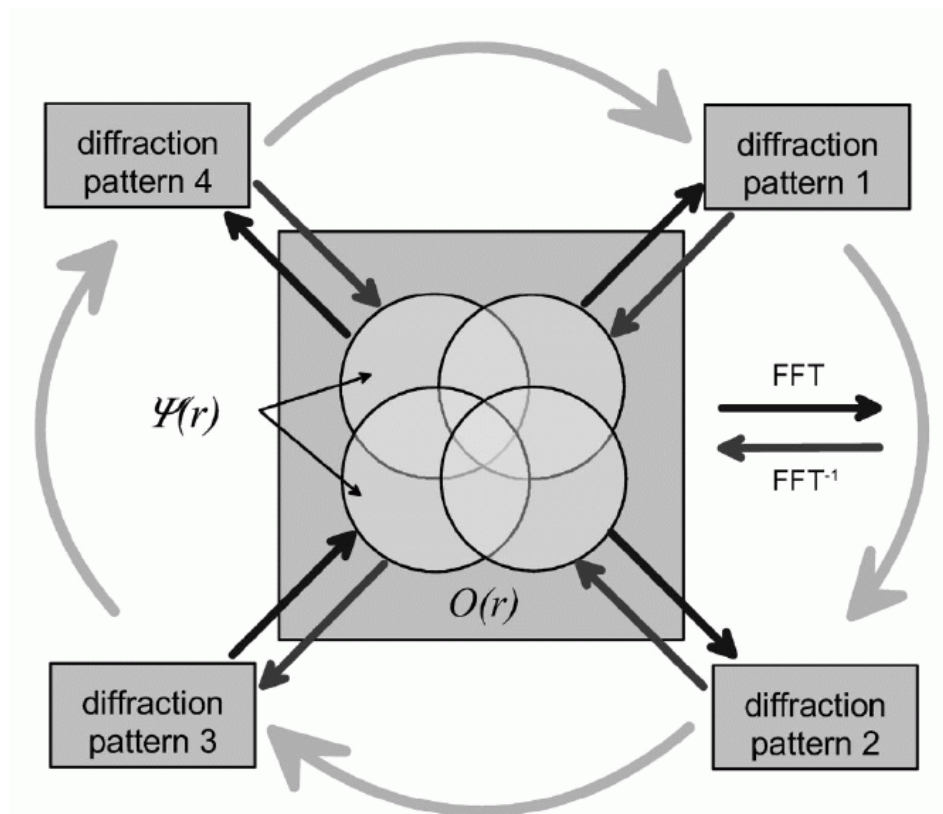


Figure 7.11: Typical reconstructed phases from runs with different combinations of algorithms and supports derived from the 2D Gaussian fit of the illumination function. Numbers in brackets denote how many iterations of the particular algorithm were done each cycle. Graphs on the left are from reconstruc-

Future of CXD: Ptychography

Rodenburg & Pfeiffer, PRL (2007)



Conclusions

- Strain fields imaged from asymmetric patterns
- Surface strain has orientation dependence
- Coherent diffraction from rough surfaces
- Nanowire “barcode” from stacking faults
- Wire cross sections show strain
- Refraction effects can be important