Strain Mapping in Nanocrystals 3D imaging through Diffraction

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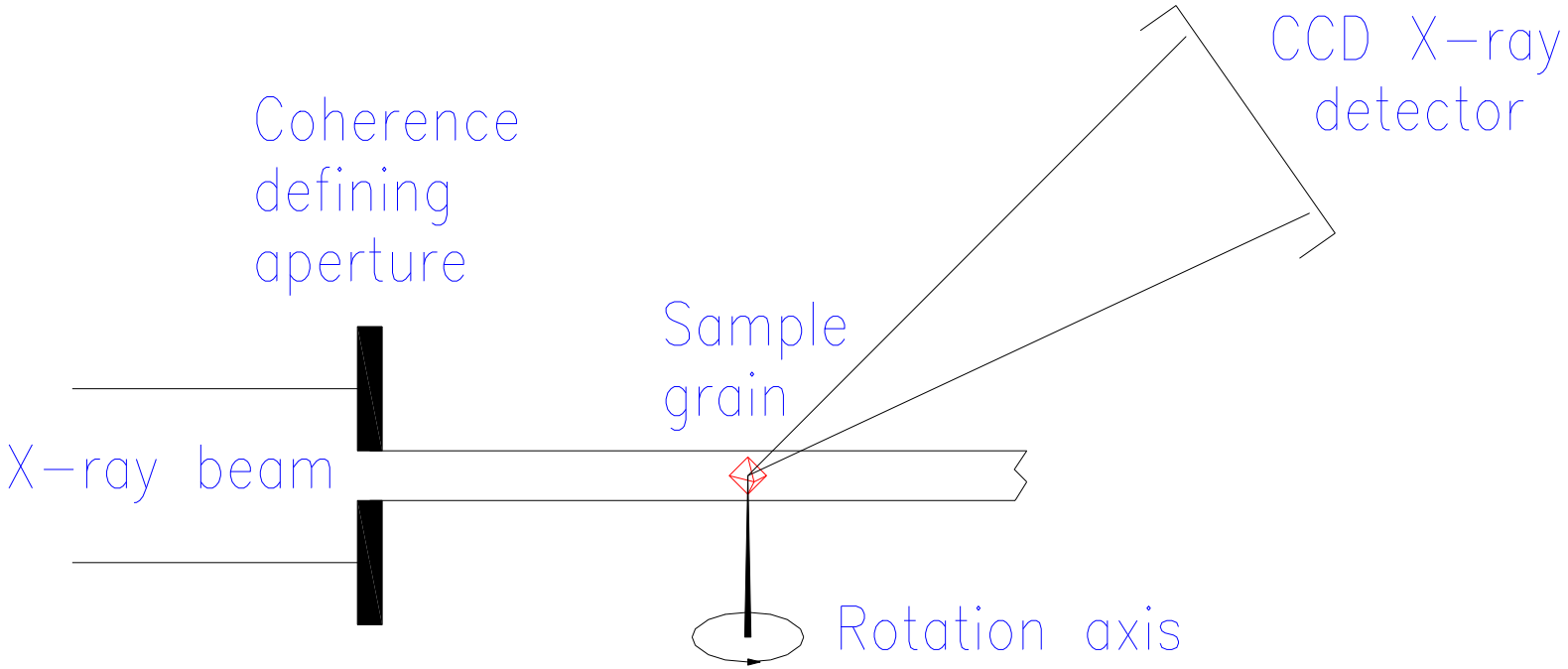
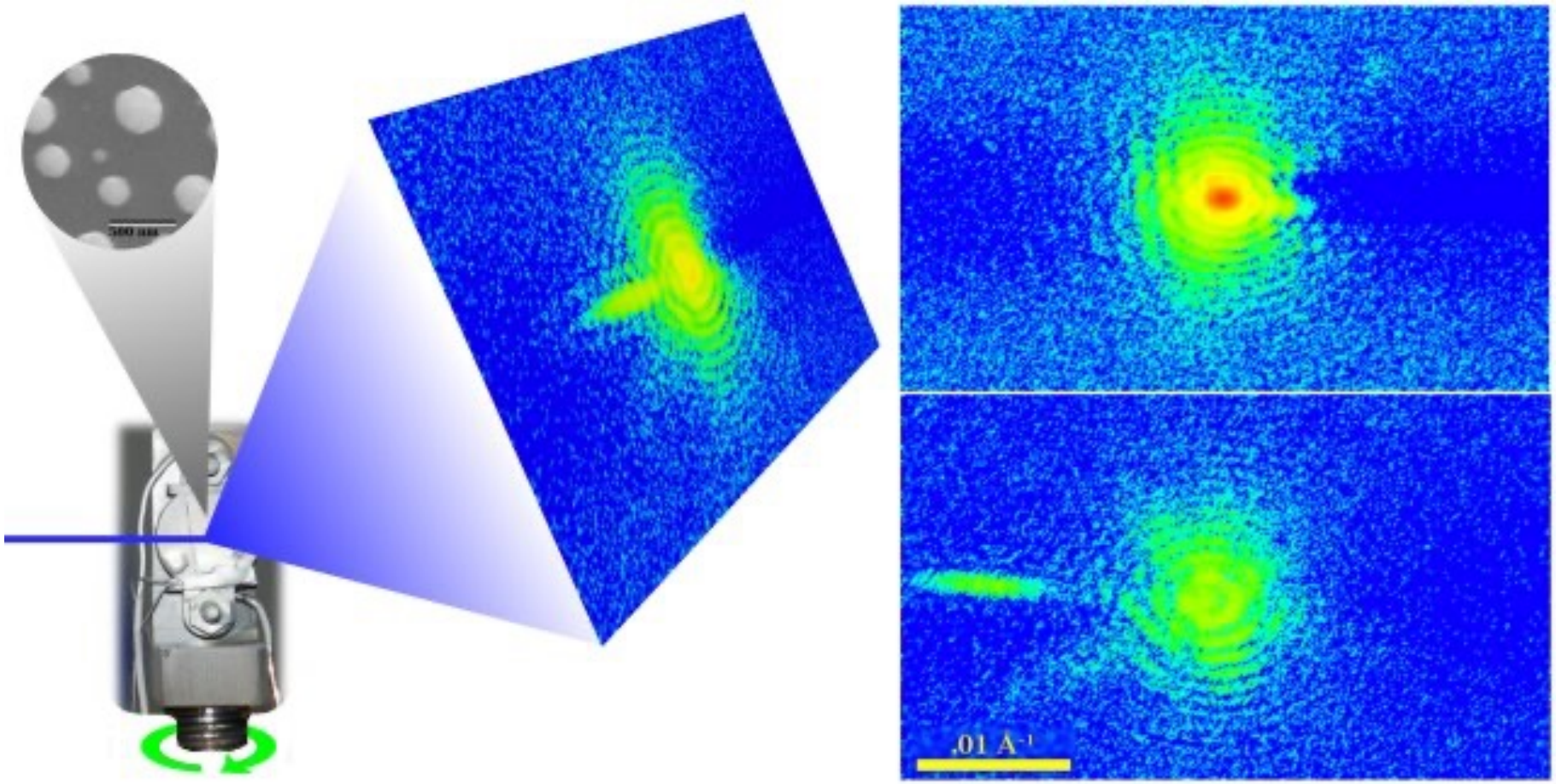
University College London

Diamond Light Source

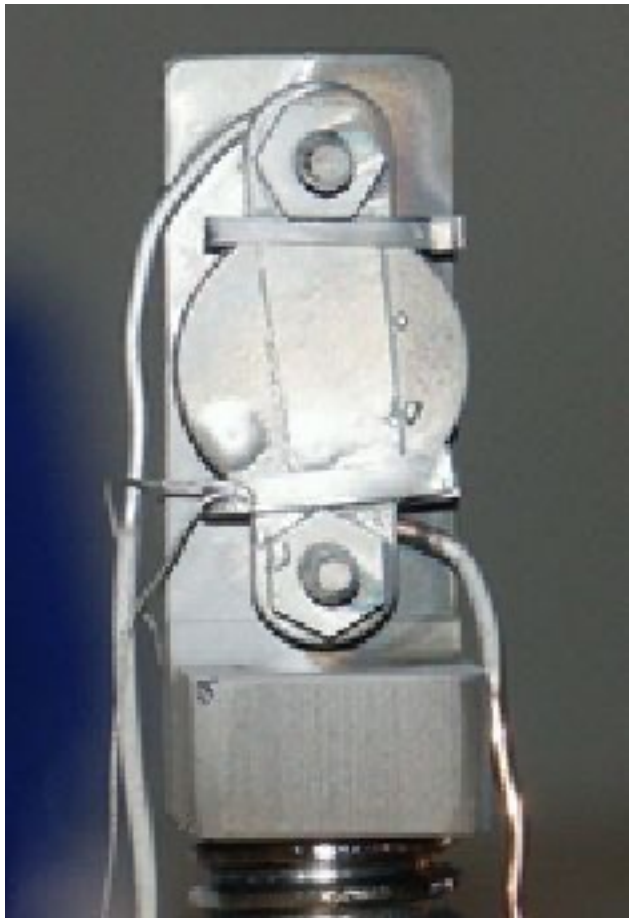
Lensless X-ray Microscope

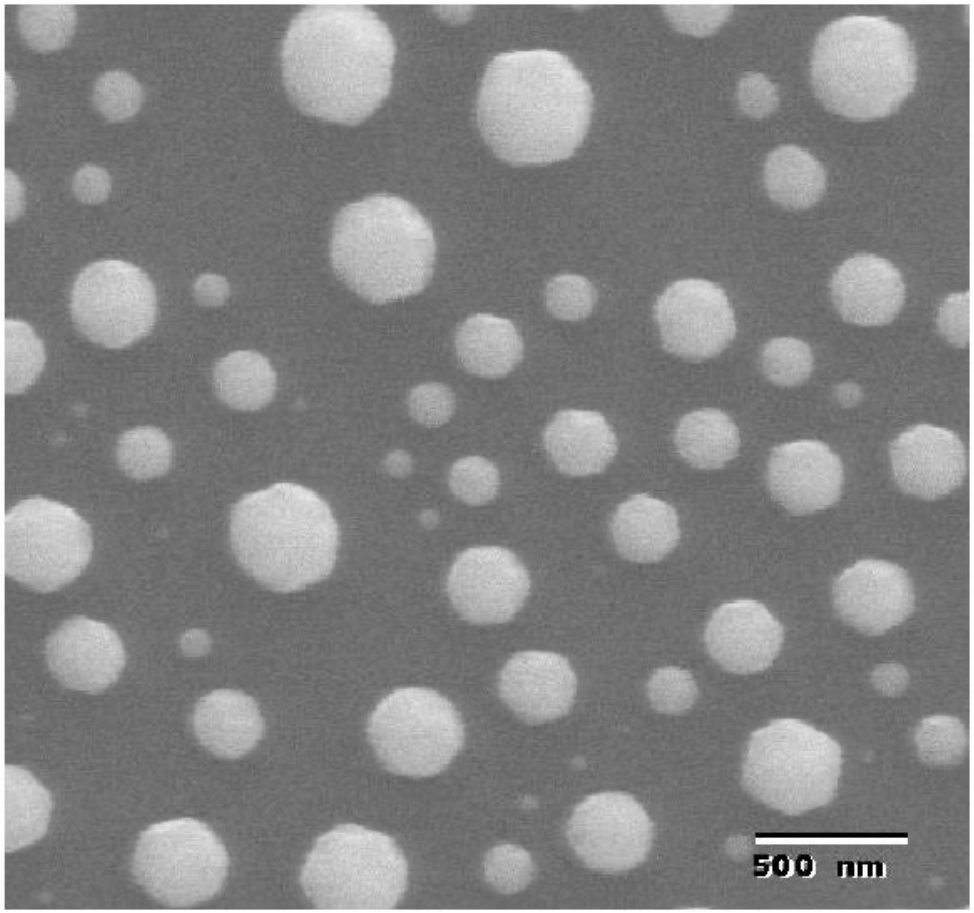


Lensless Imaging setup in UHV

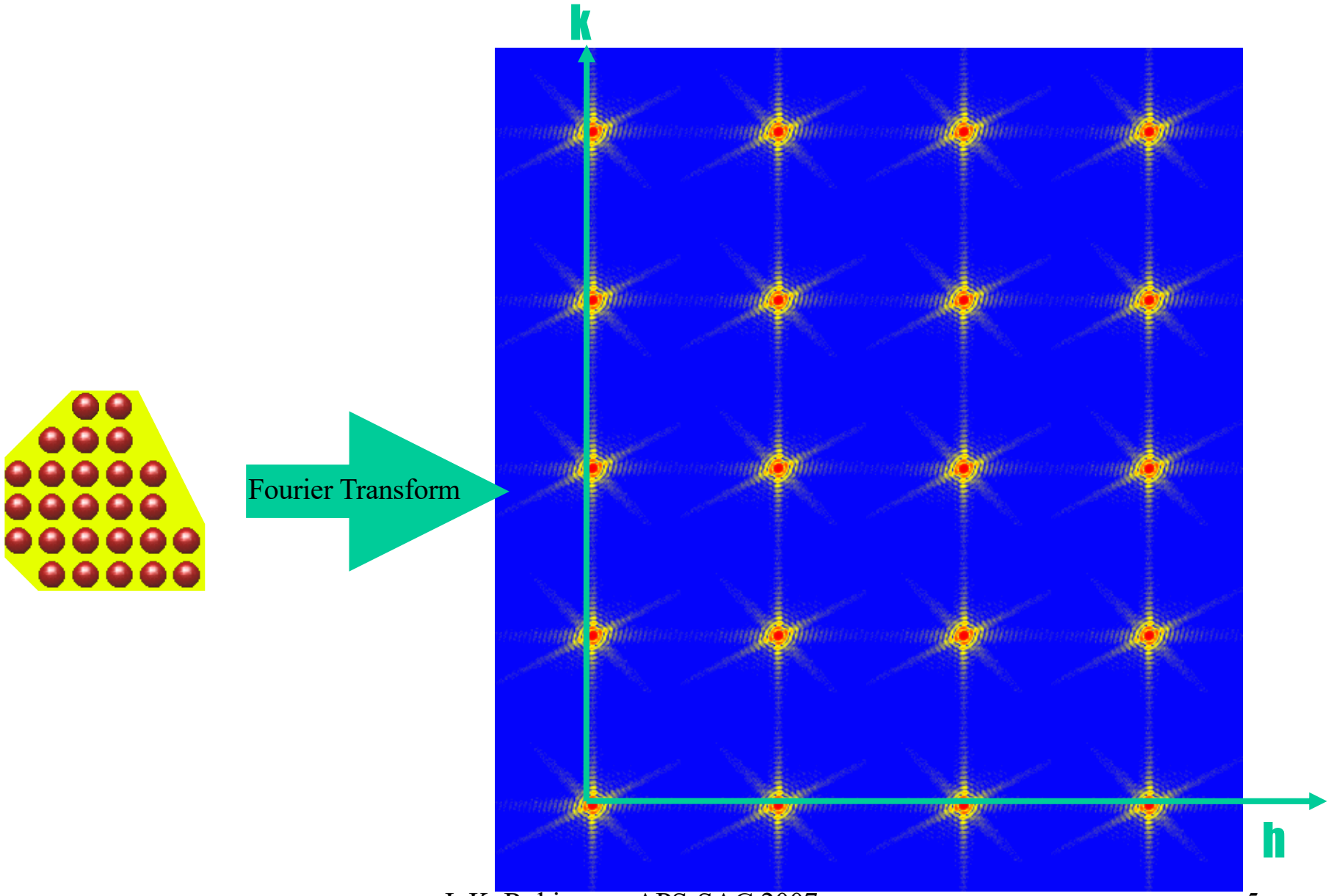


In situ growth of Pb crystals





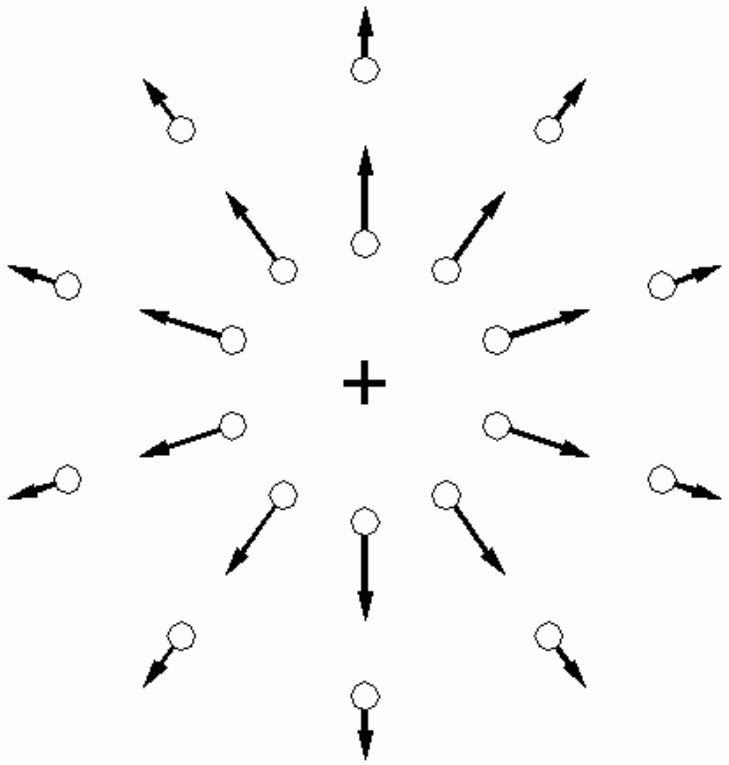
Coherent Diffraction from Crystals

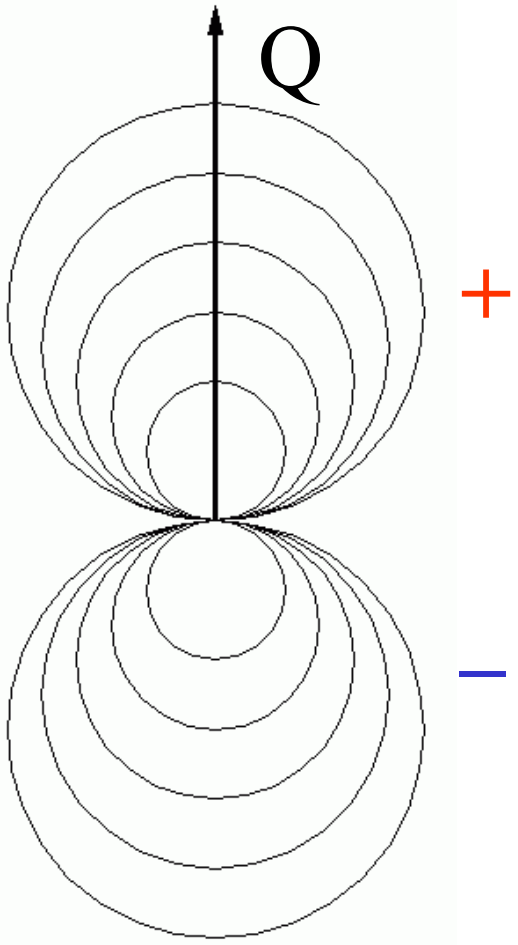


Diffraction by Strain of Point Defect

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

Imaginary density





Good statistics, 3D diffraction data

Mark Pfeifer, Garth Williams, Ivan Vartaniants, Ross Harder

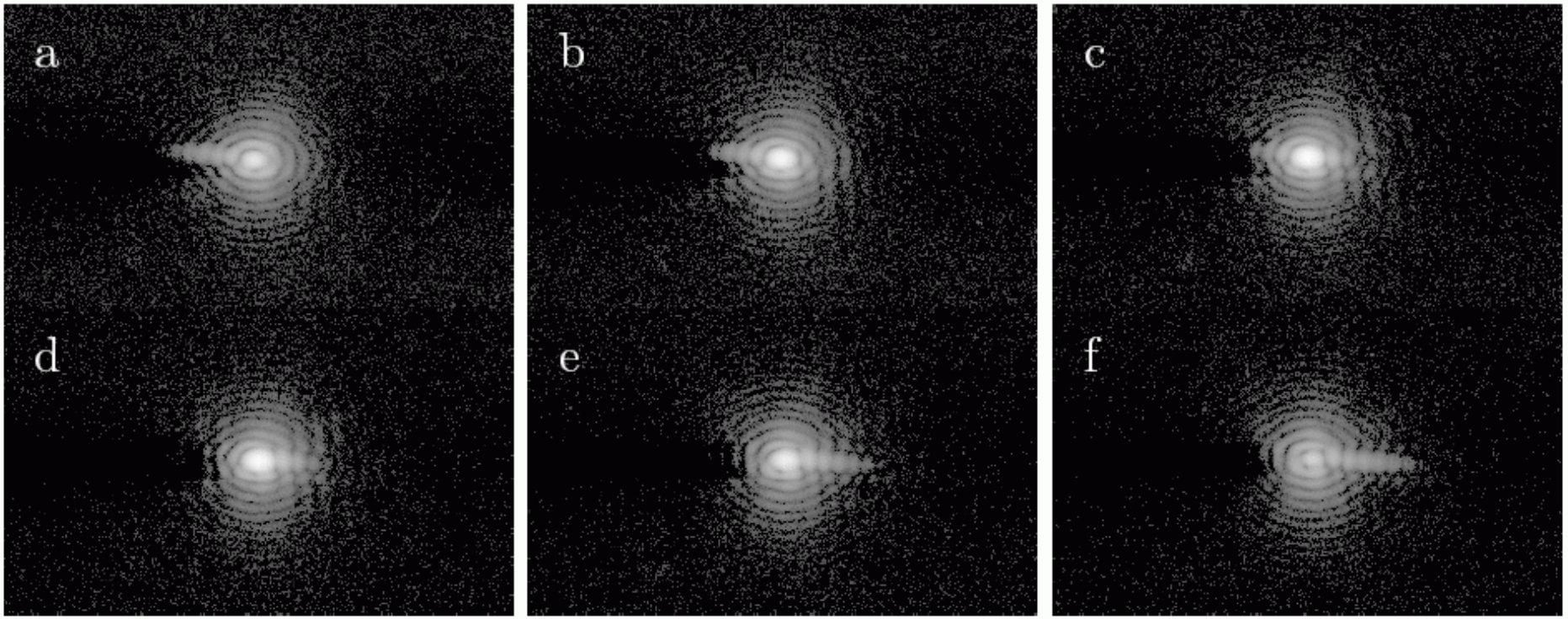
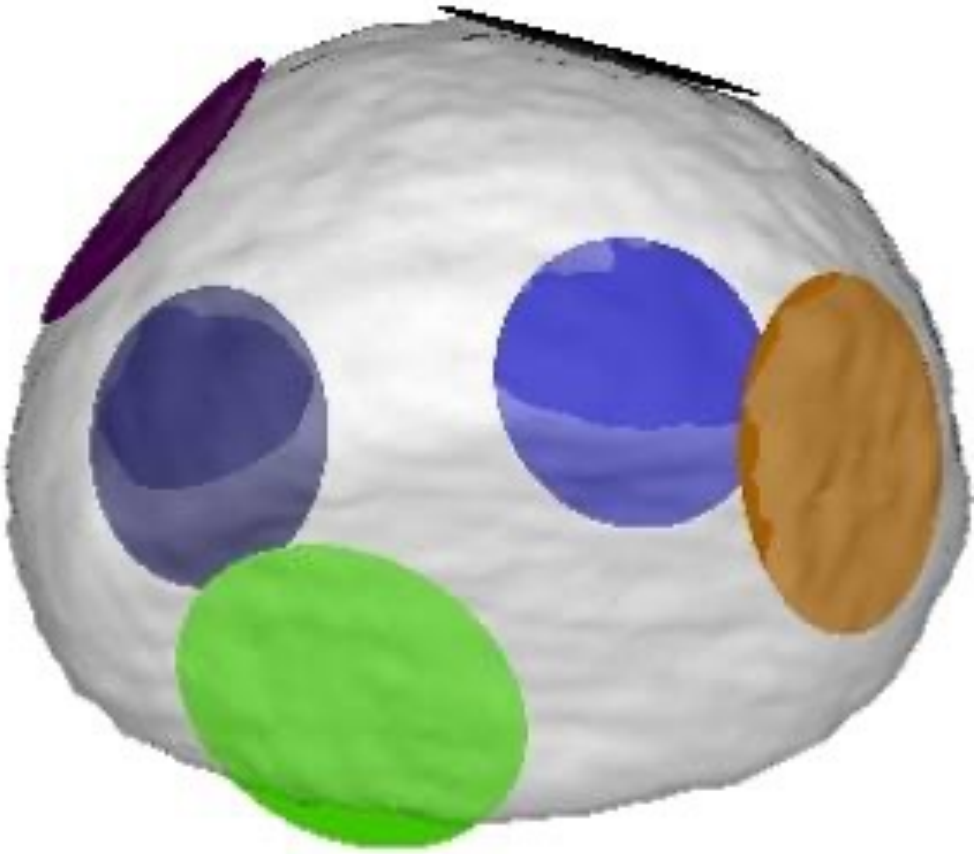
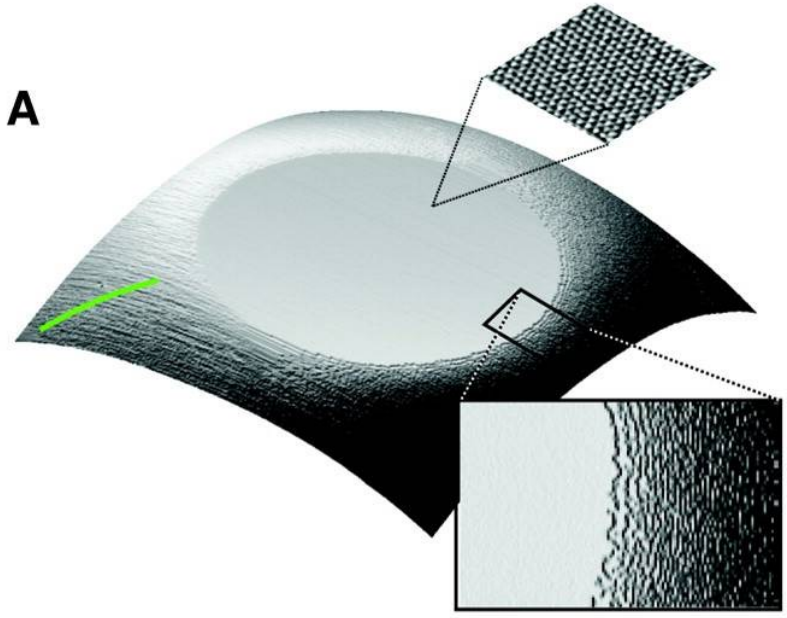


Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

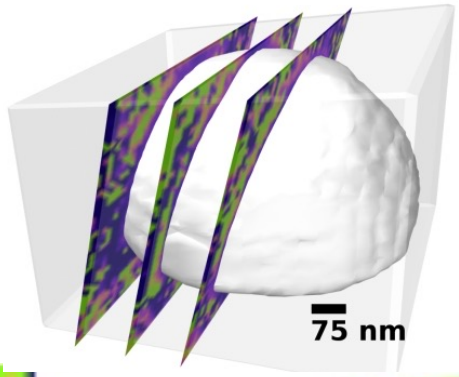
Facets of Equilibrium Crystal Shape

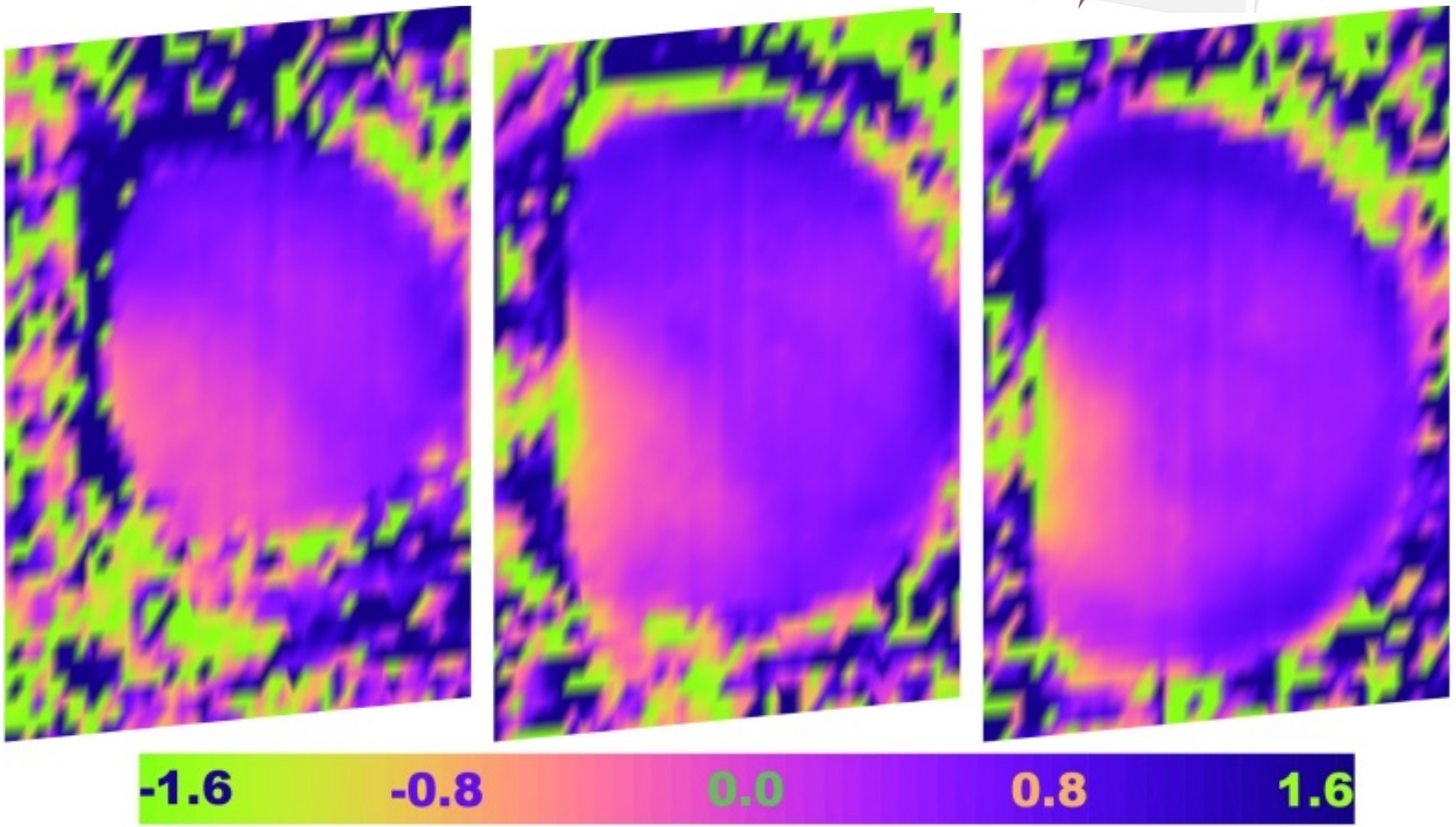


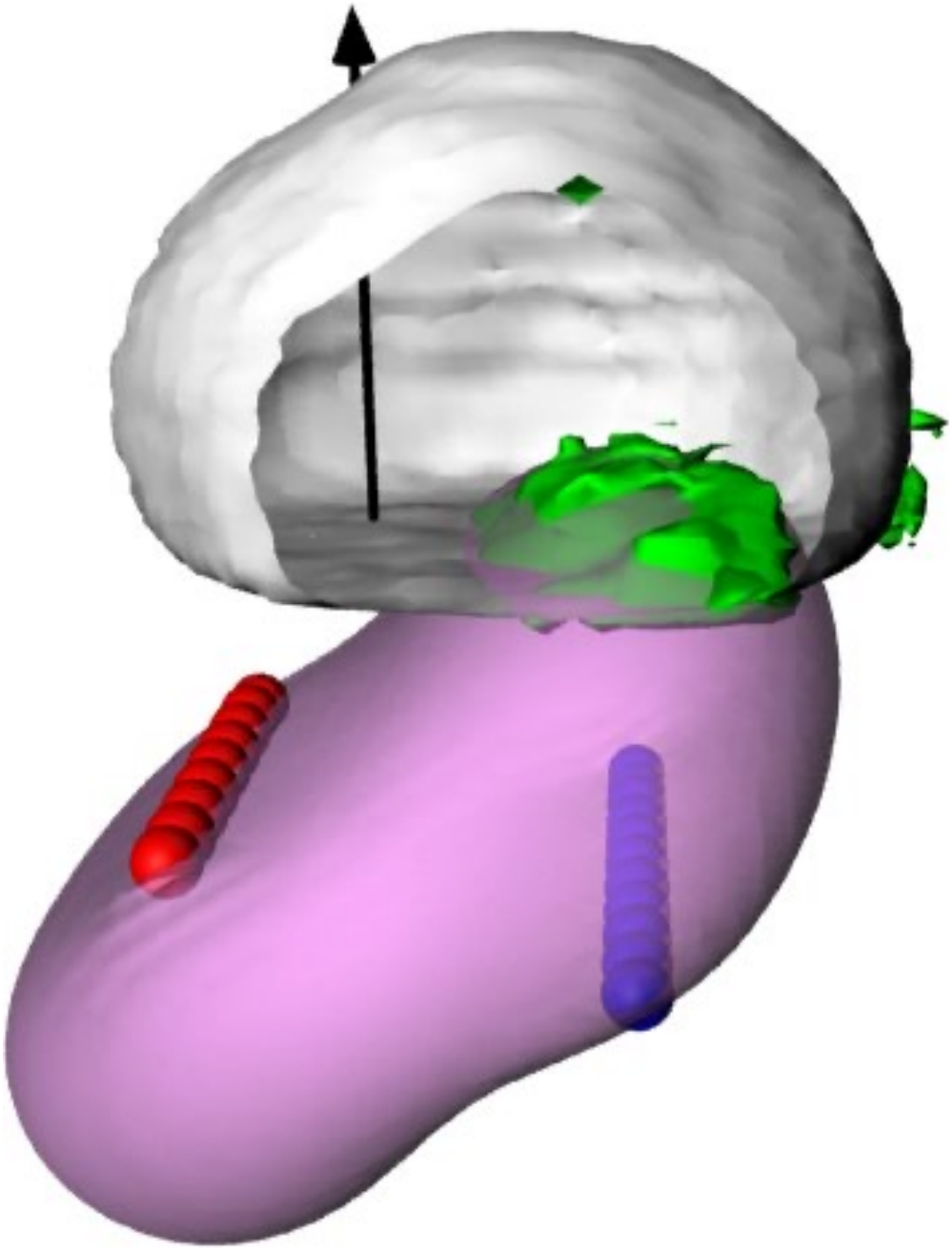


Thurmer K, Williams E, Reutt-Robey J
Science **297** 2033 (2002)

3D phase map sections







Refraction effects in Lead at 8.9keV

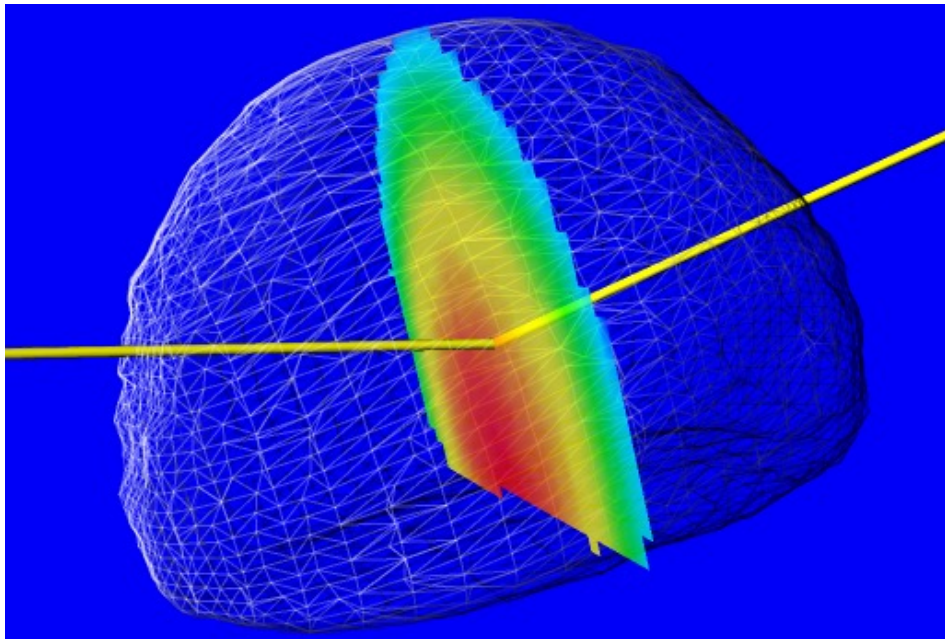
Phase accumulation due to refraction along scattering path

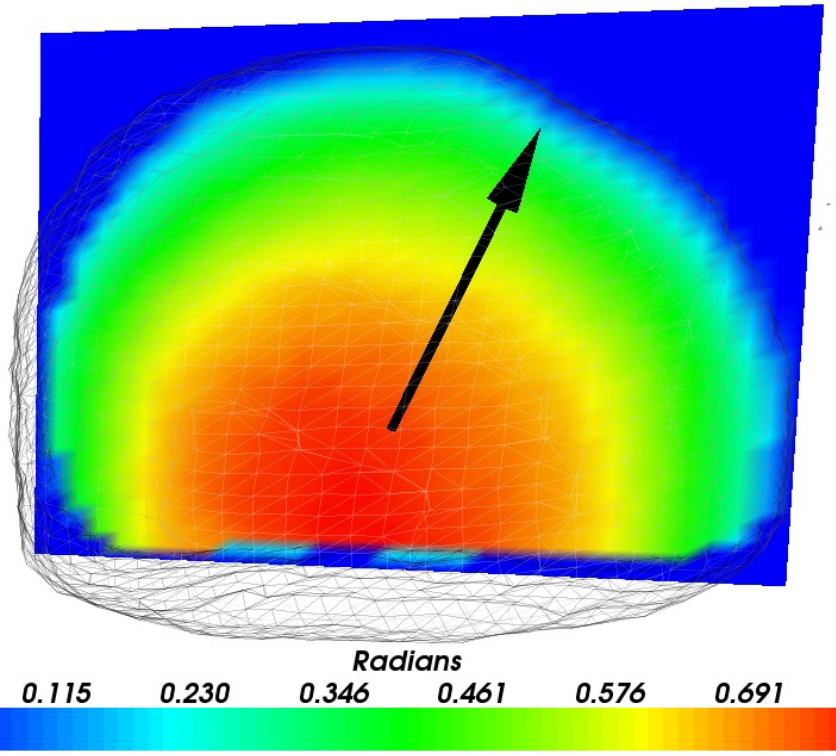
d=750nm: $kd\delta = 0.76$rad

$kd\beta = 0.07$

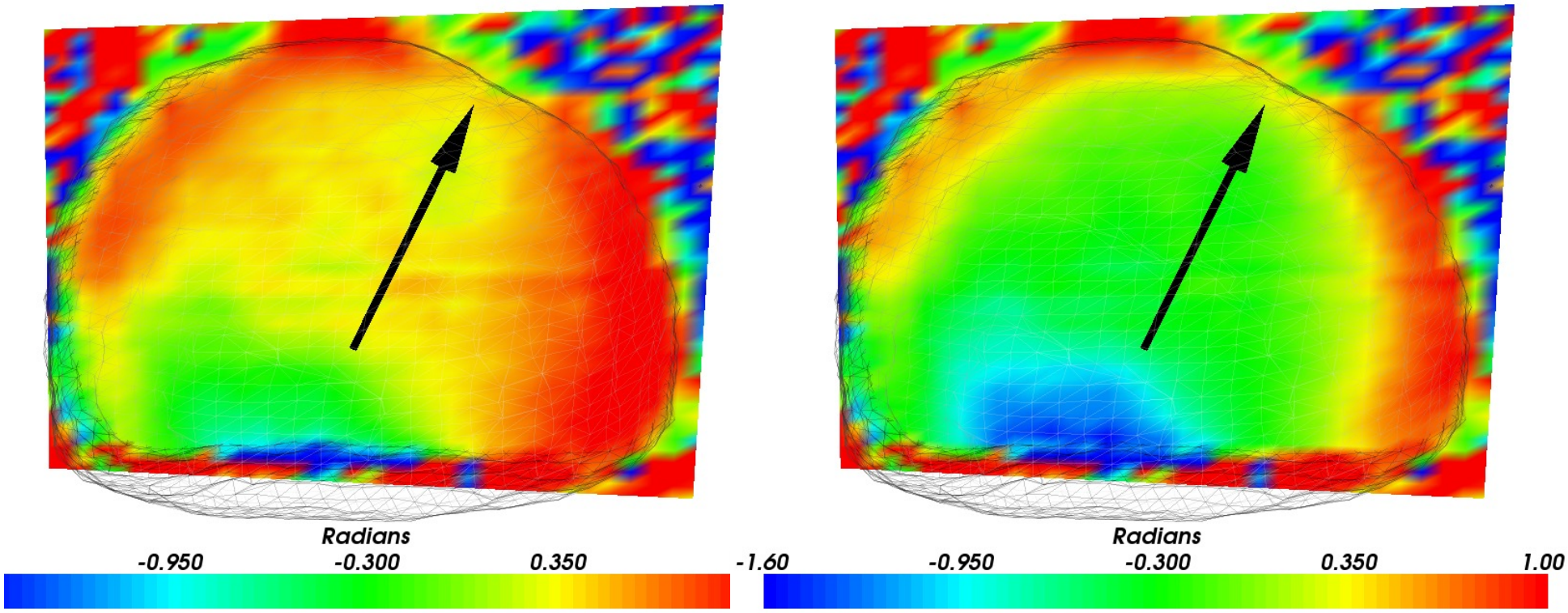
$\delta = 2.23 \times 10^{-5}$

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



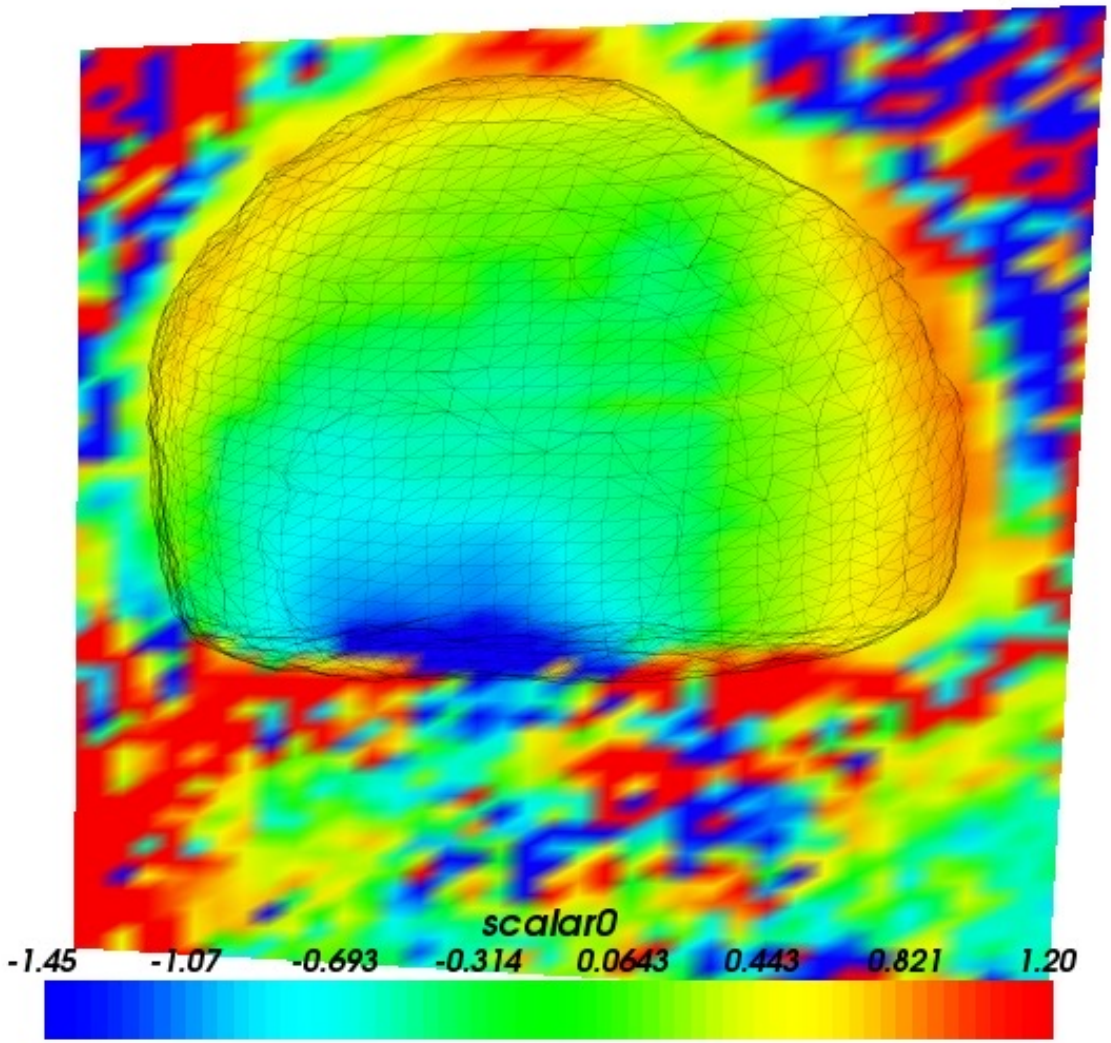


Phase Maps before and after Correction



Positive Phase is Surface Expansion

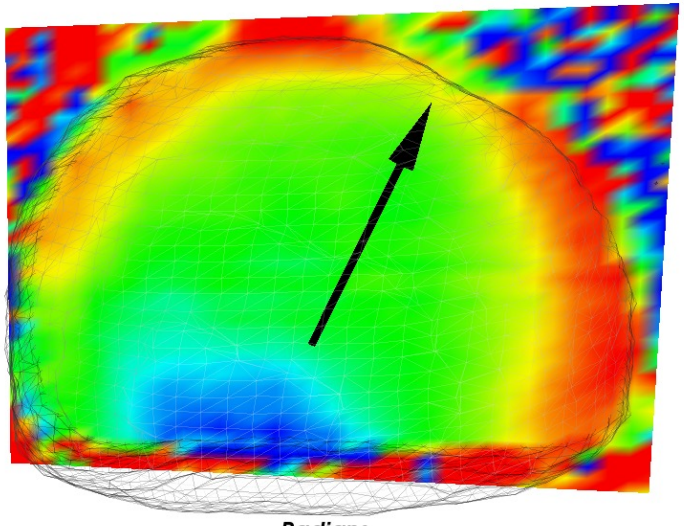
including correction for refraction by crystal

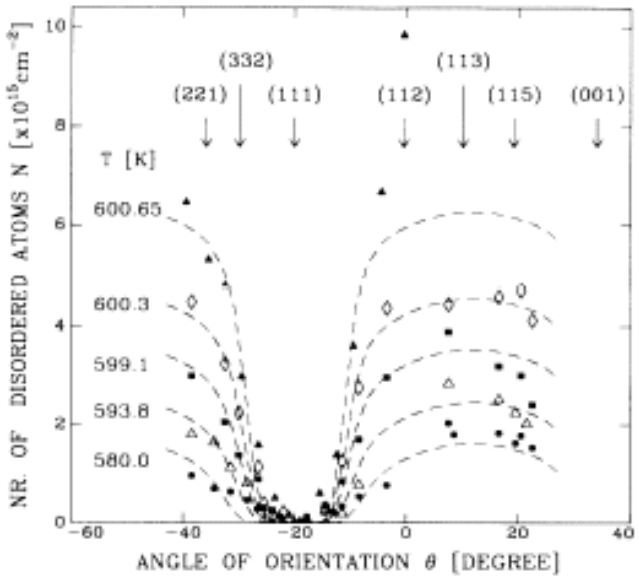


Max phase = 1.15rad
= 0.052nm

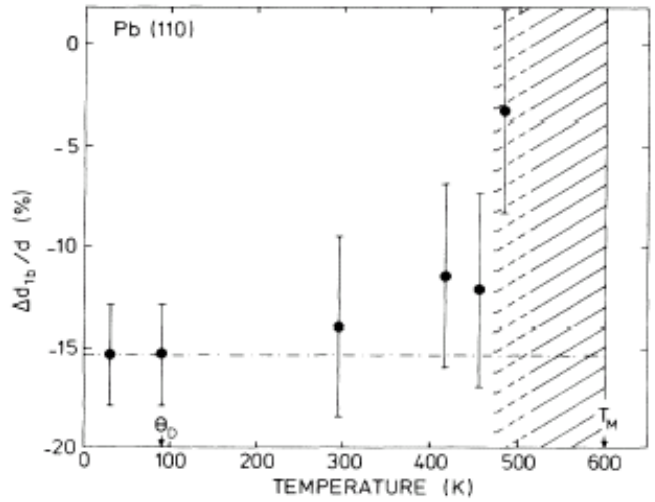
Phase on (111) facet:
= 0.47 rad
= 0.02nm

Surface Thermal Expansion: ion channeling + theory

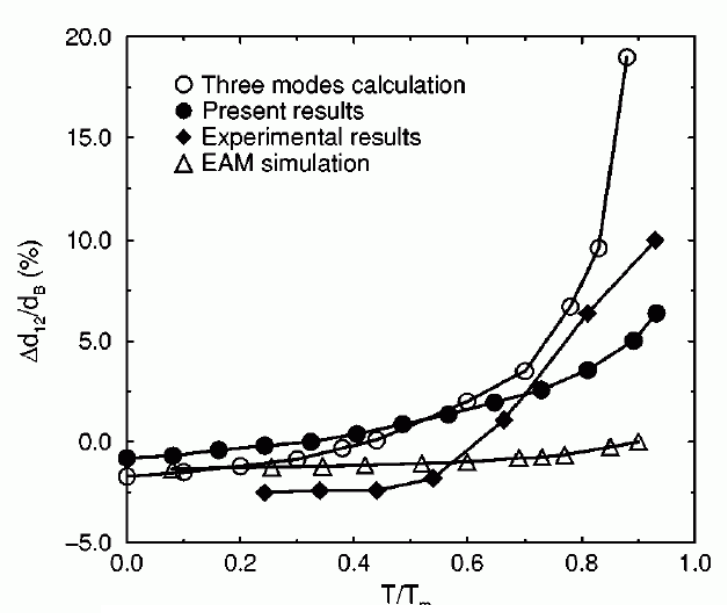




Pluis, van der Gon, Frenken, van der Veen
PRL 59 401(1987)



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

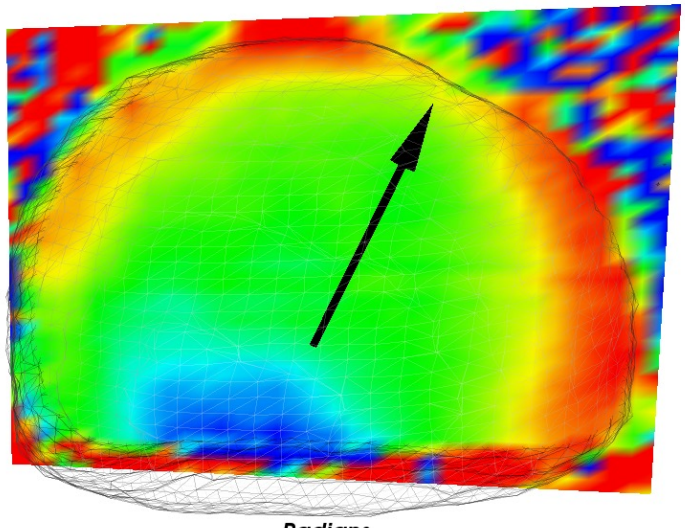


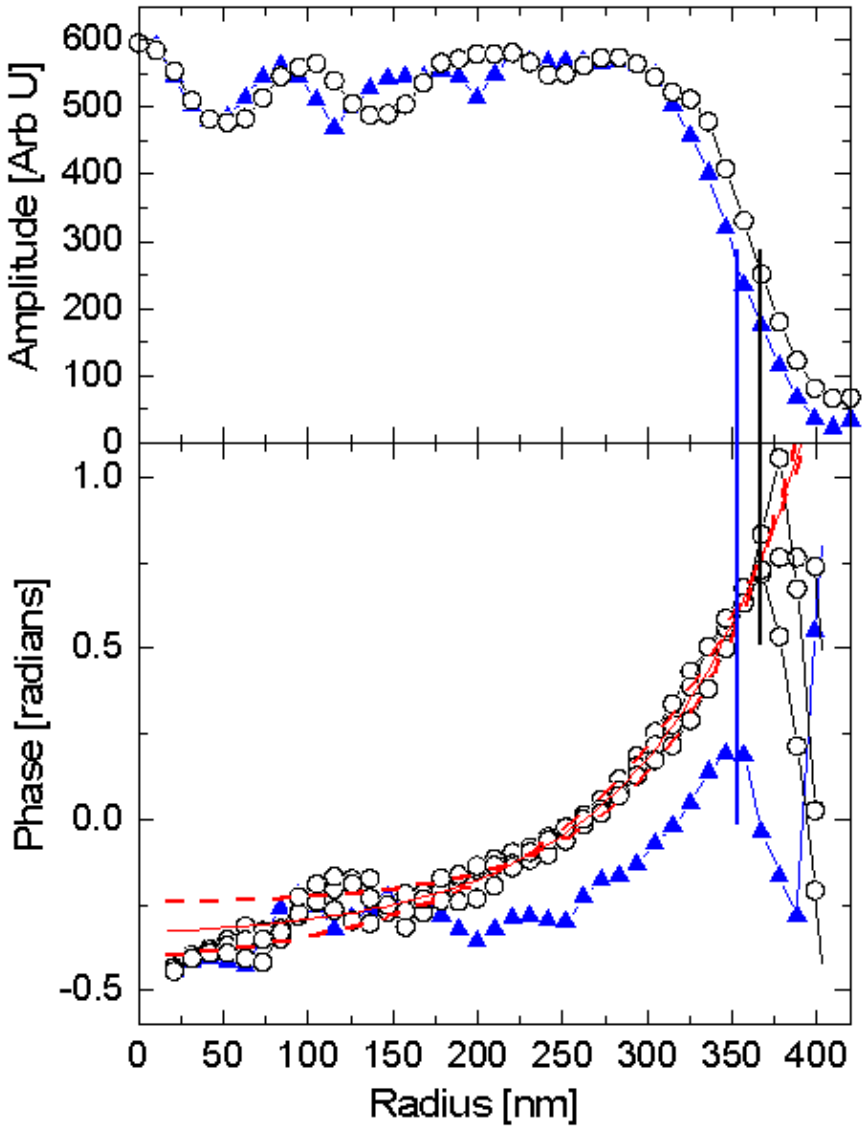
Ag(111) theory J. Xie (Scheffler group)
PRB 59 970 (1999)

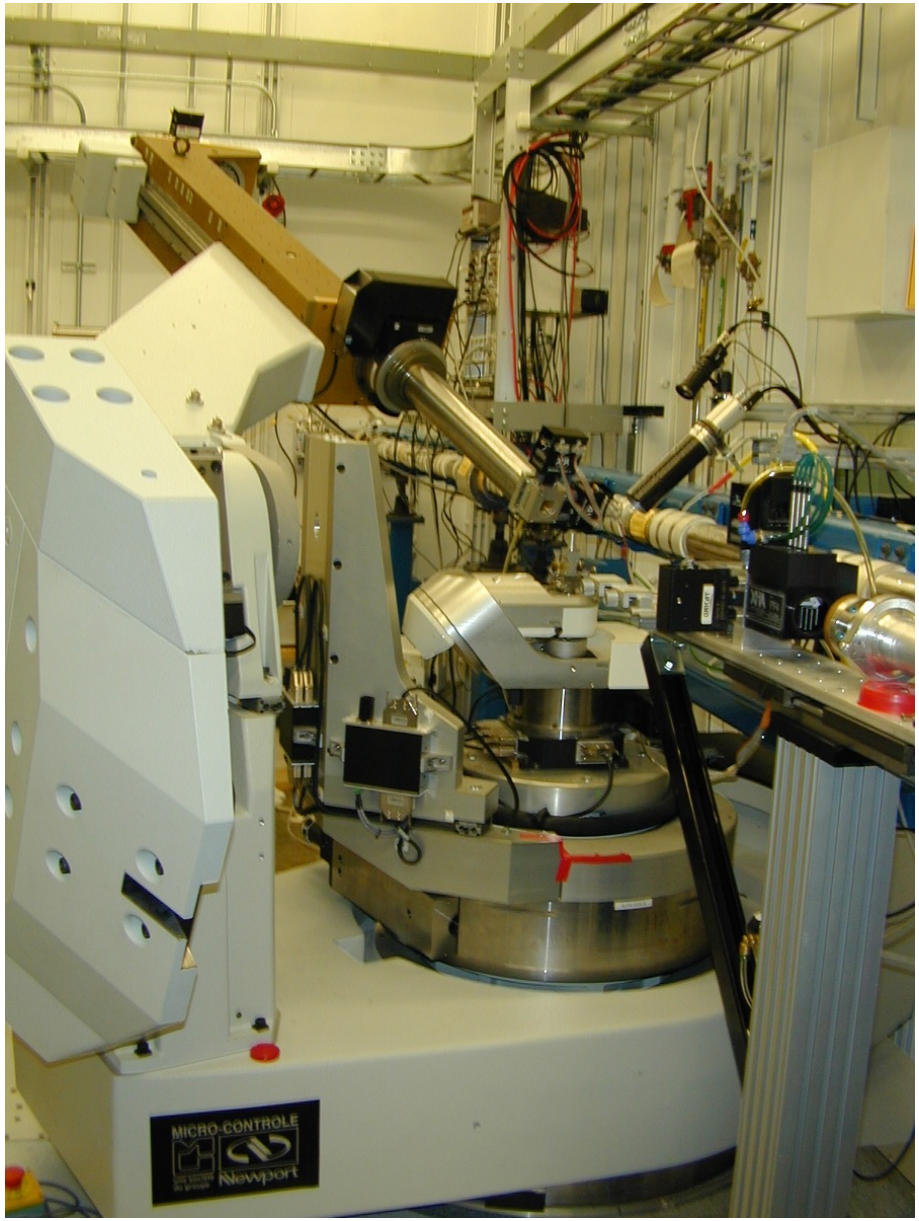
Depth Variation of Distortion

Facets subtend 18.6 ±2.6°
ECS predicts 14°

Depth measured 90 ± 20nm
Theory says 75nm






MICRO-CONTROLE
Newport

Planning for 34-ID-C (CXD)

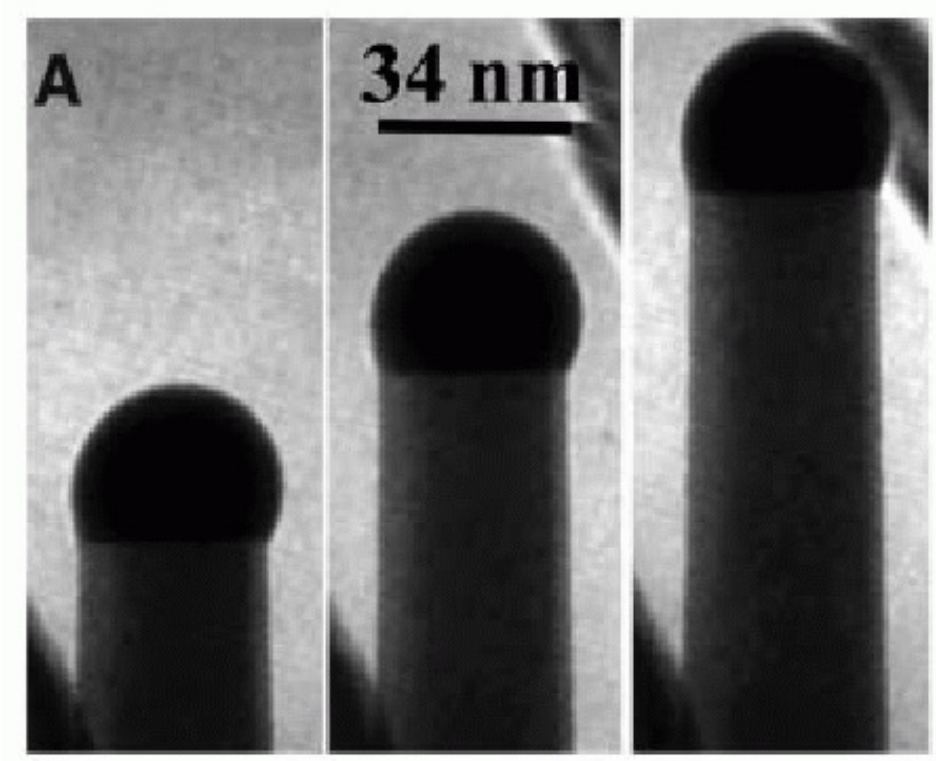
- Instrument fully developed for CXD
  - diffractometer repairs
  - removable UHV/KB mirrors/detectors
  - dismantle quickly to allow new uses
- Engage new beamline scientist
- Transition time until December 2008
- Access via GUPs and PUPs afterwards

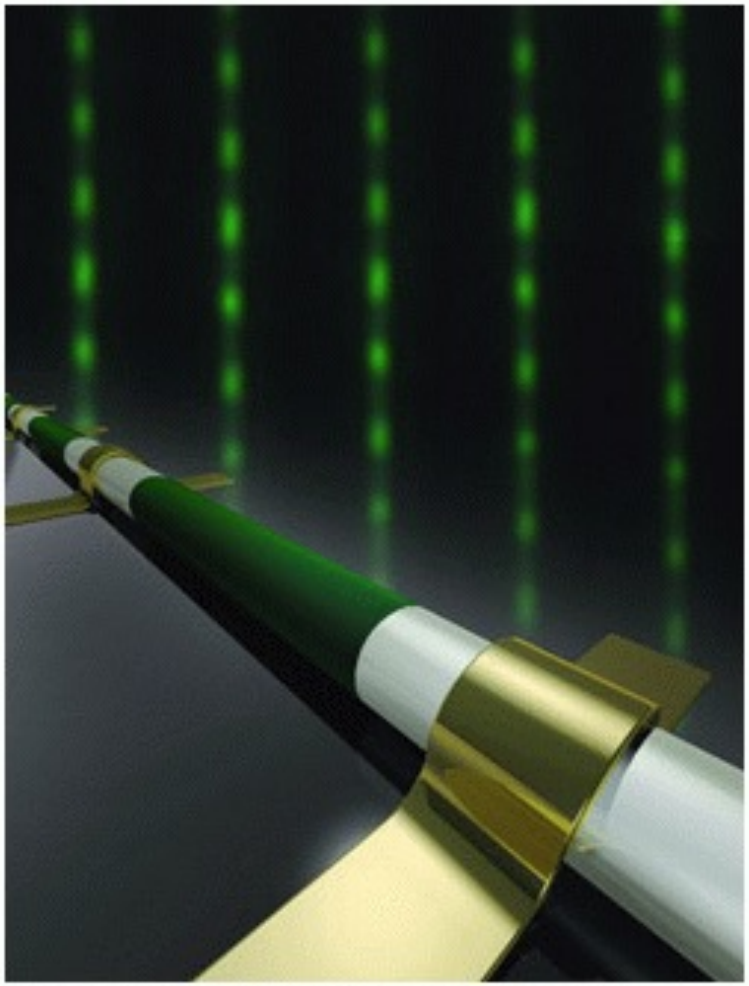
Science Areas to be Pursued

- Generation of strain in Nanocrystals
  - catalysts, in situ
  - ion irradiation
  - gettering to introduce oxygen vacancies
  - mechanical deformation, sintering
- Look for defects unique to Nanophase

VLS growth of nanowires

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

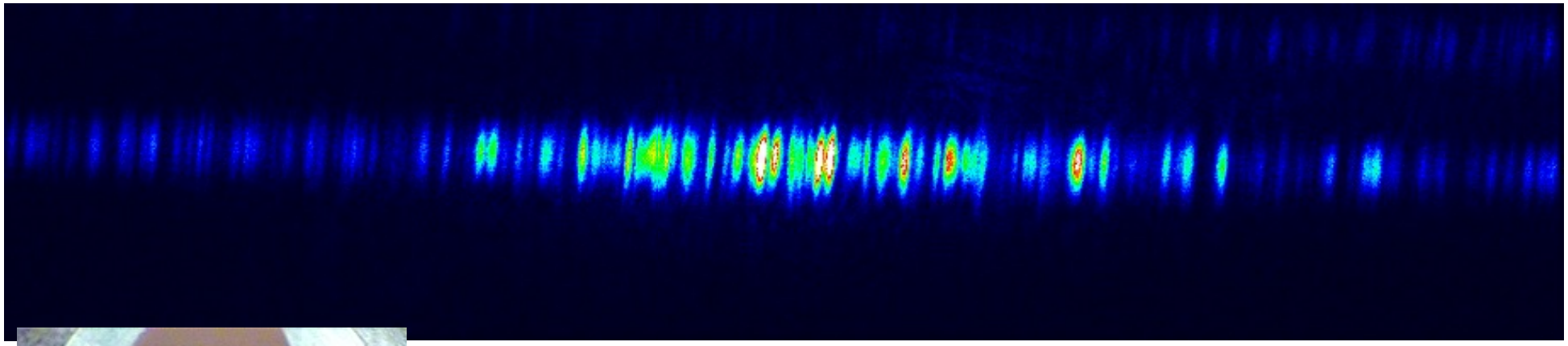


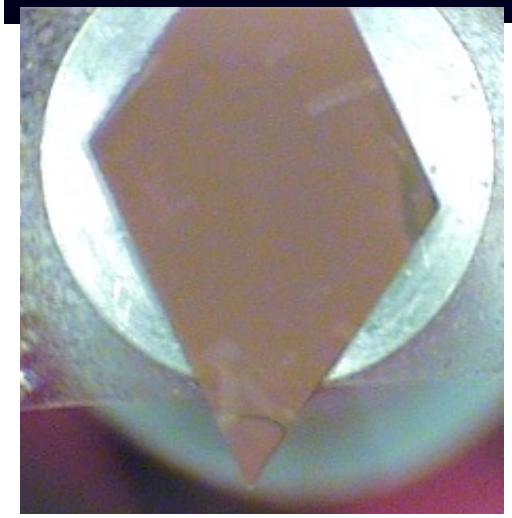


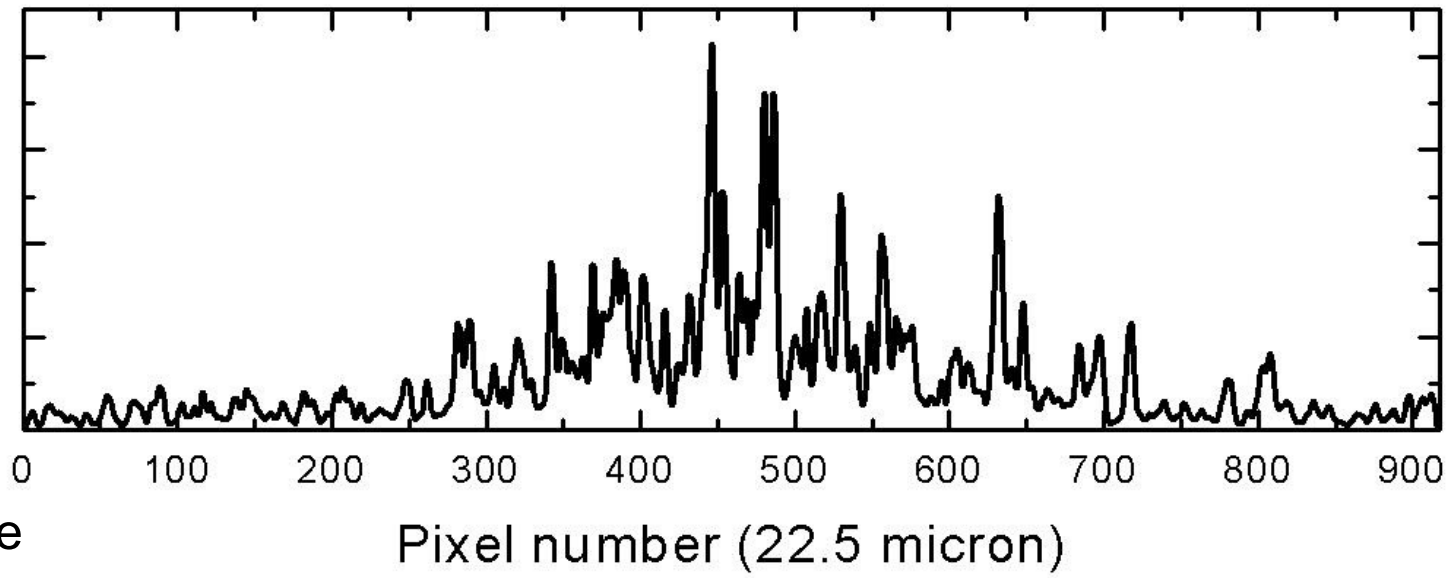
NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

GaAs Nanowire "Barcode"

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





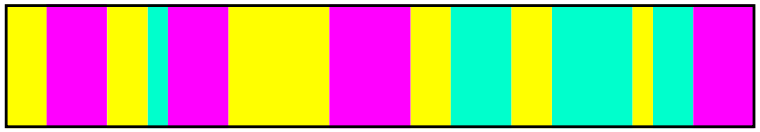


GaAsNW1106-22.spe
B9348 from Philips

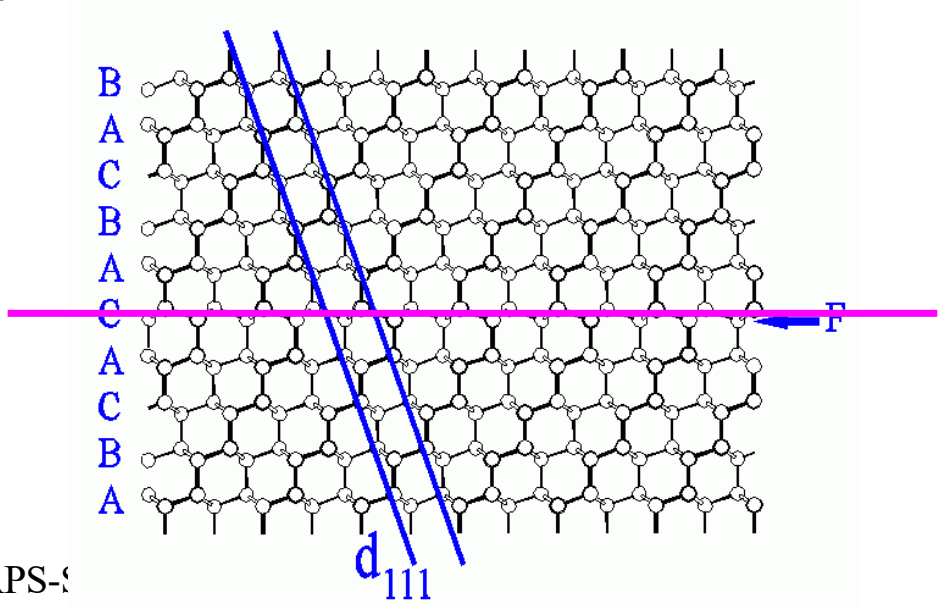
Models of Barcode Diffraction

(111) wires at (11-1) reflection

- Twinned stacking sequence

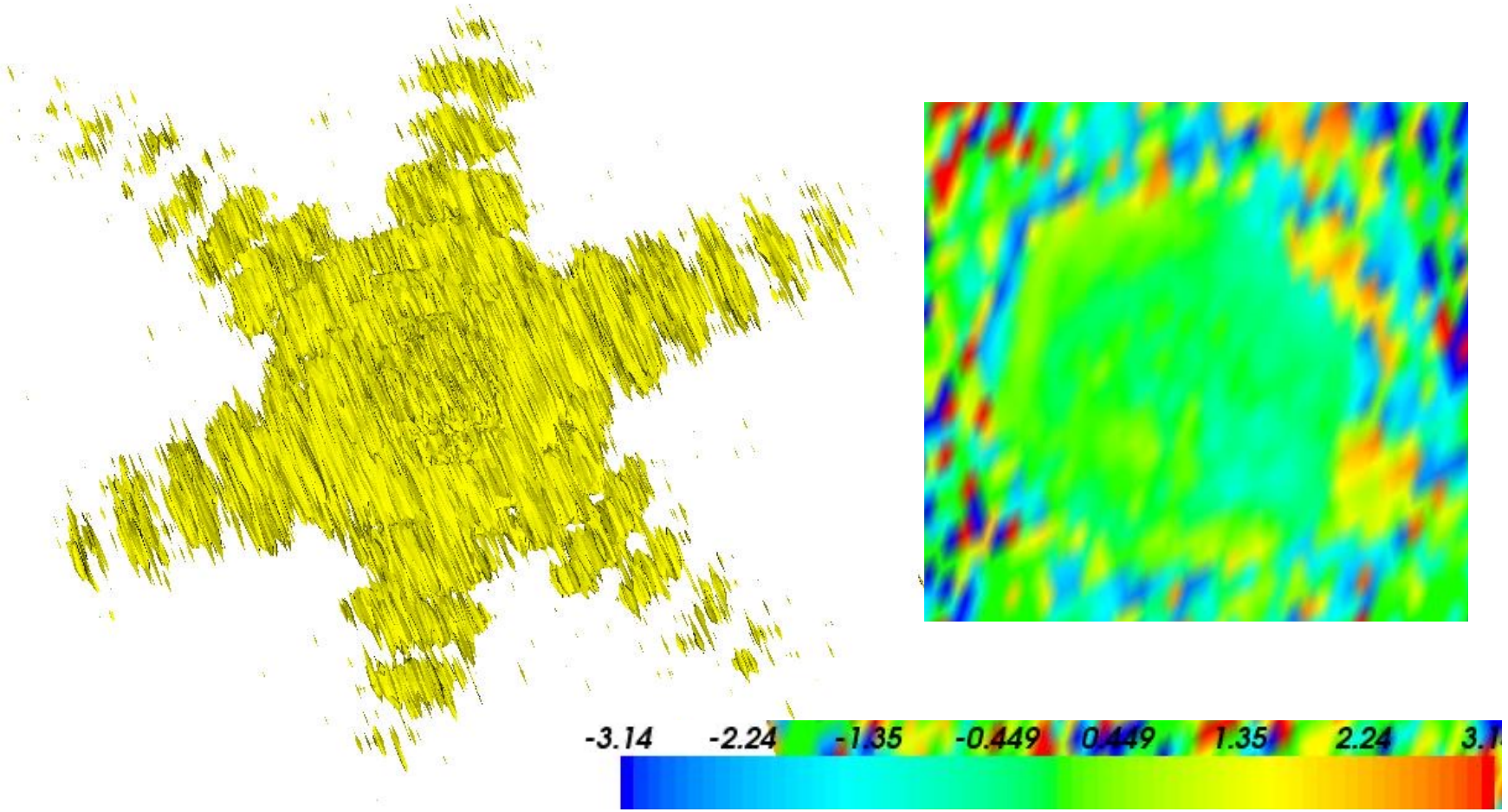


- Deformation faults



ZnO Nanowire Reconstruction

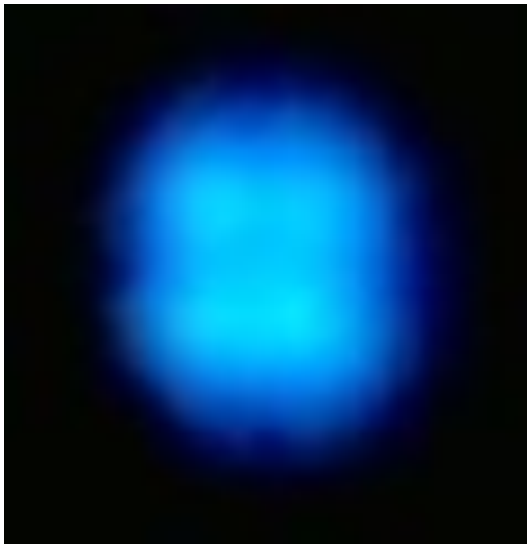
Ross Harder, Steven Leake, PhD project at UCL

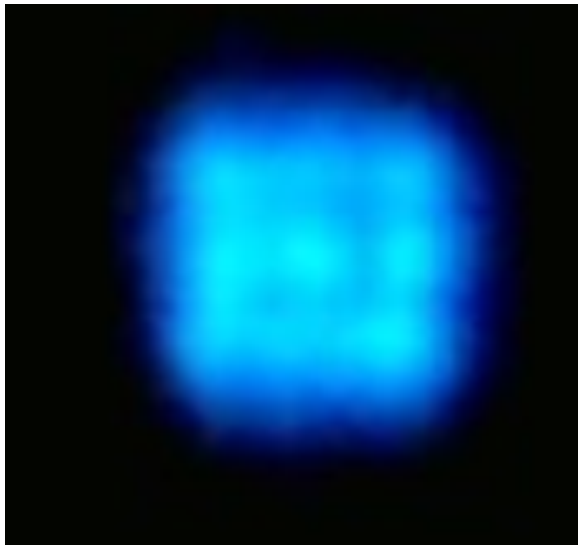


Phase Images using CXD

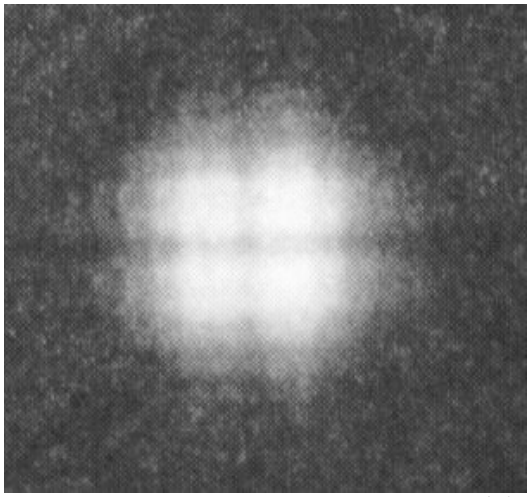
- Strain, displacements along **Q**-vector
- Chemical contrast (especially at resonance)
- Lattice shifts due to stacking faults
- Height of a reflecting surface
- Antiphase domain structures
- Refraction along path through object
- Illuminating wavefront, resulting from slits, focussing optics

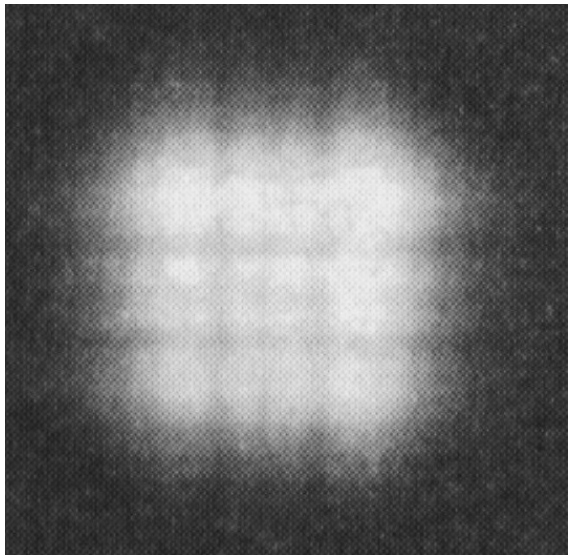
Fresnel Diffraction when $d^2 \sim \lambda D$





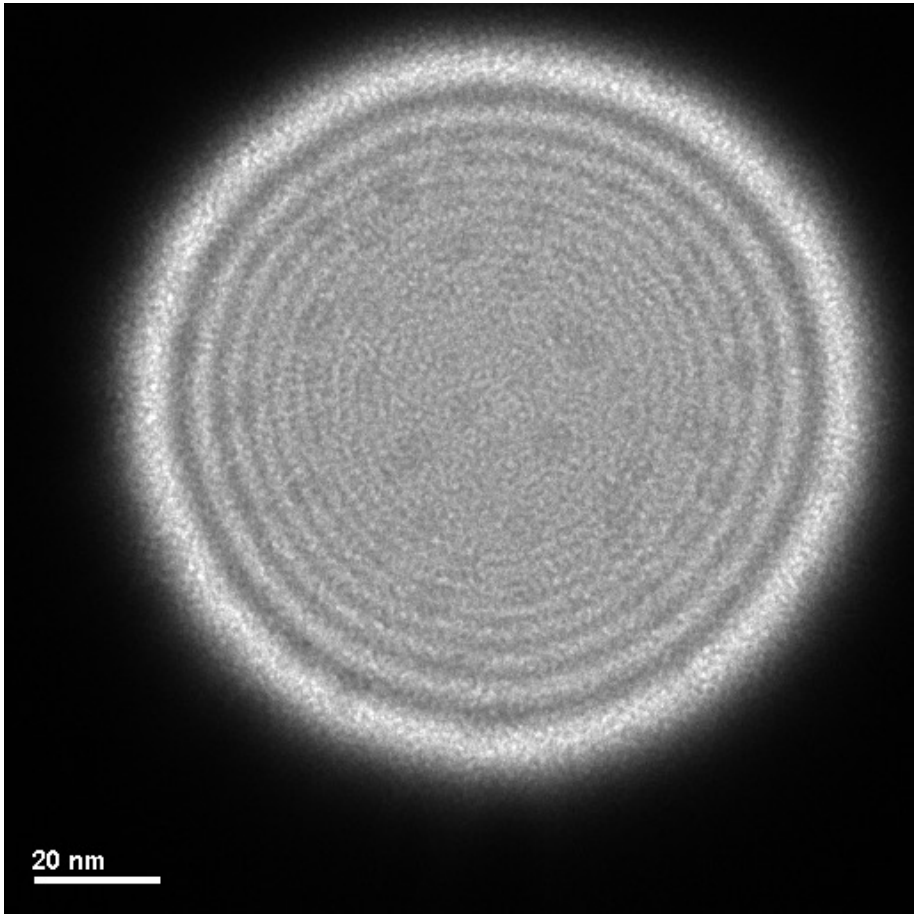
X-ray beam defined by RB slits 5um





Visible Fresnel diffraction from Hecht "Optics"

100nm Electron Microscope probe



FeAl antiphase domains (001)

Lorenz Stadler, PhD dissertation, TU Wien (2005)

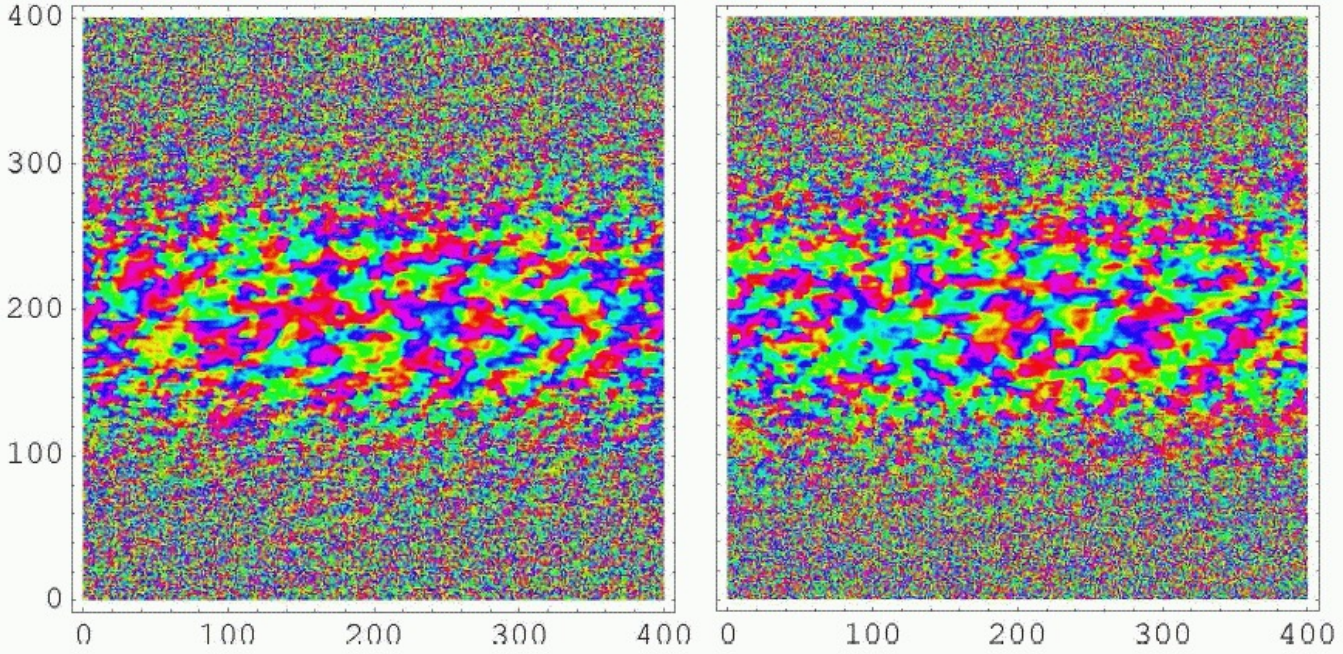
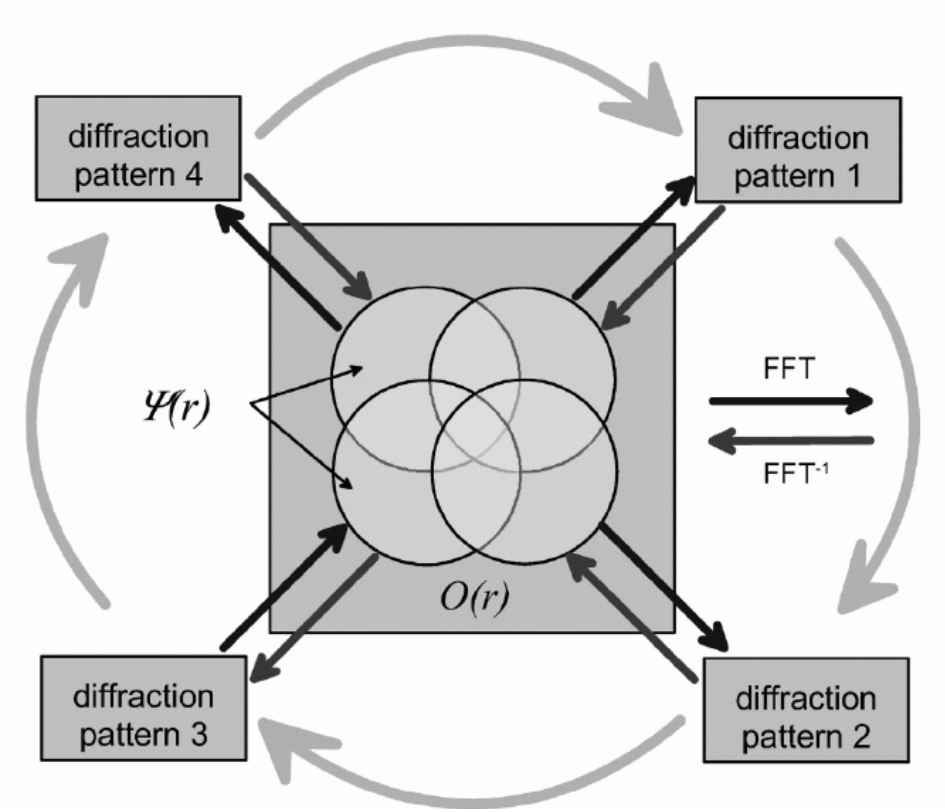
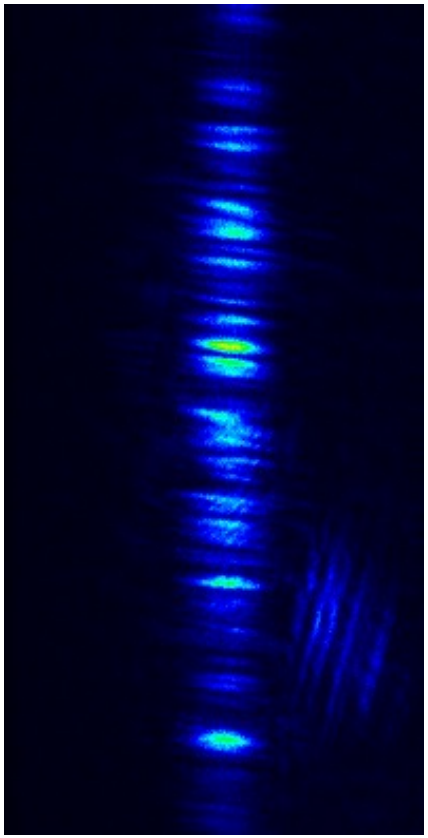


Figure 7.11: Typical reconstructed phases from runs with different combinations of algorithms and supports derived from the 2D Gaussian fit of the illumination function. Numbers in brackets denote how many iterations of the particular algorithm were done each cycle. Graphs on the left are from reconstruc-

Future of CXD: Ptychography

Rodenburg & Pfeiffer, PRL (2007)





Conclusions

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

GUPs active at 34-ID-C

- Hyunjung Kim Sogang U
- Darren Dale Cornell
- Vincent Favre-Nicolin CEA
- Jack Sadlier NASA
- Brent Heuser UIUC
- Bob Averback UIUC
- Jim Zuo UIUC

Possible Upgrades

- Better positioning, hexapod
- Better focusing
- In-vacuum focusing
- Better detectors
- Integrated software