

Opportunities for using coherence for studying strain

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Diamond Light Source

X-ray coherent diffraction Workshop

Soleil, Ormes des Merisiers

December 2009

Outline

- Coherent x-ray diffraction
- CXD can solve the **phase** problem
- Nanocrystal structures
- Extension to **phase** objects
- Exploration of crystal strain
- Effects of partial coherence

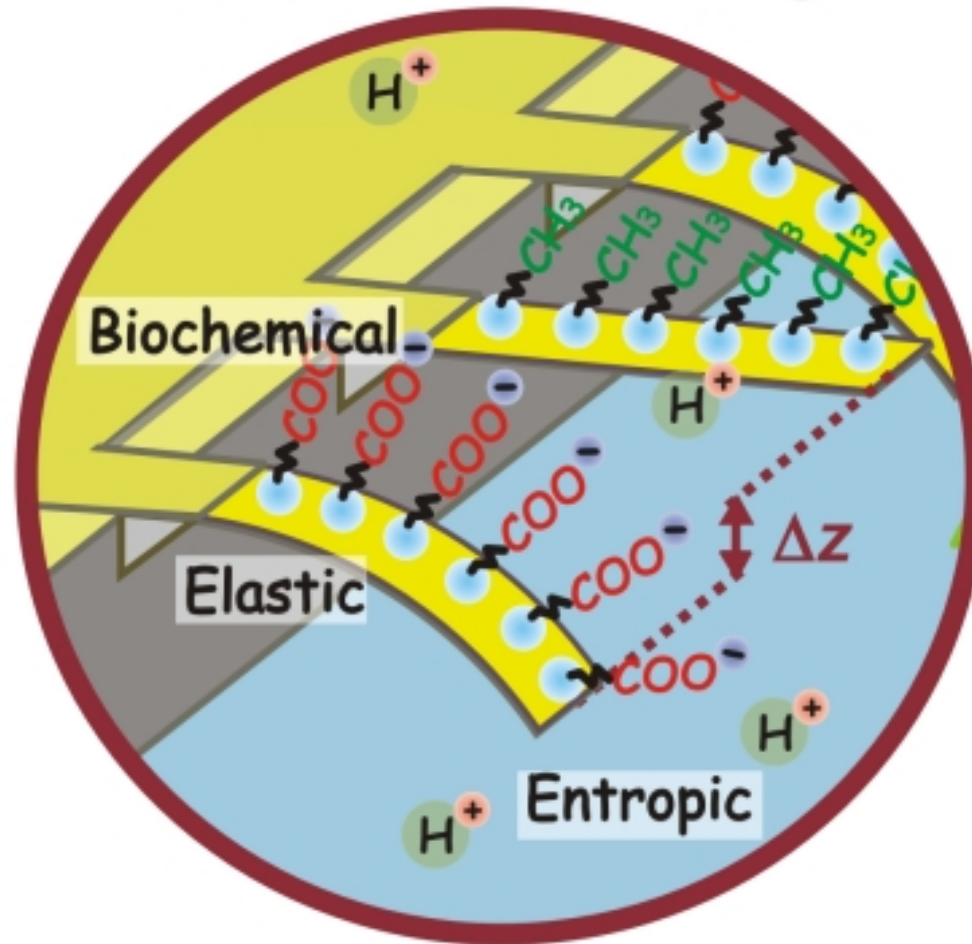
London Centre for Nanotechnology

- Clean Rooms
- Low-T STM
- Lithography
- 3-beam FIB
- Visualisation
- CLS?



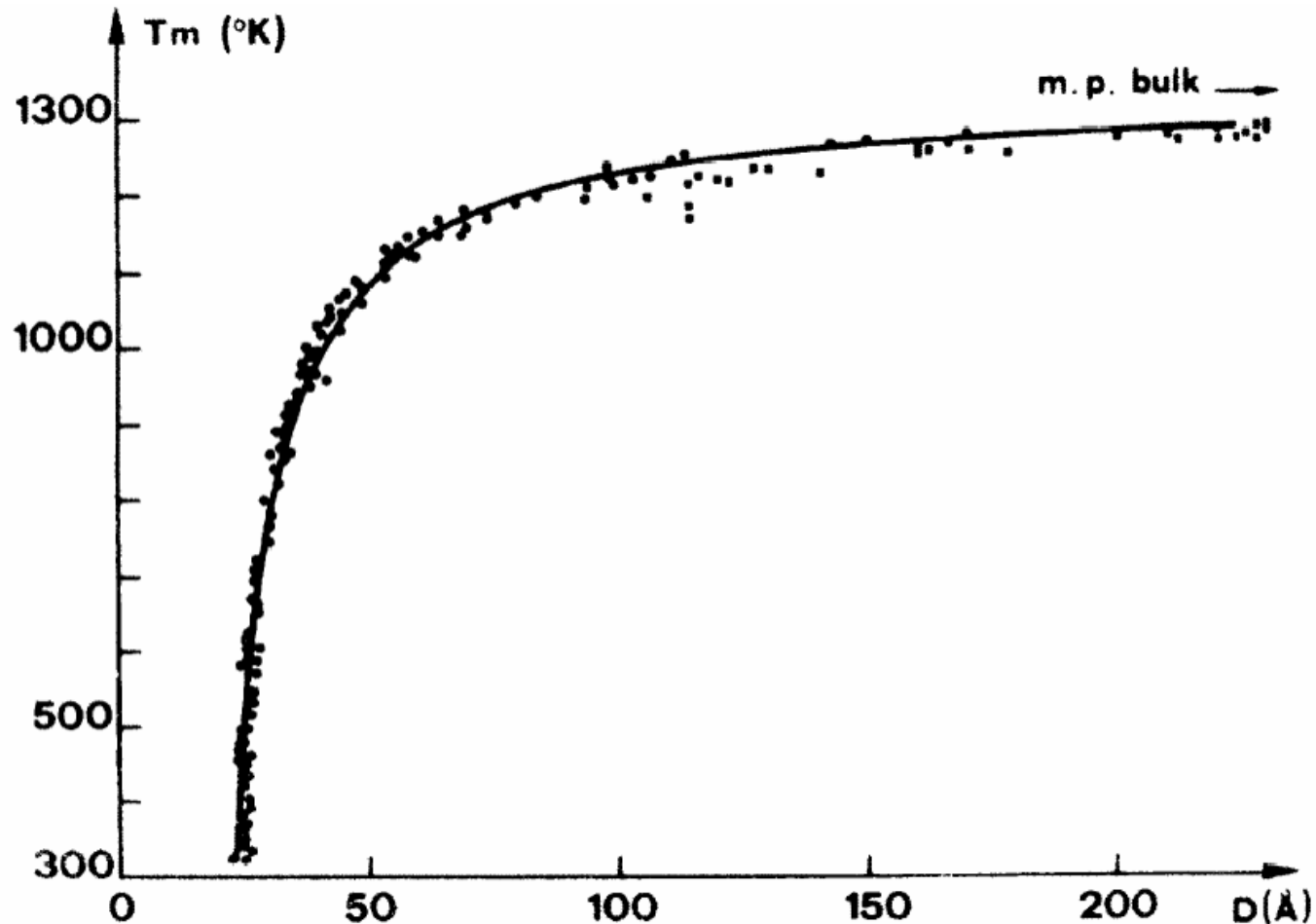
Nanocantilevers

Dr Rachel McKendrie

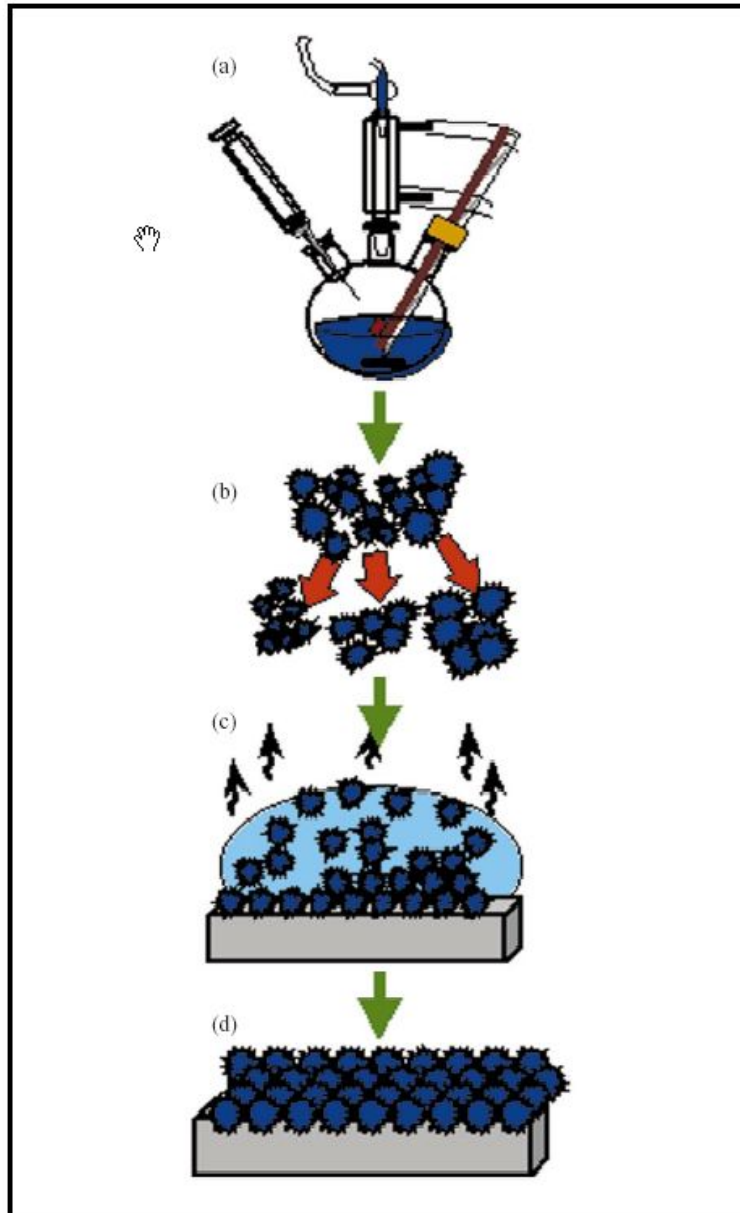


Size-dependent Melting of Au Particles

P. Buffat and J-P. Borel, Phys. Rev. A 2287-97 (1975)

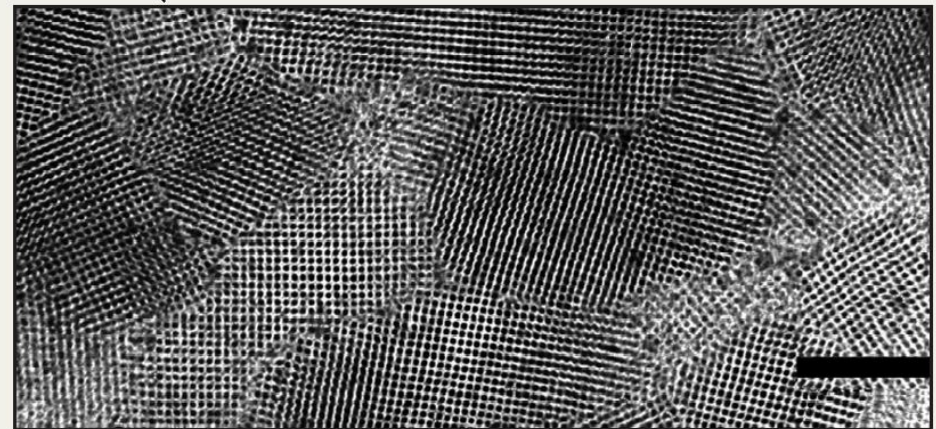


Chemical Synthesis of Nanocrystals



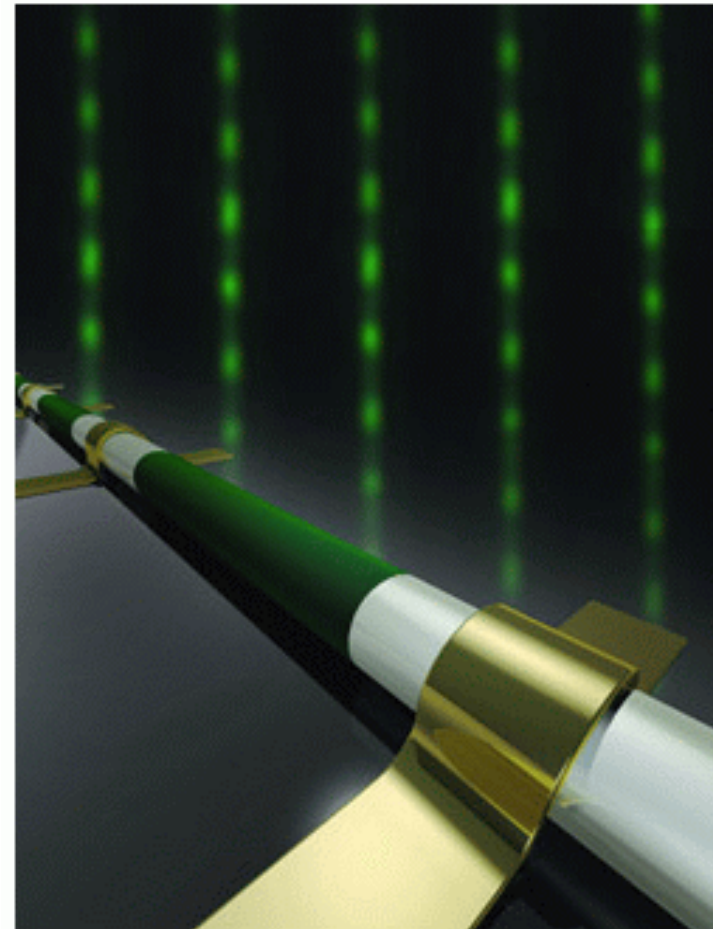
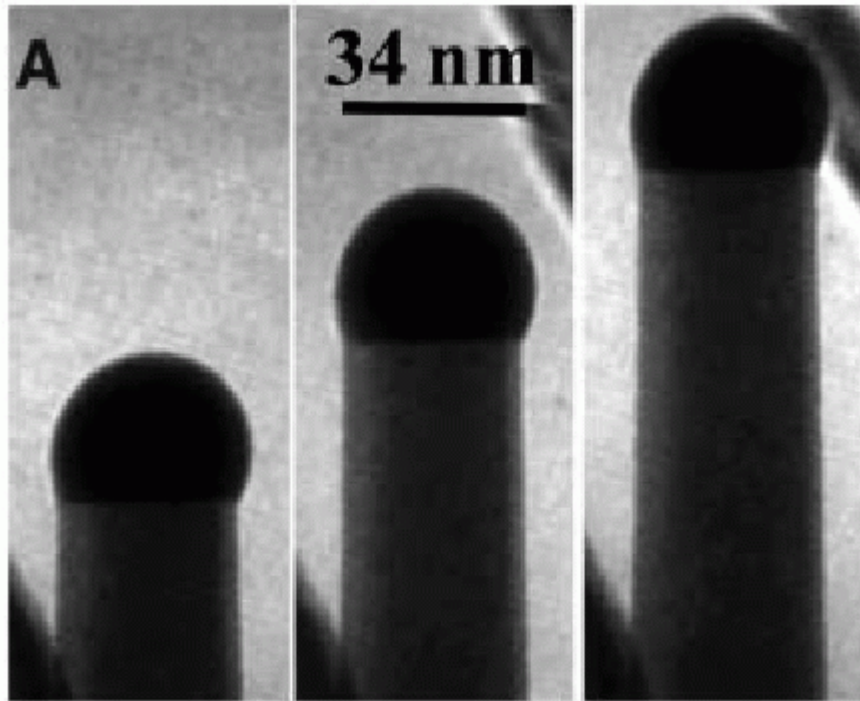
- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

C. B. Murray, *IBM J. Res. & Dev.*
45 47 (2001)



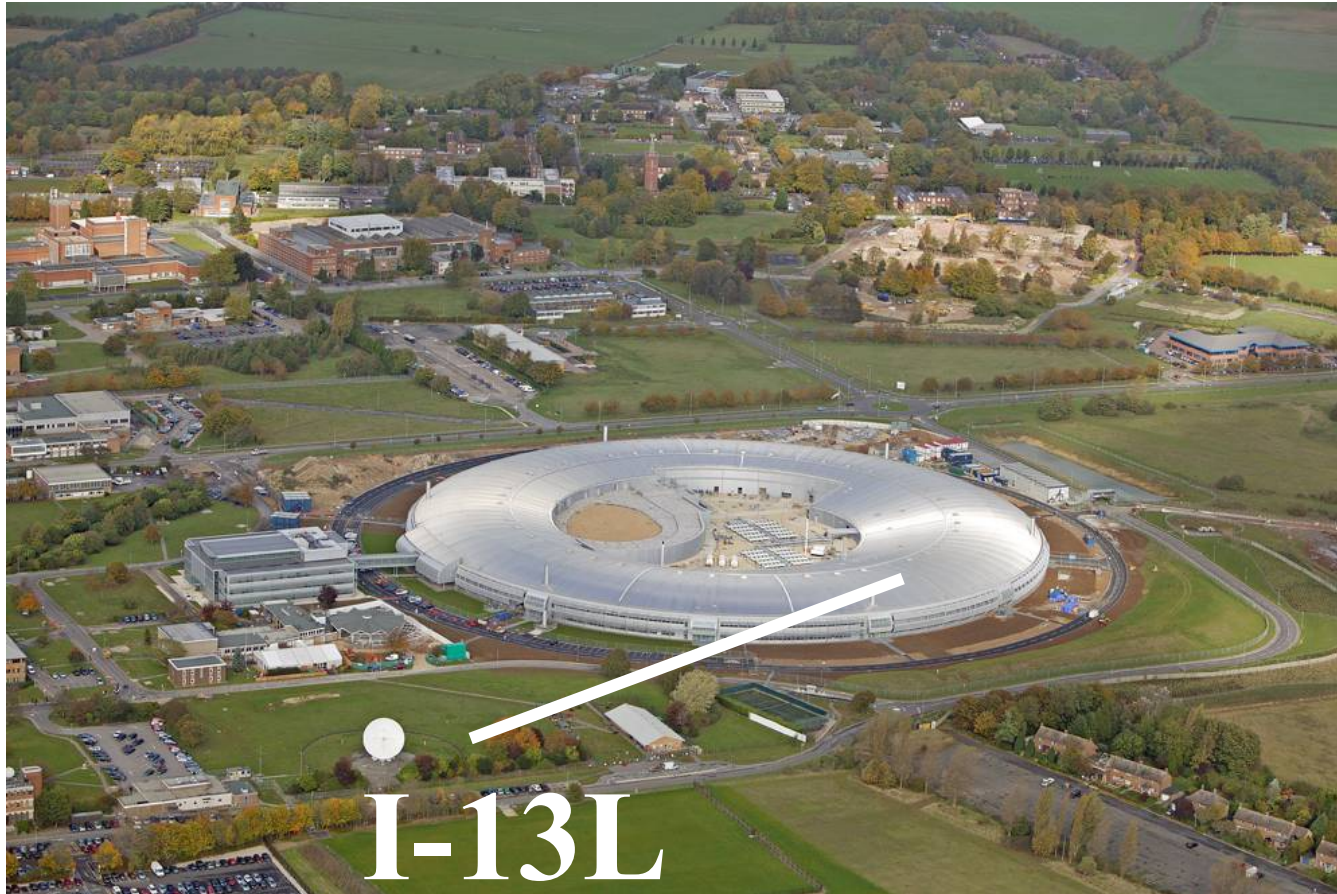
VLS growth of nanowires

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



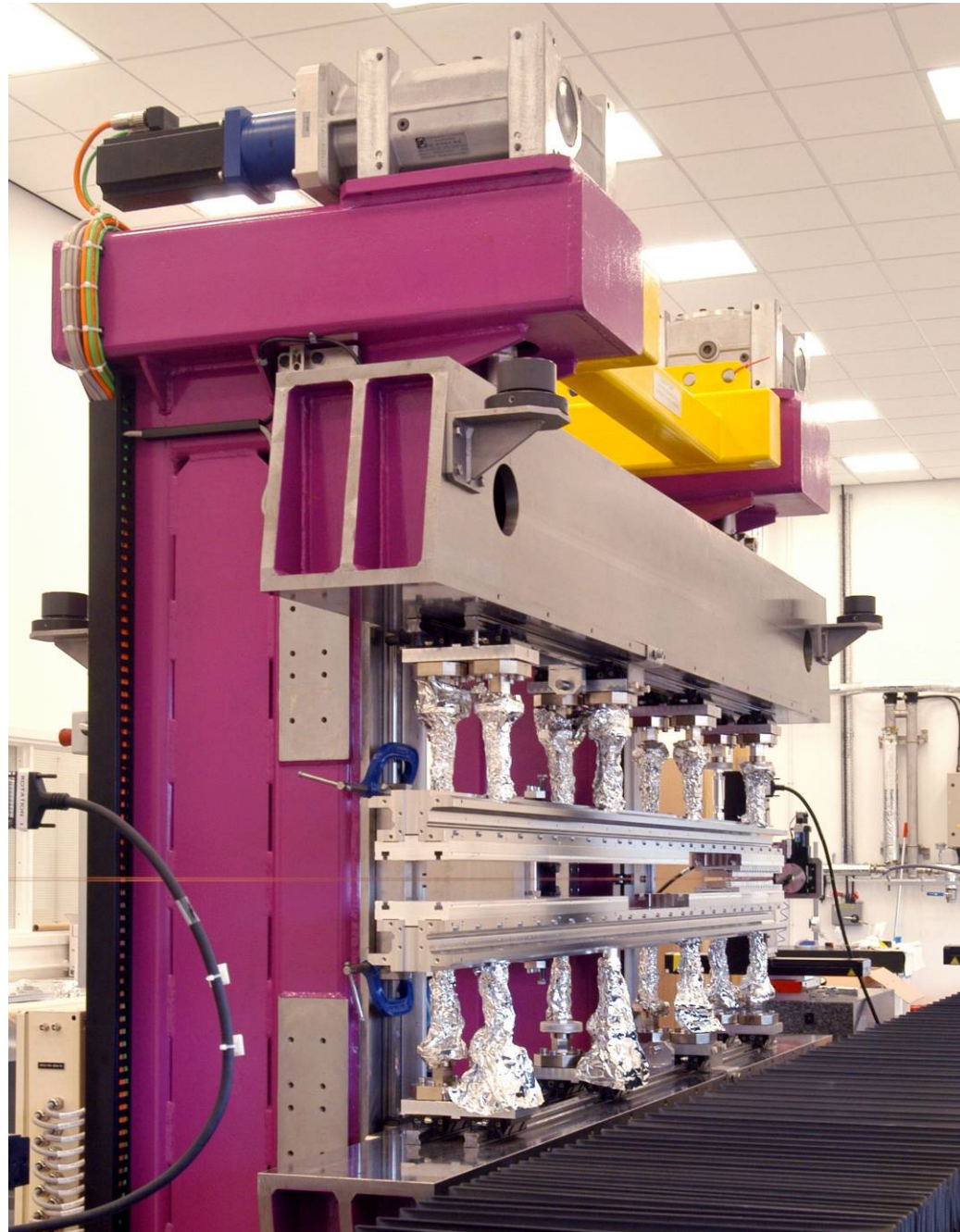
I. K. Robinson, Solei NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

Diamond Light Source (RAL)

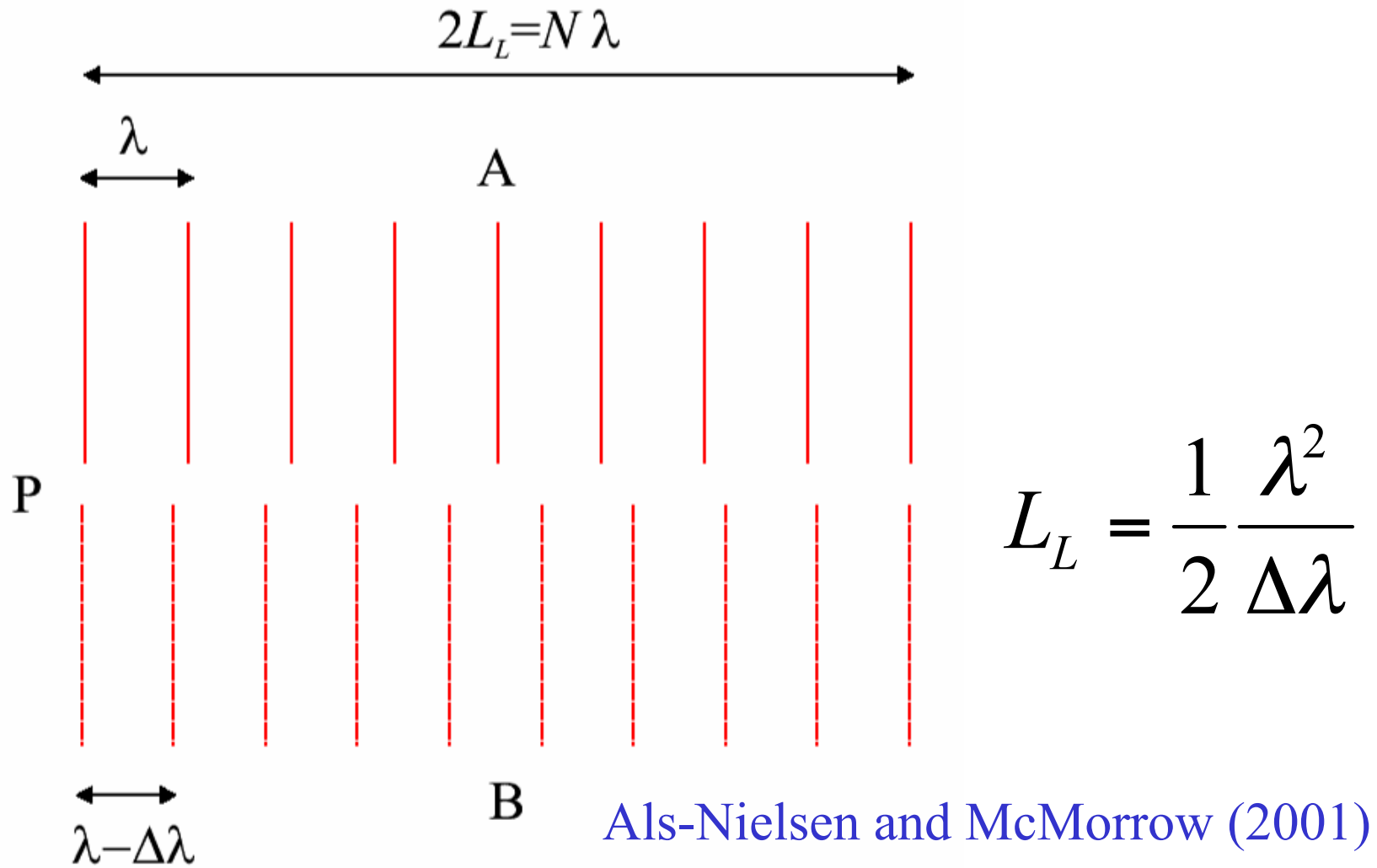


I. K. Robinson, Soleil 2009

Diamond
in-vacuum
X-ray
Undulator

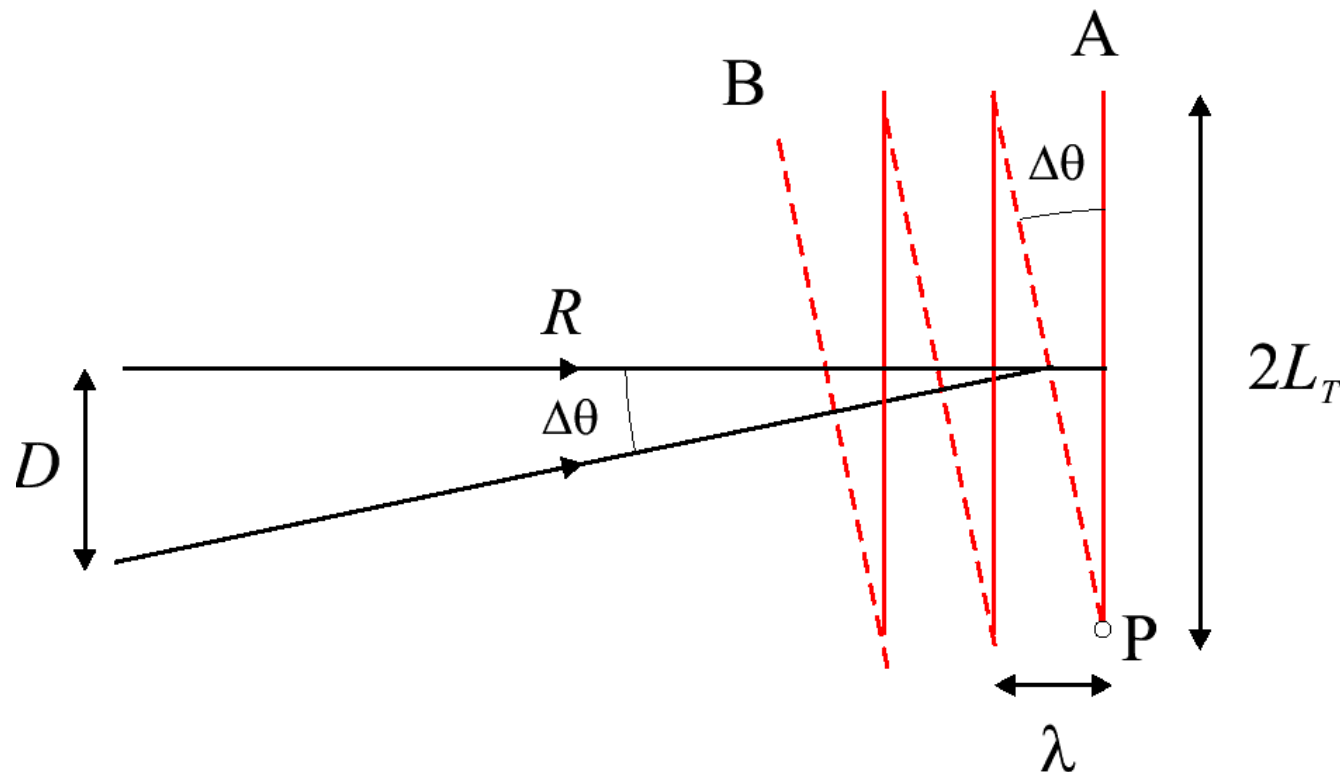


Longitudinal Coherence



Als-Nielsen and McMorrow (2001)

Lateral (Transverse) Coherence



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

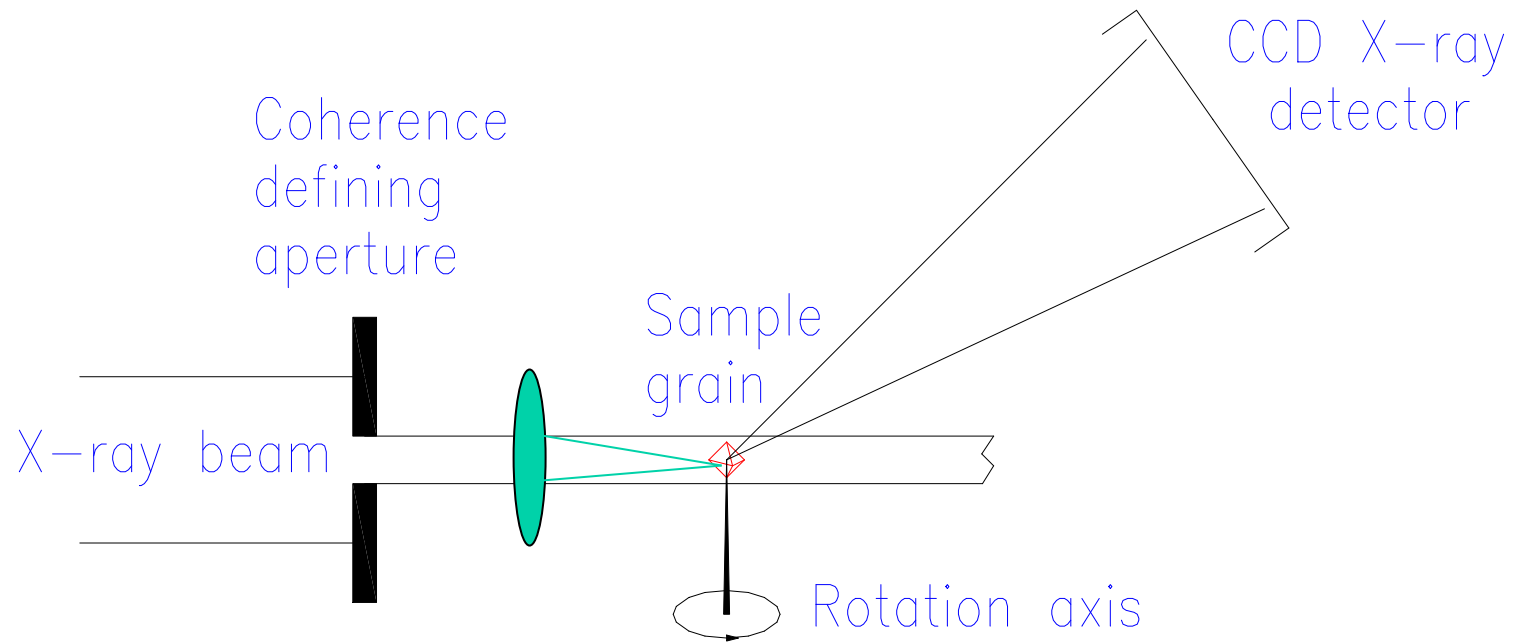
Als-Nielsen and McMorrow (2001)

Robert Hooke's microscope, 1665

National Museum of Health
and Medicine, Washington
DC

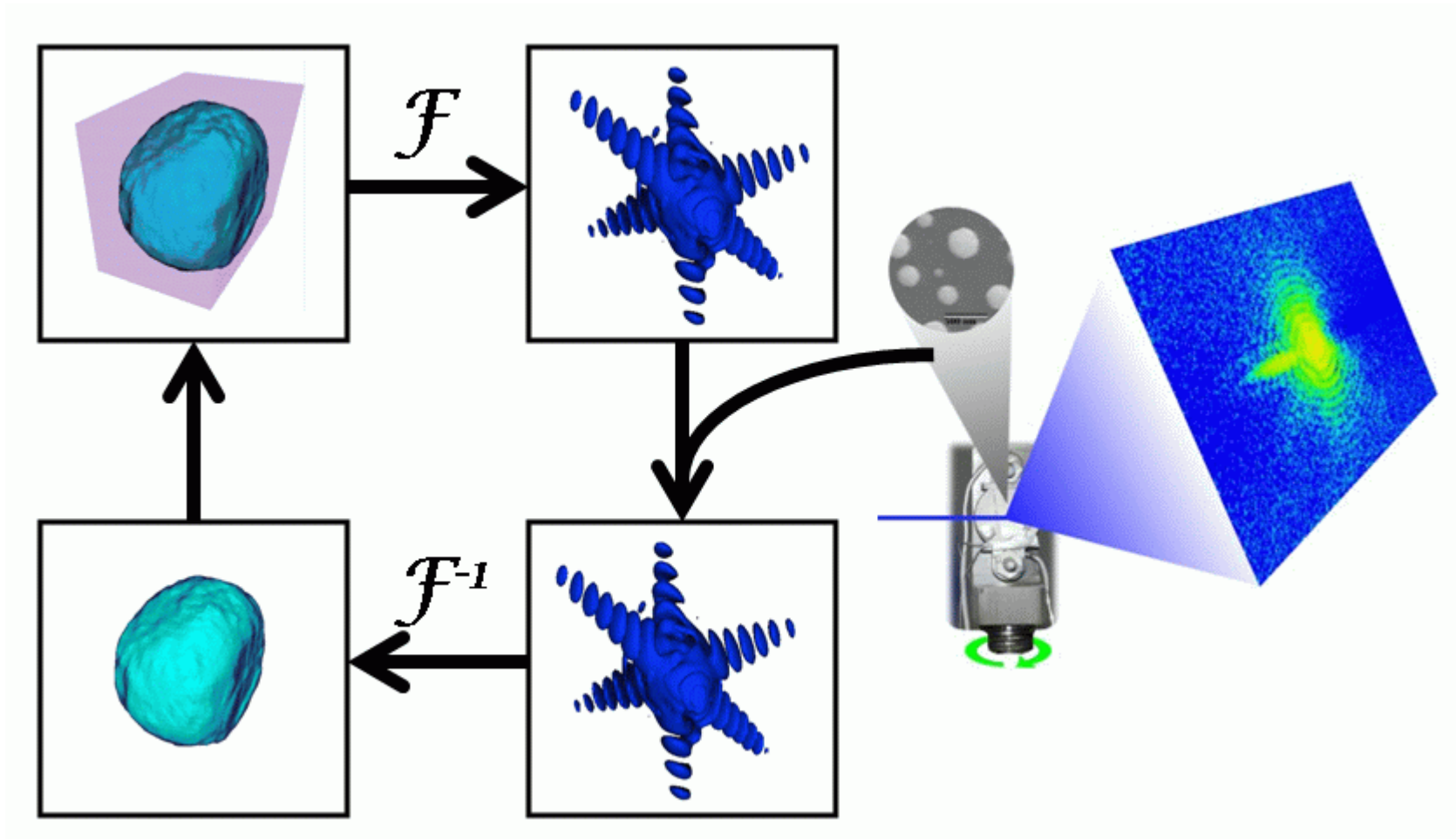


Lensless X-ray Microscope, 2003



Oversampling solves Phase Problem

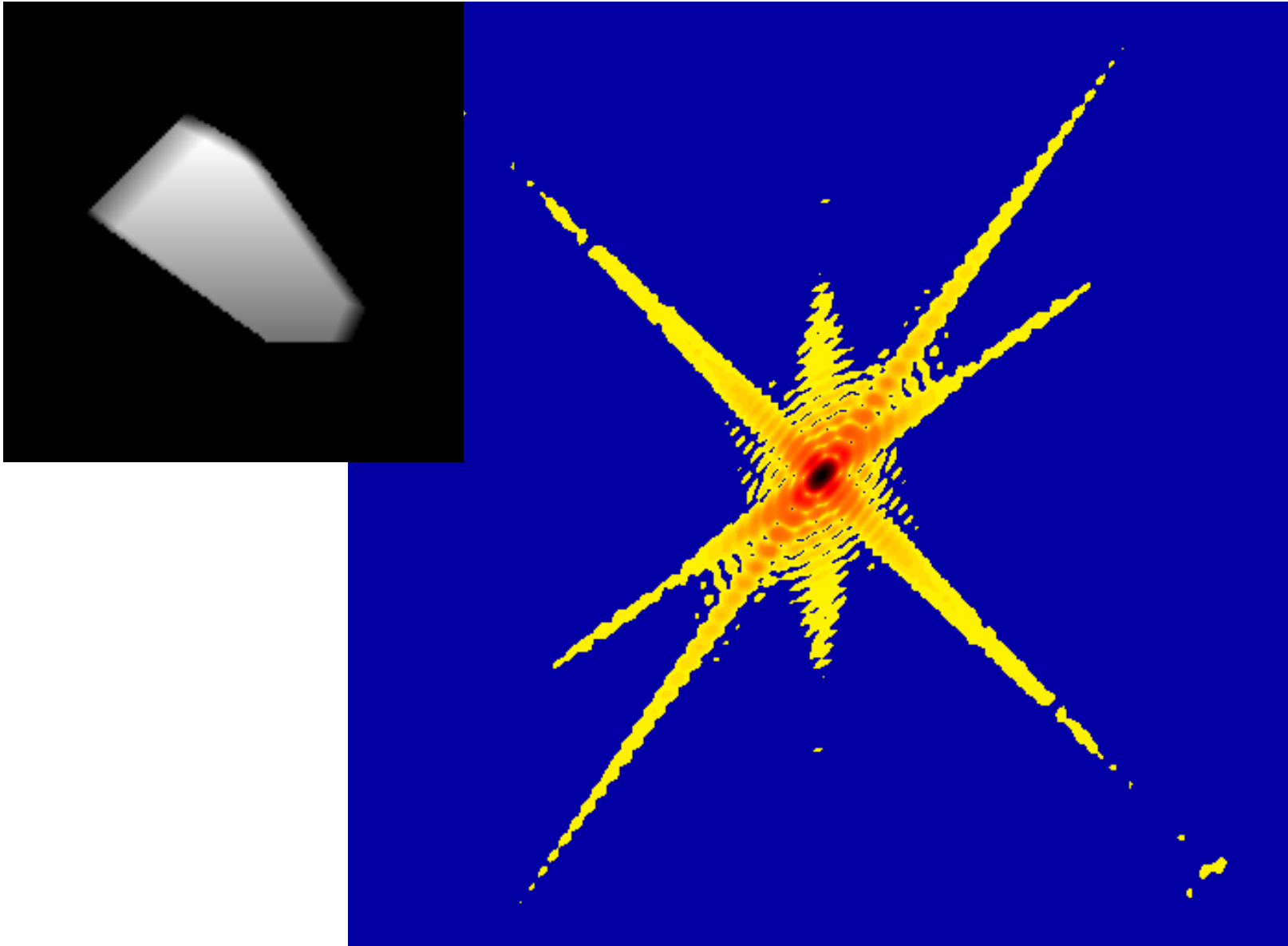
Generic “Error Reduction” method



J. R. Fienup *Appl. Opt.* 21 2758 (1982)

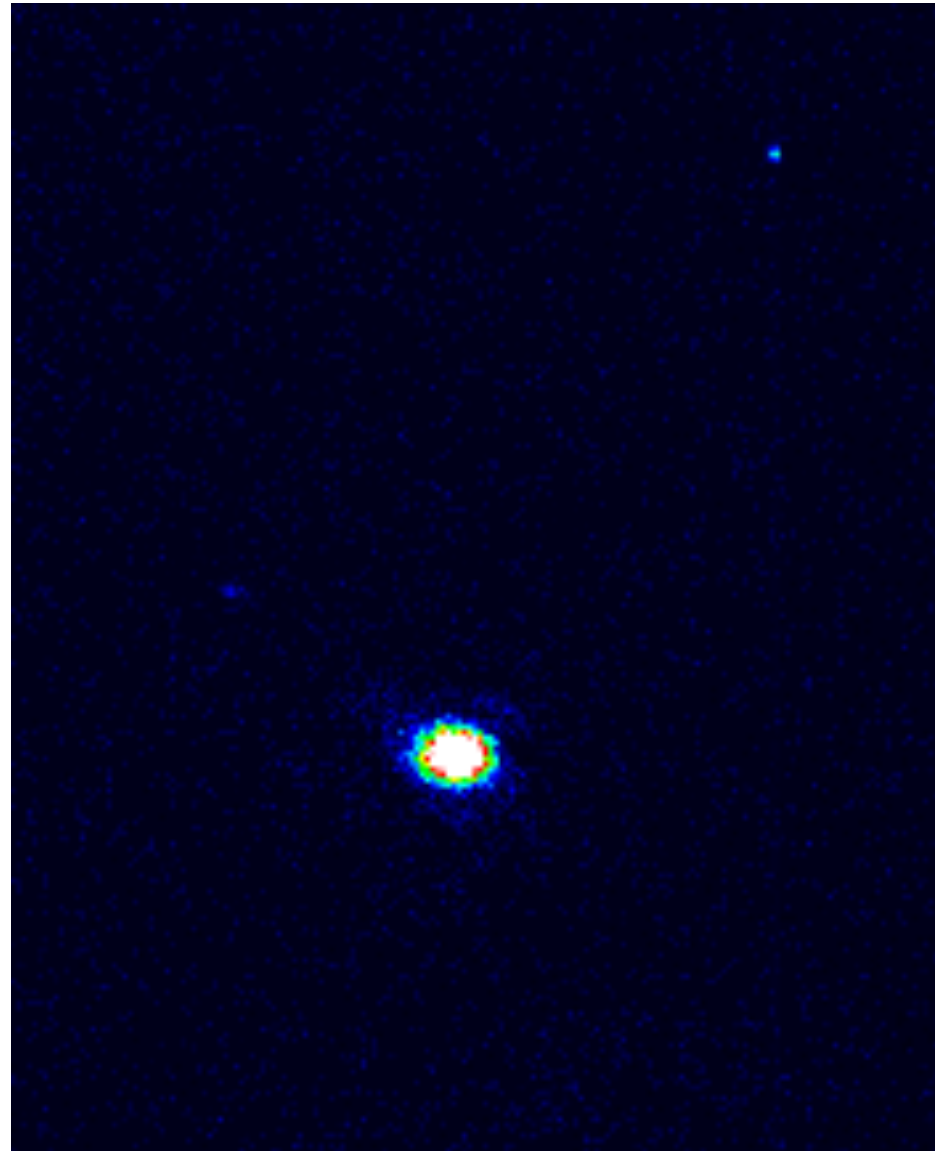
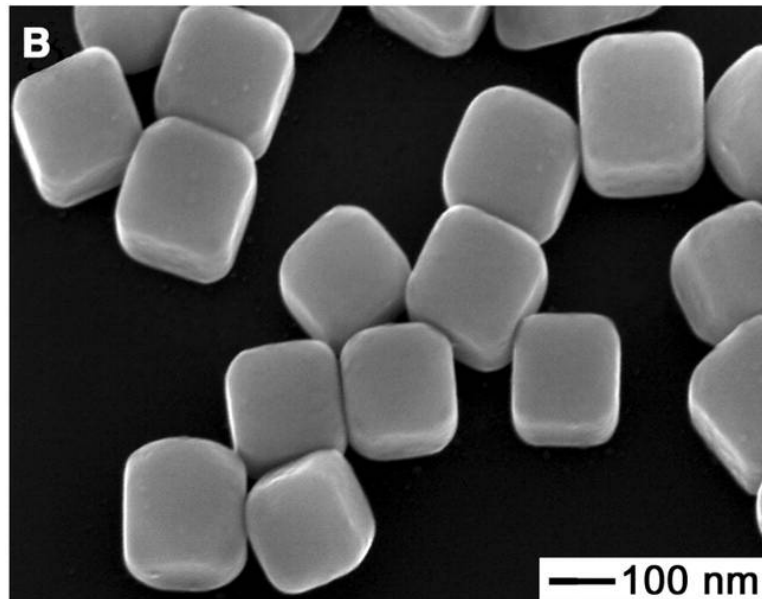
R. W. Gerchberg and W. O. Saxton *Optik* 35 237 (1972)

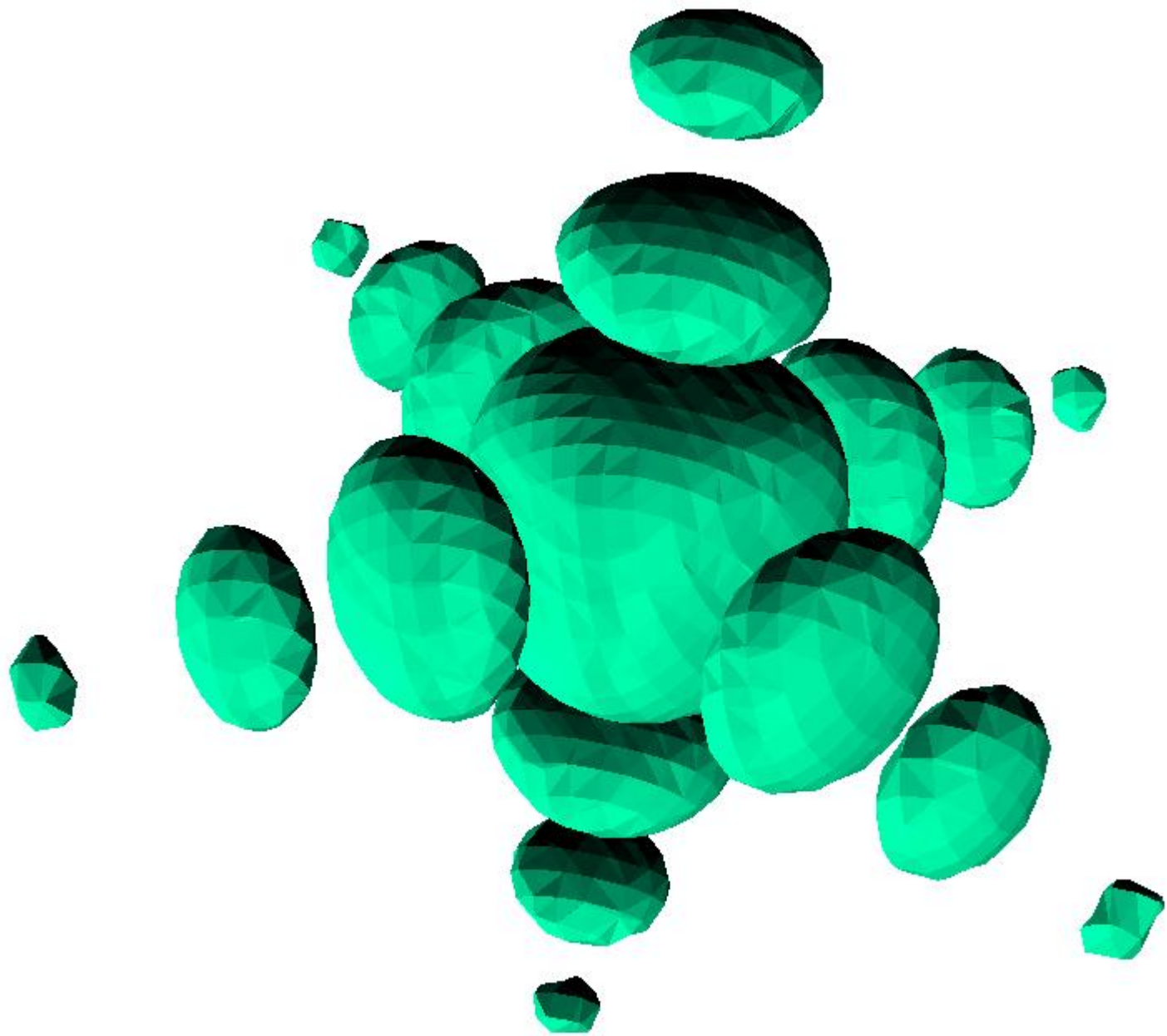
I. K. Robinson, *Soleil* 2009

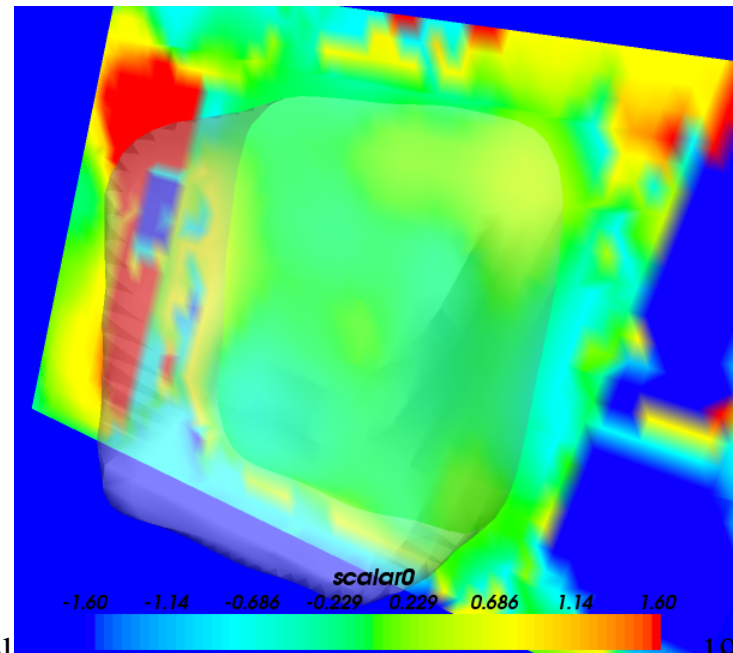
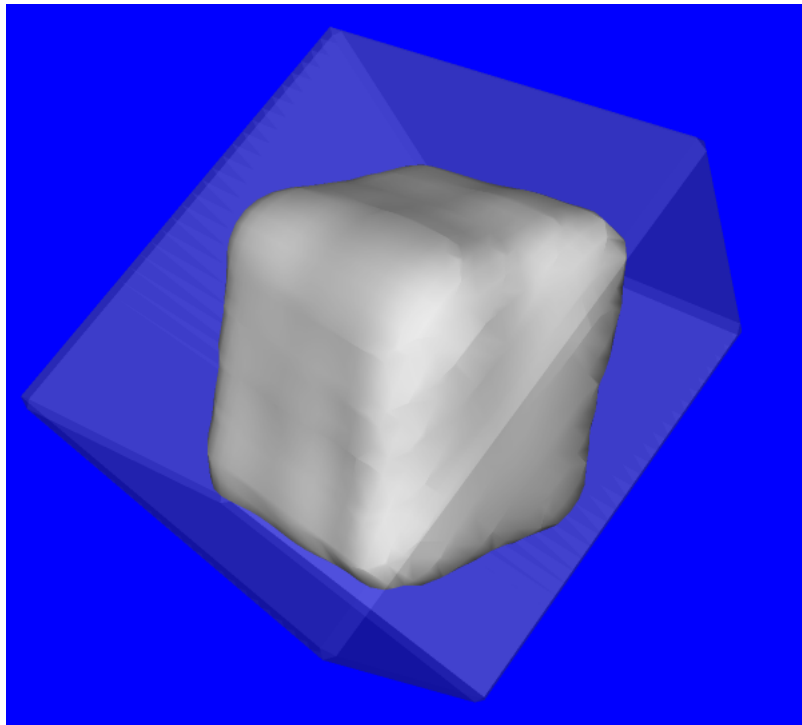
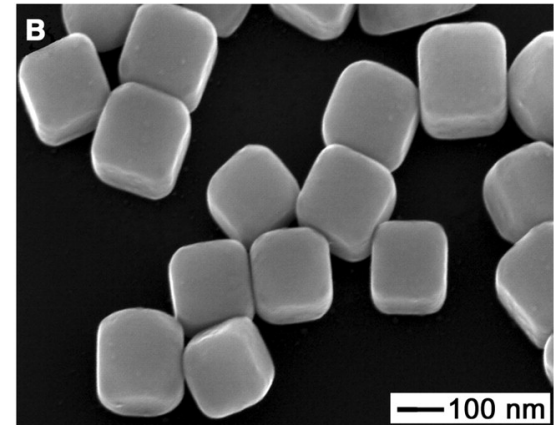
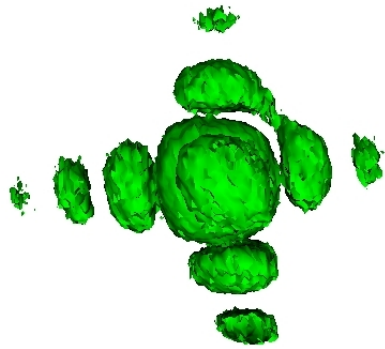
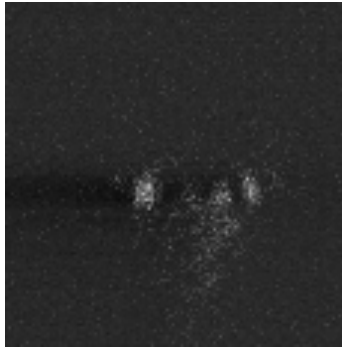


Chemically Synthesized Silver Nanocube Rock with 0.01° steps

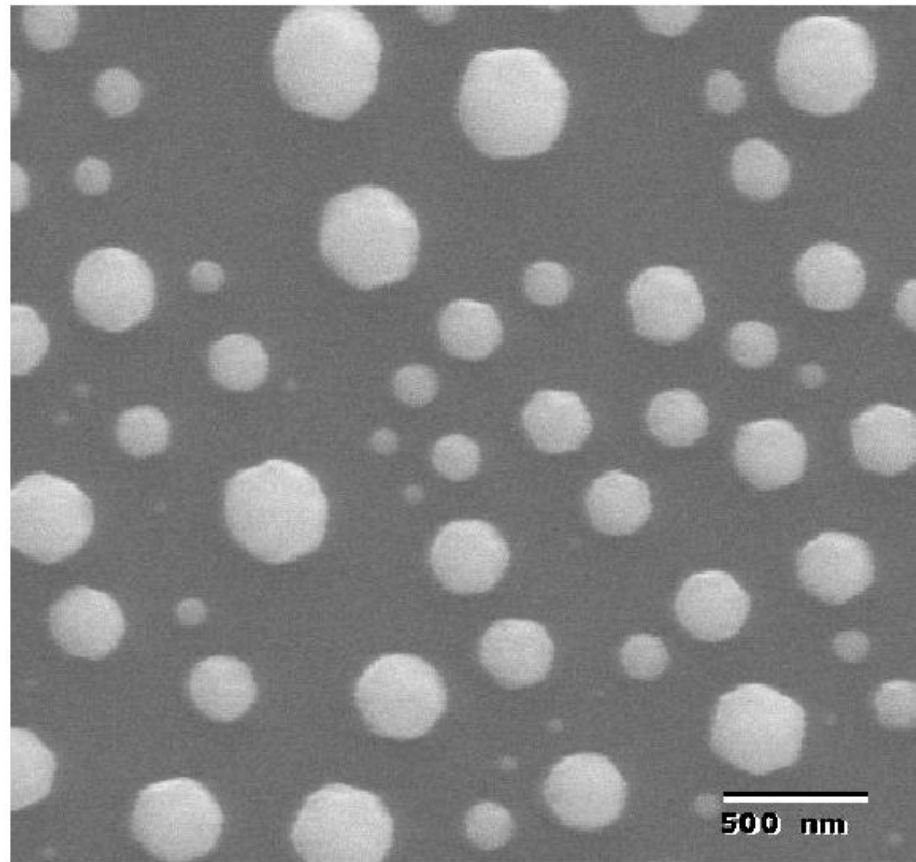
Yugang Sun and Younan Xia,
Science 298 2177 (2003)



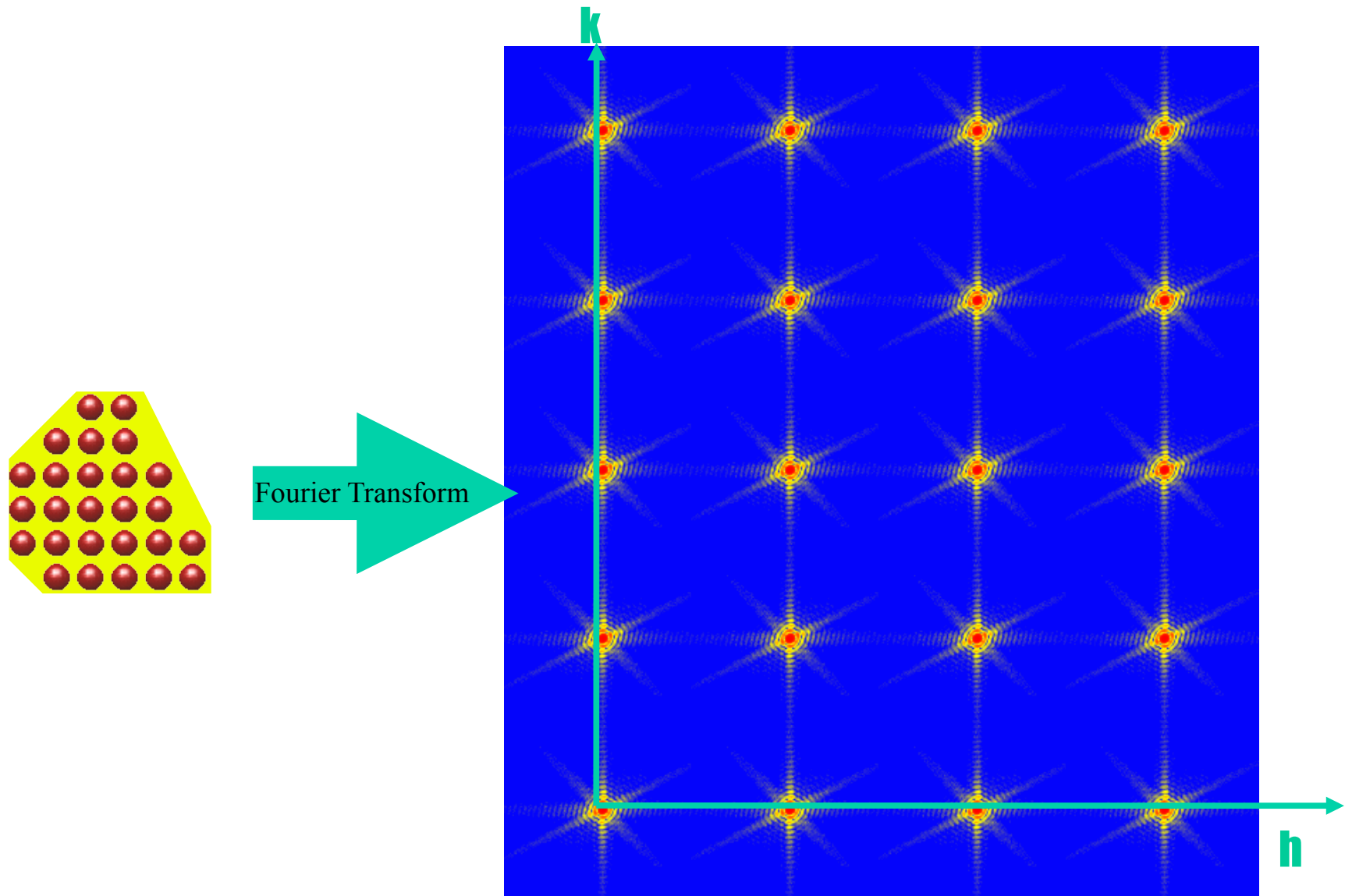




In situ growth of Pb crystals

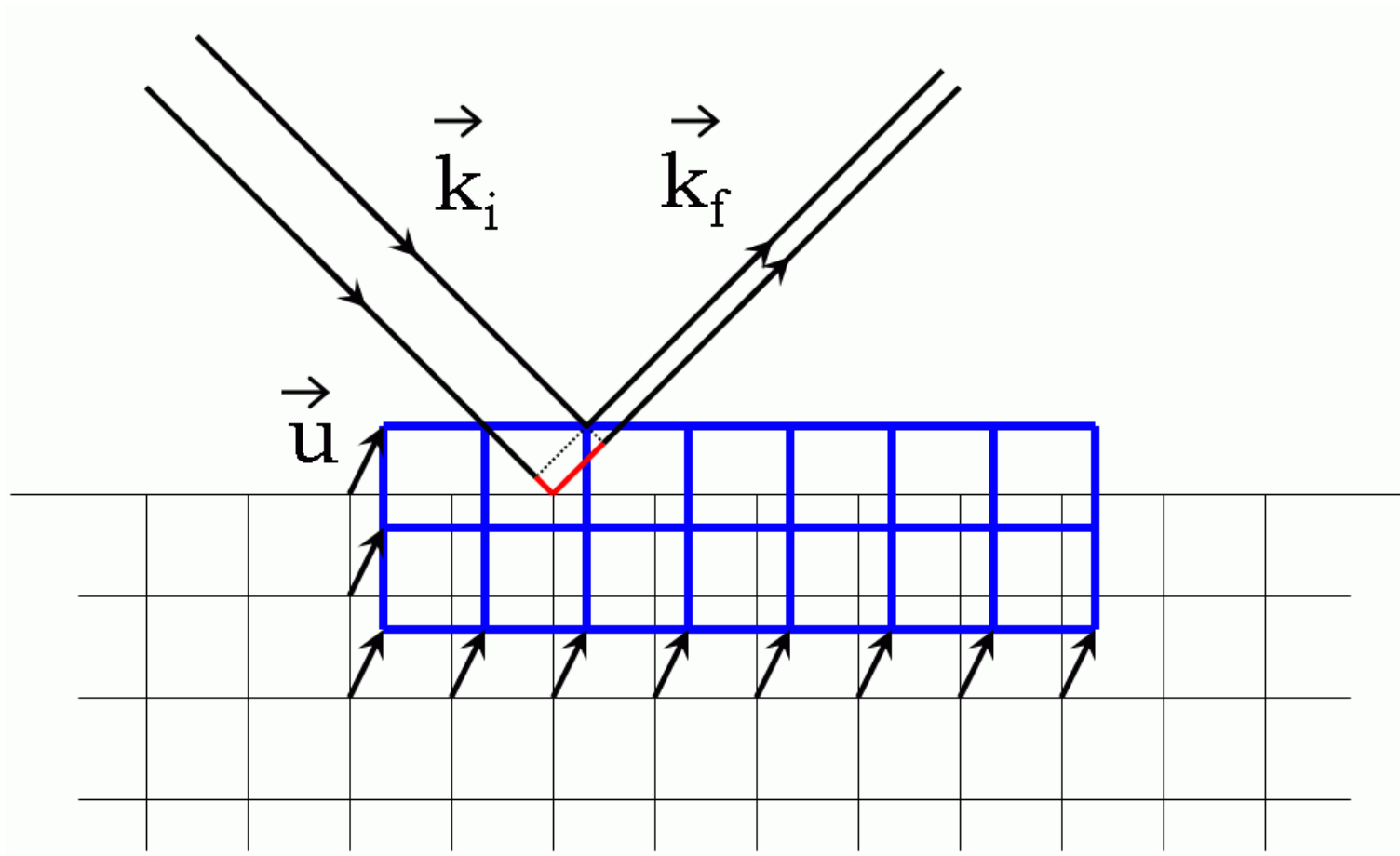


Coherent Diffraction from Crystals



Sensitivity to strain

$$\Delta\varphi = \mathbf{k}_f \cdot \mathbf{u} - \mathbf{k}_i \cdot \mathbf{u} = \mathbf{Q} \cdot \mathbf{u}$$



Good statistics, 3D diffraction data

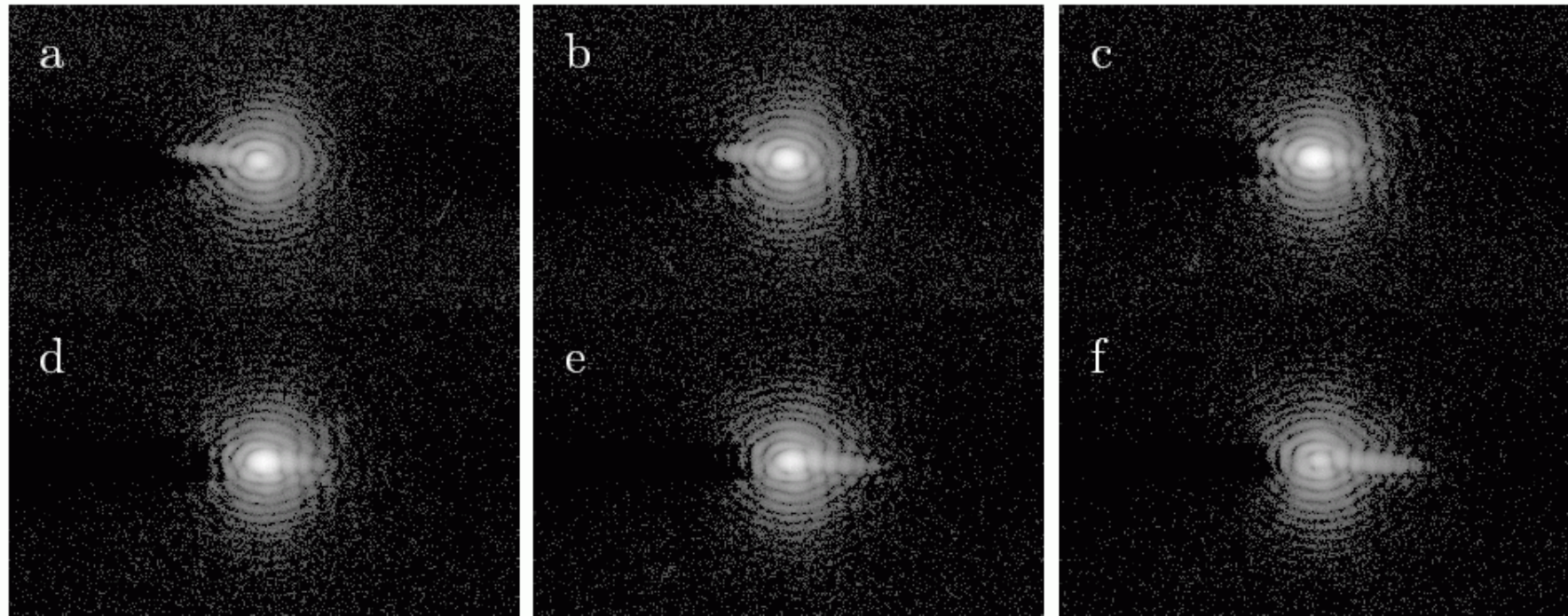
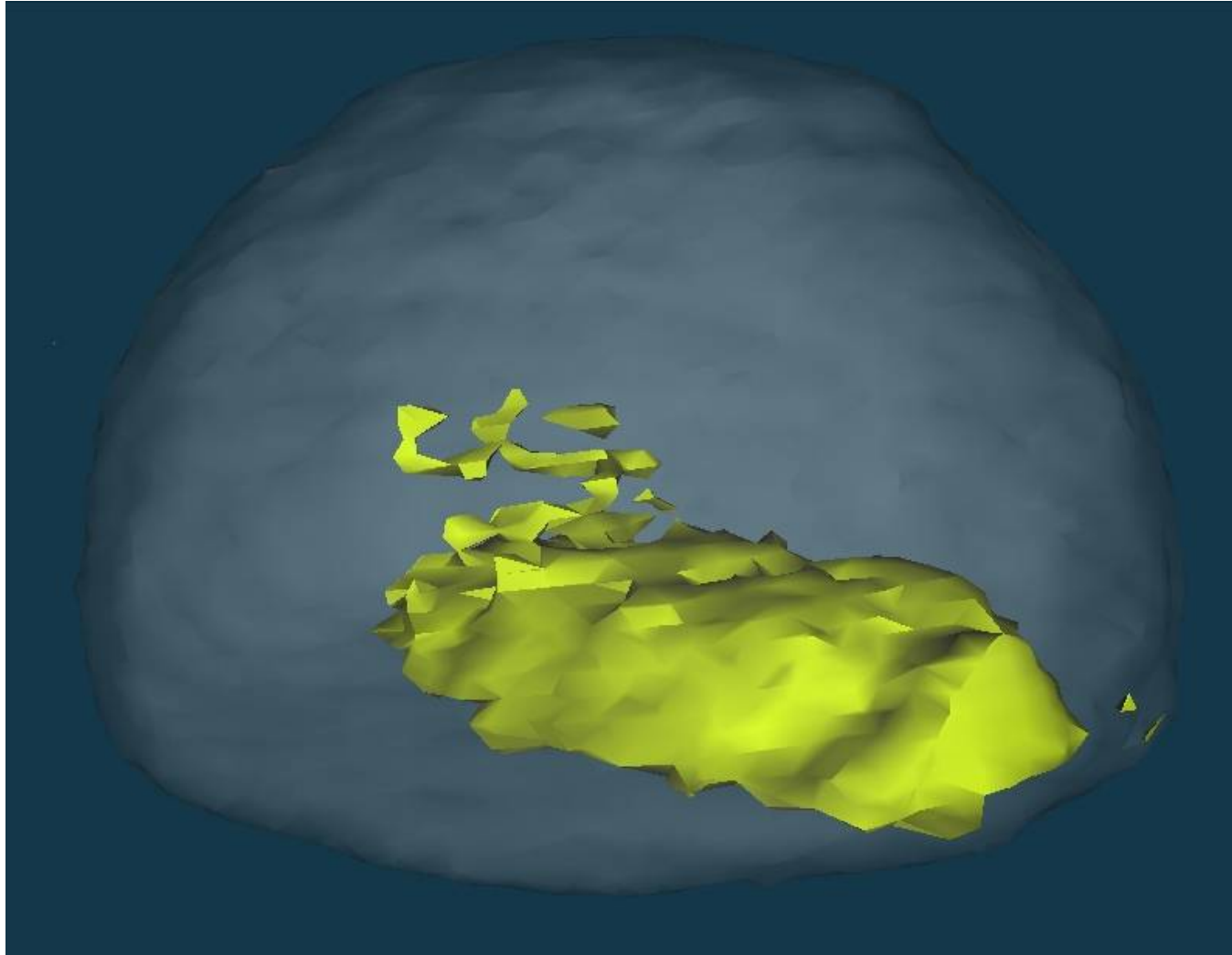


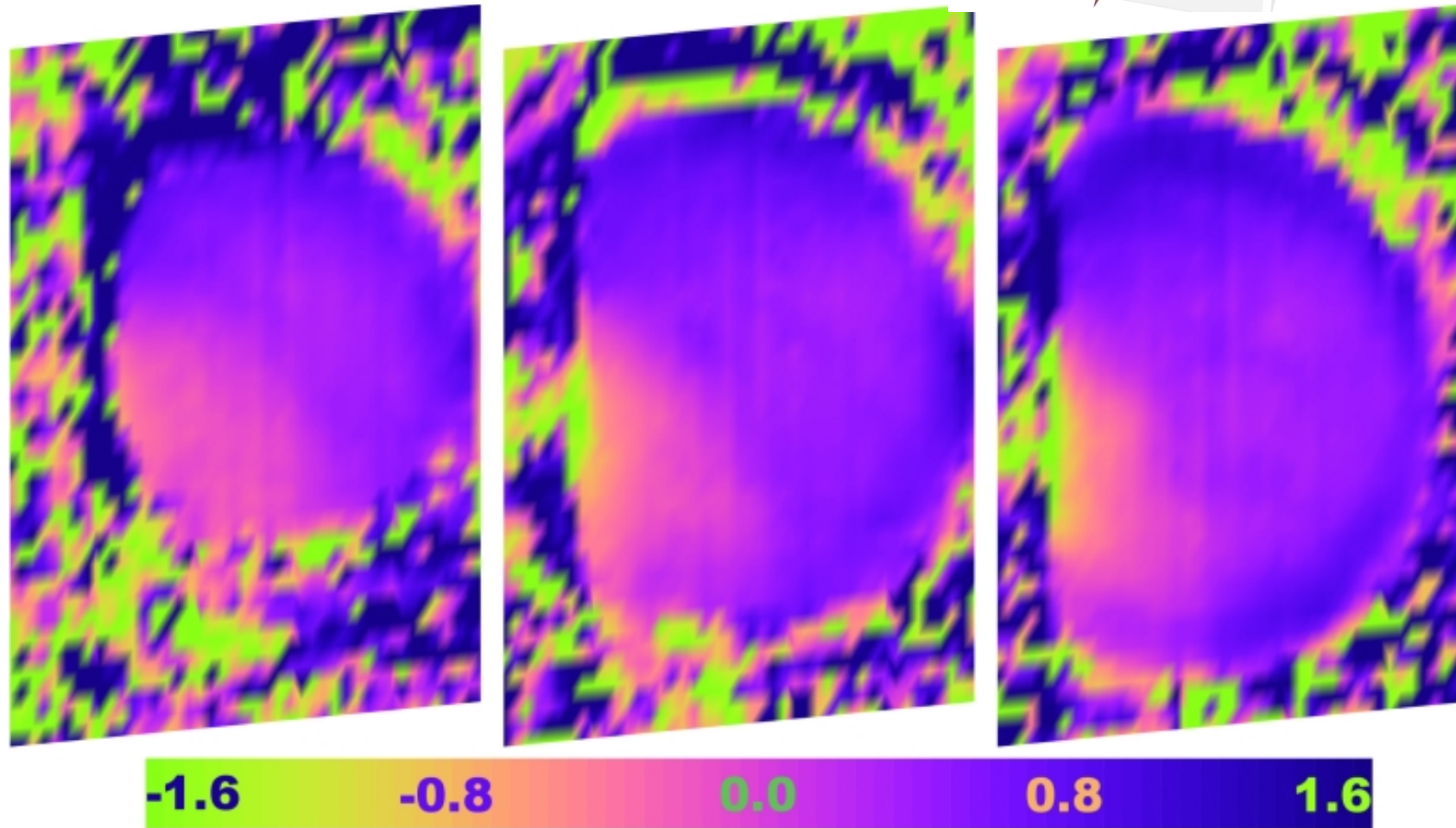
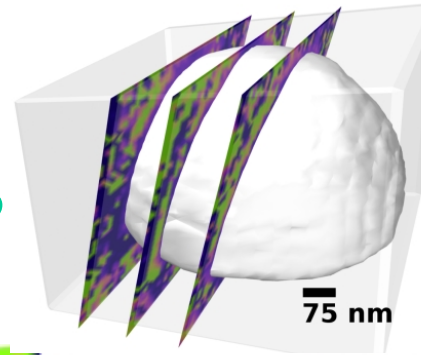
Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

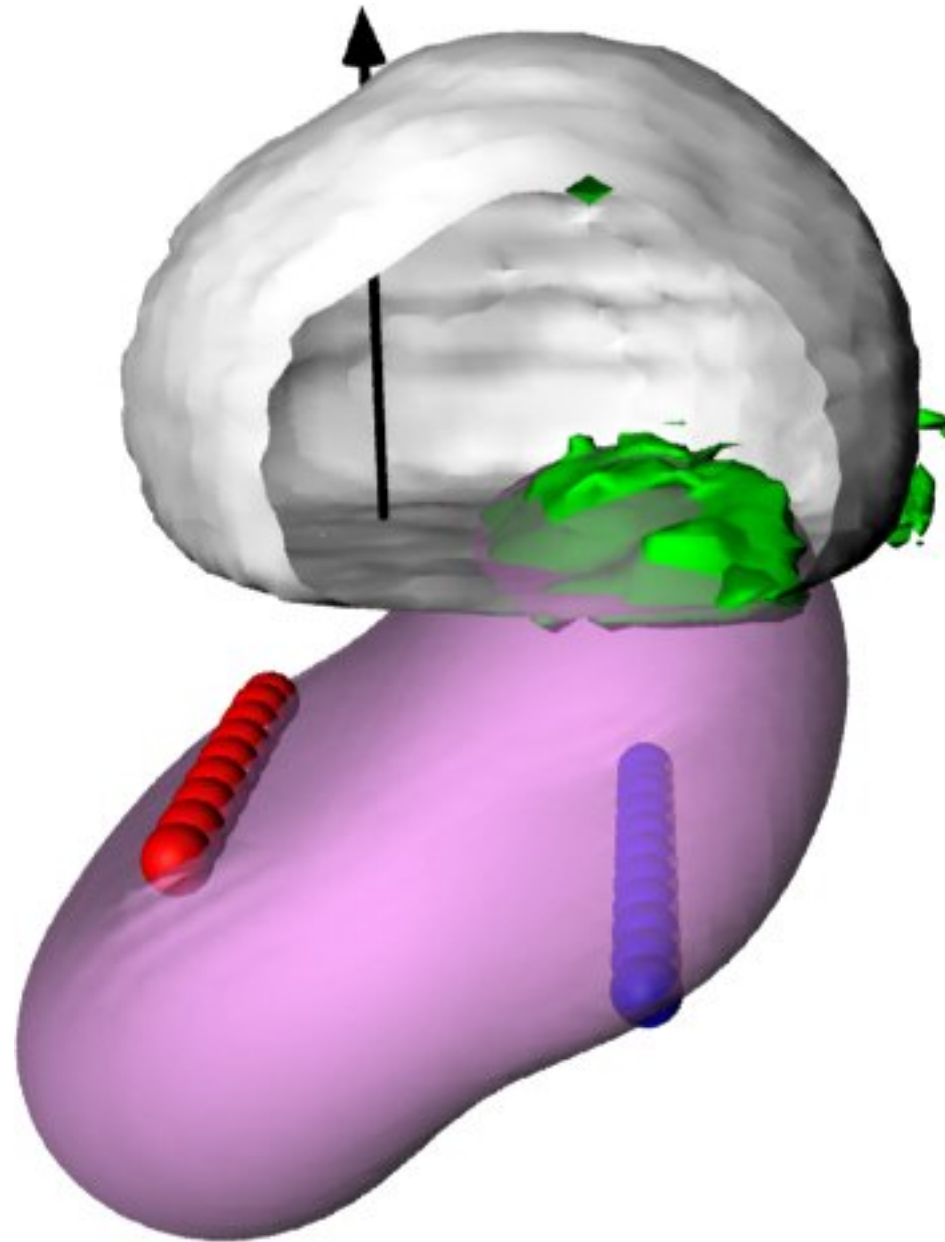
Modeling of 3D Phase Bump



I. K. Robinson, Soleil 2009

3D phase map sections

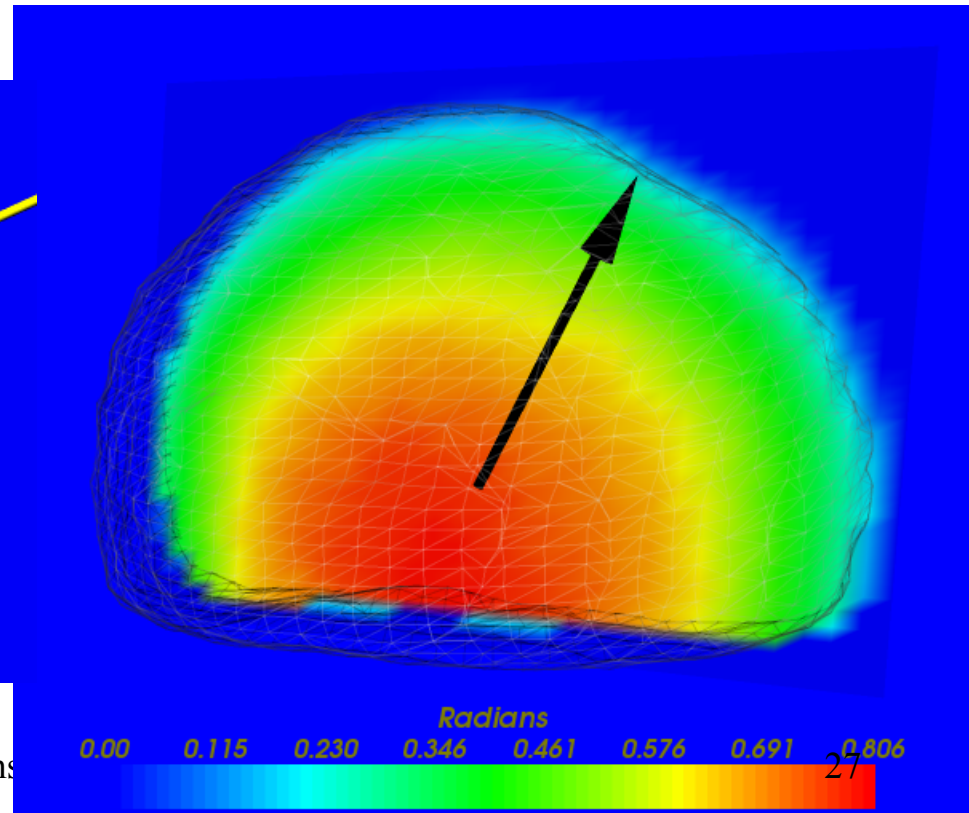
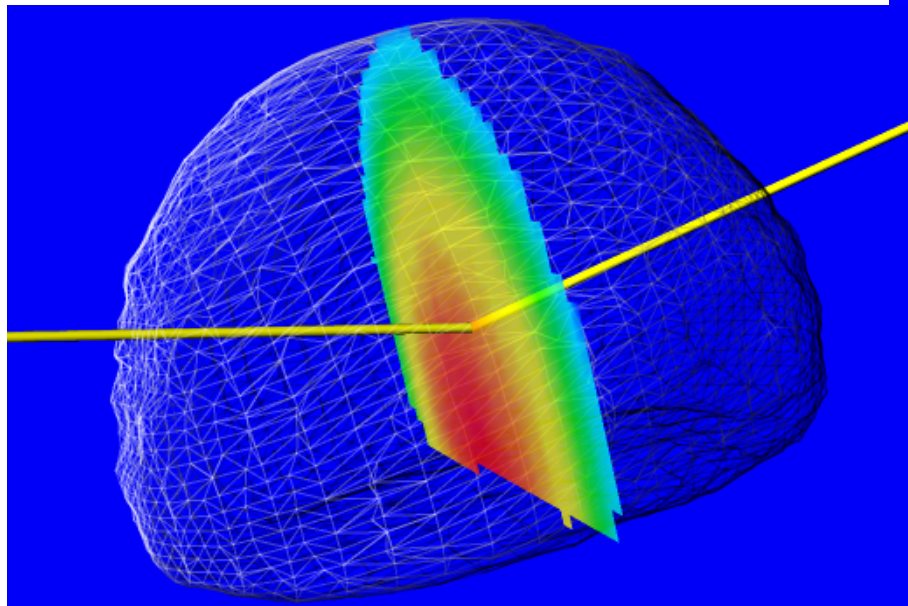




Refraction effects in Lead at 8.9keV

Phase accumulation due to refraction along scattering path
 $n=1-\delta+i\beta$

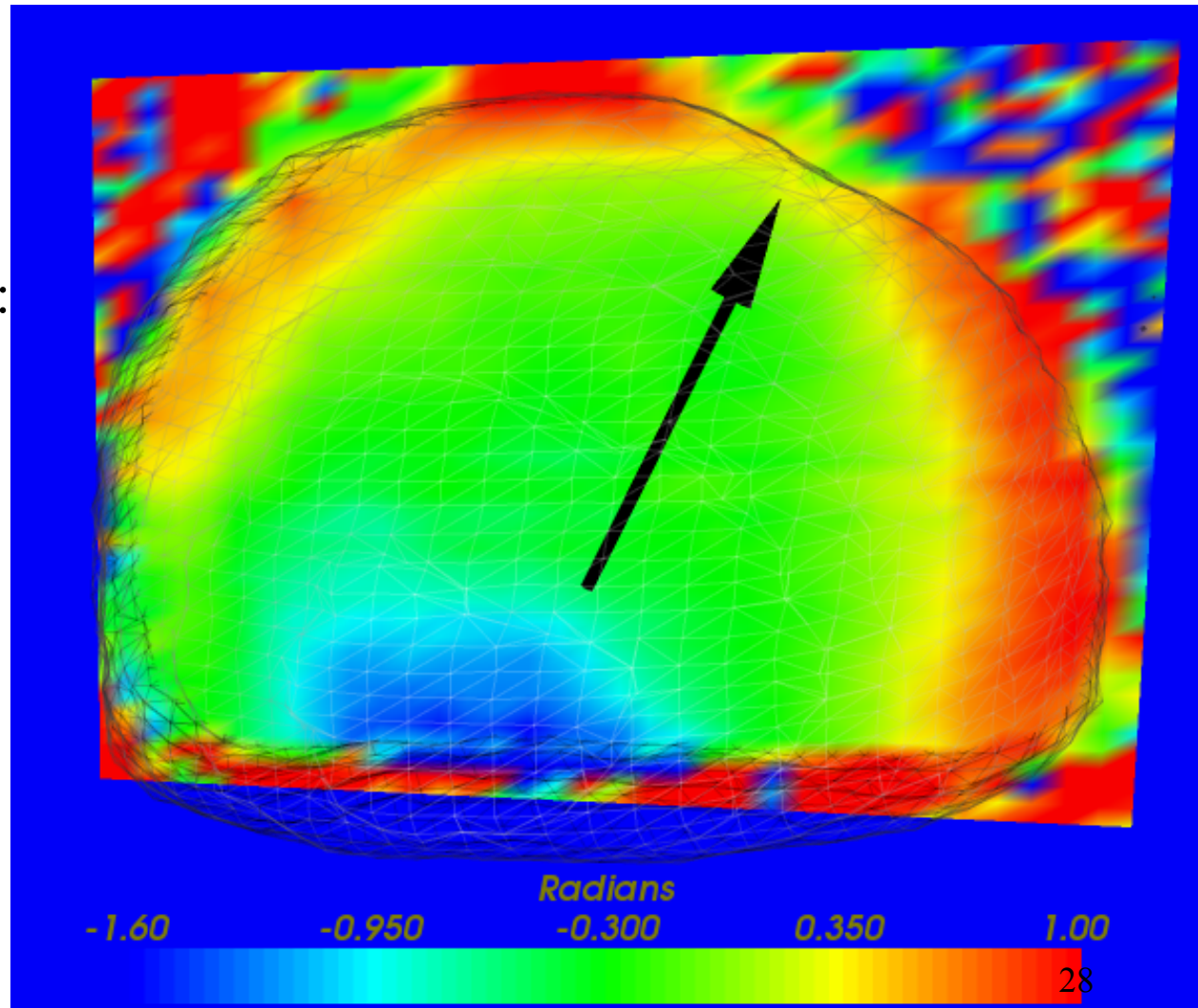
$$\delta=2.23\times 10^{-5}$$
$$\beta=2.19\times 10^{-6}$$



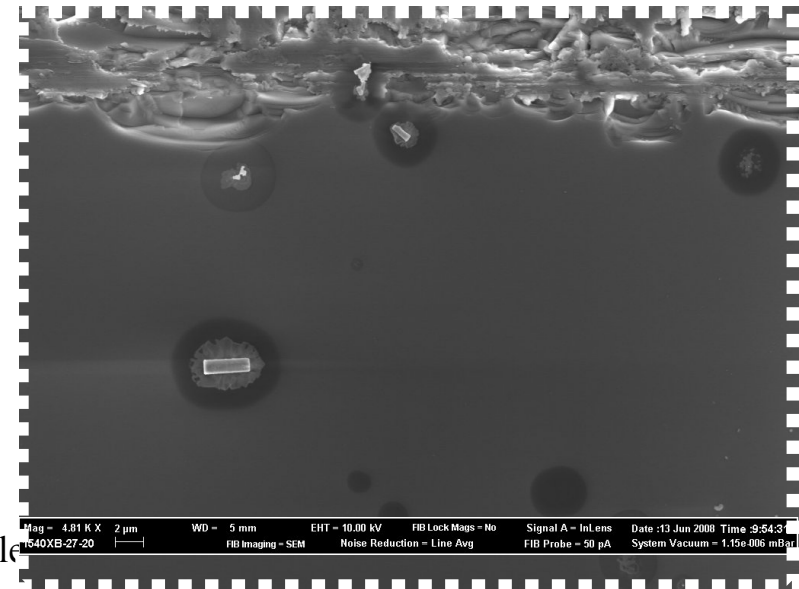
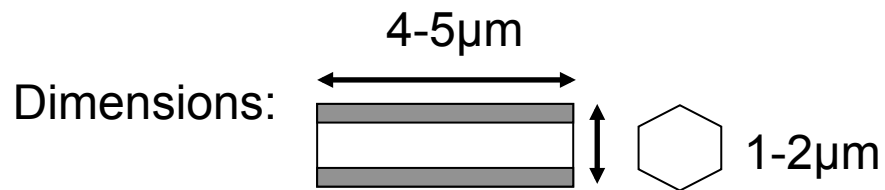
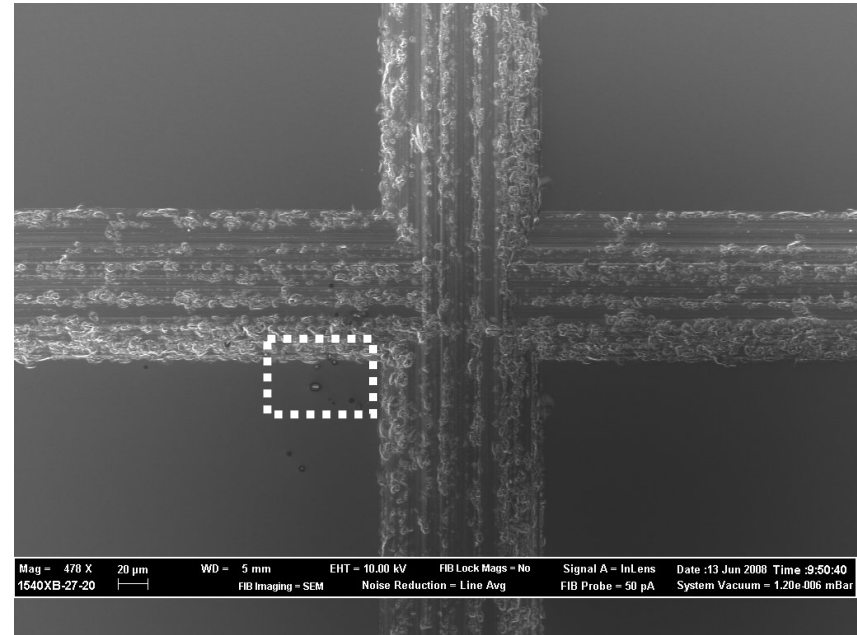
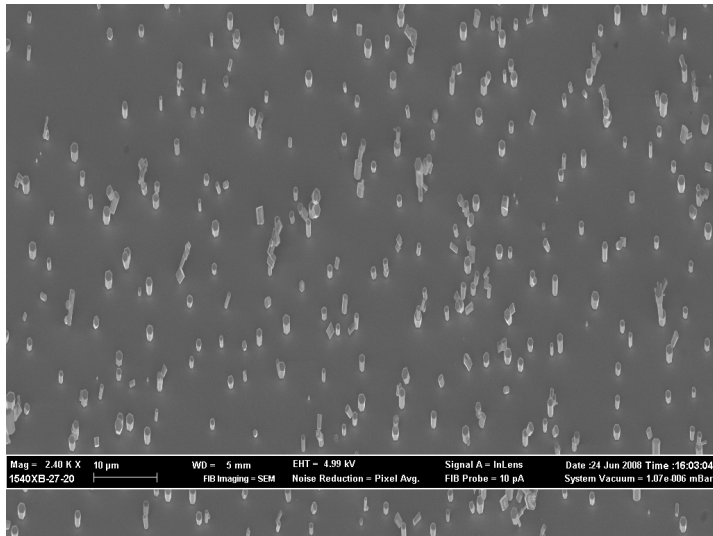
Refraction corrected phase map

Max phase = 1.15rad
= 0.052nm

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

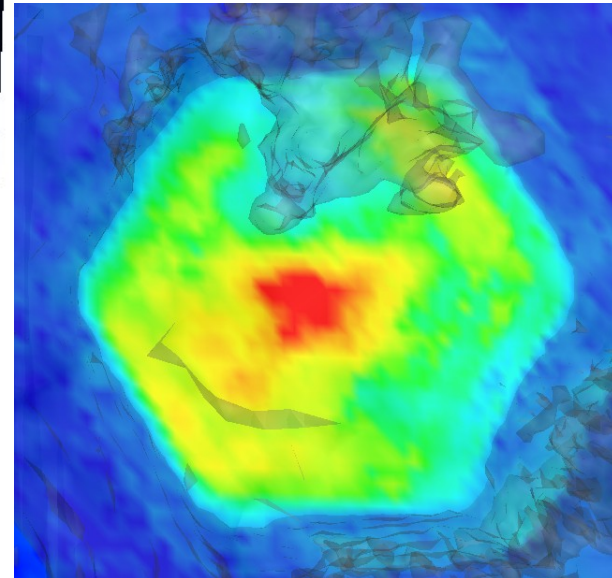
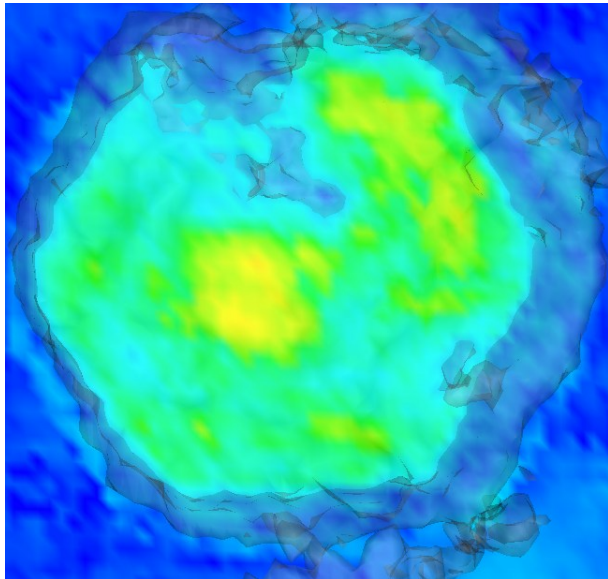
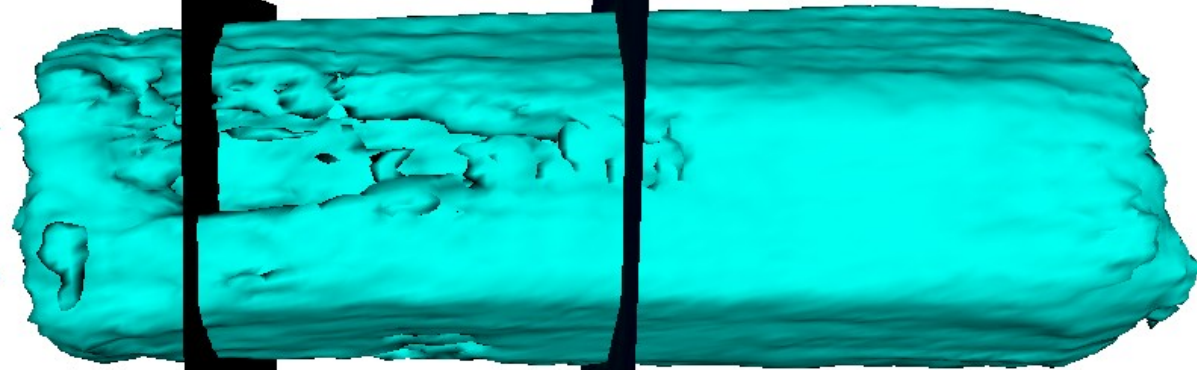


ZnO Sample Preparation



Density sections ZnO-39 (010)

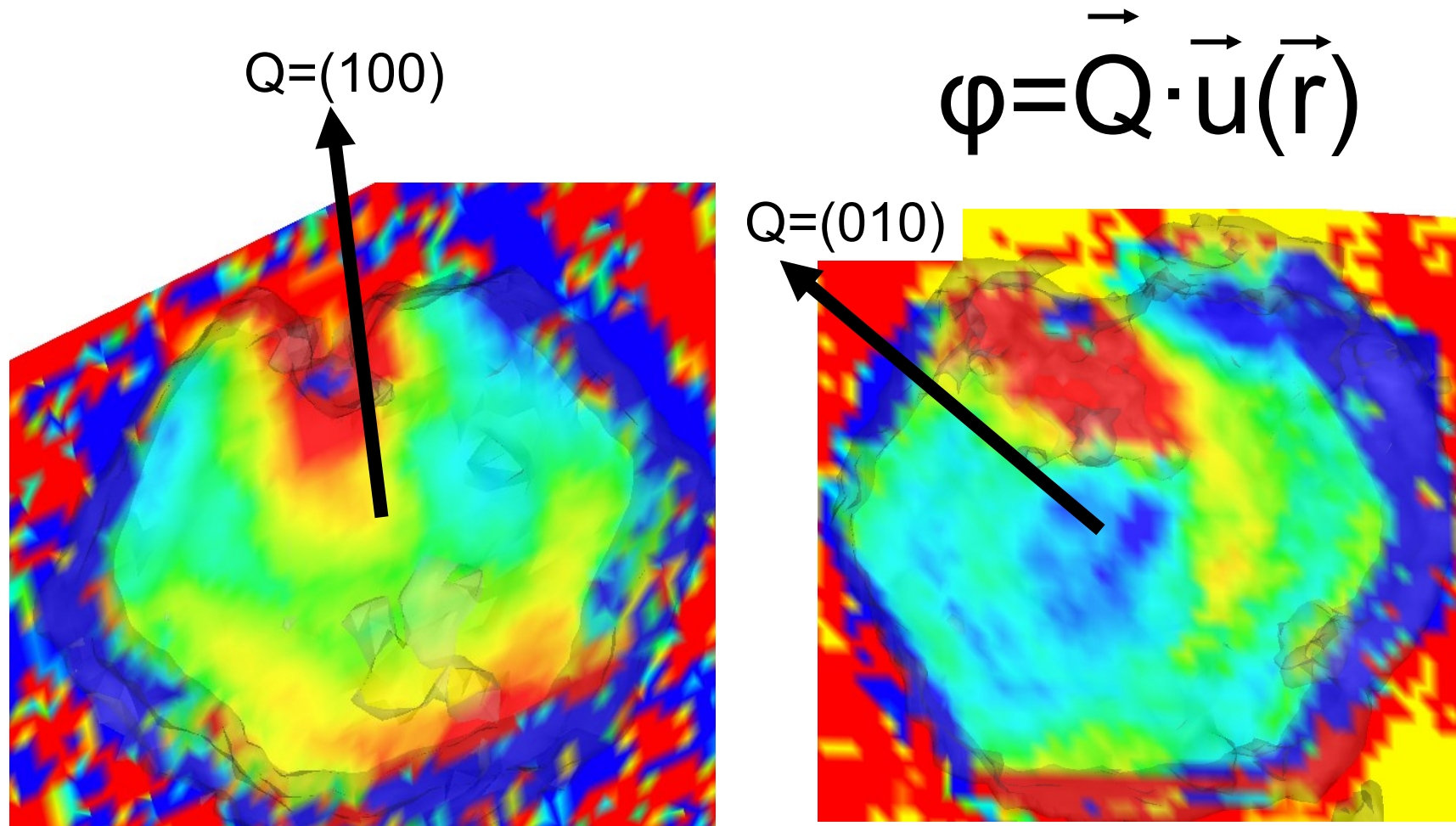
Marcus Newton and Steven Leake (in preparation, 2008)



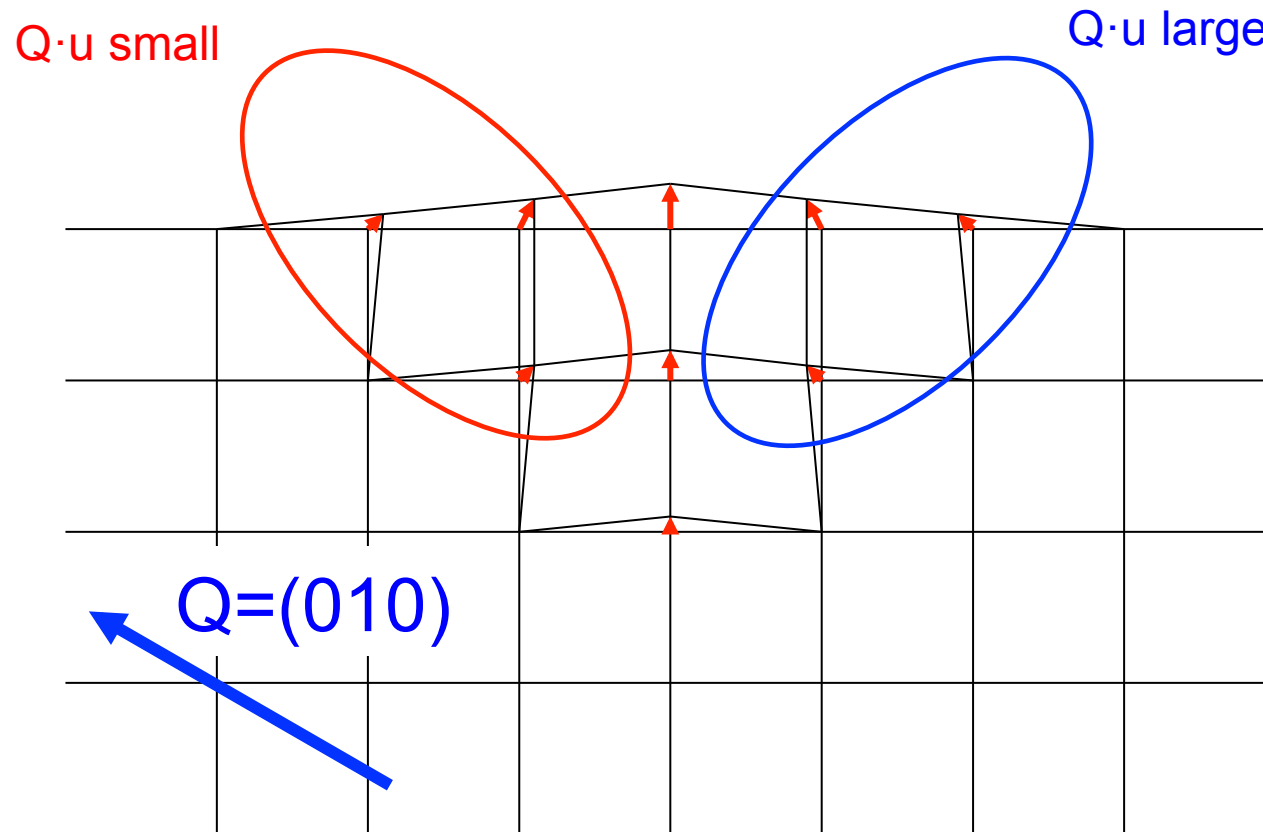
I. K. Robinson, Soleil 2009

Phase maps from 2 Bragg peaks

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

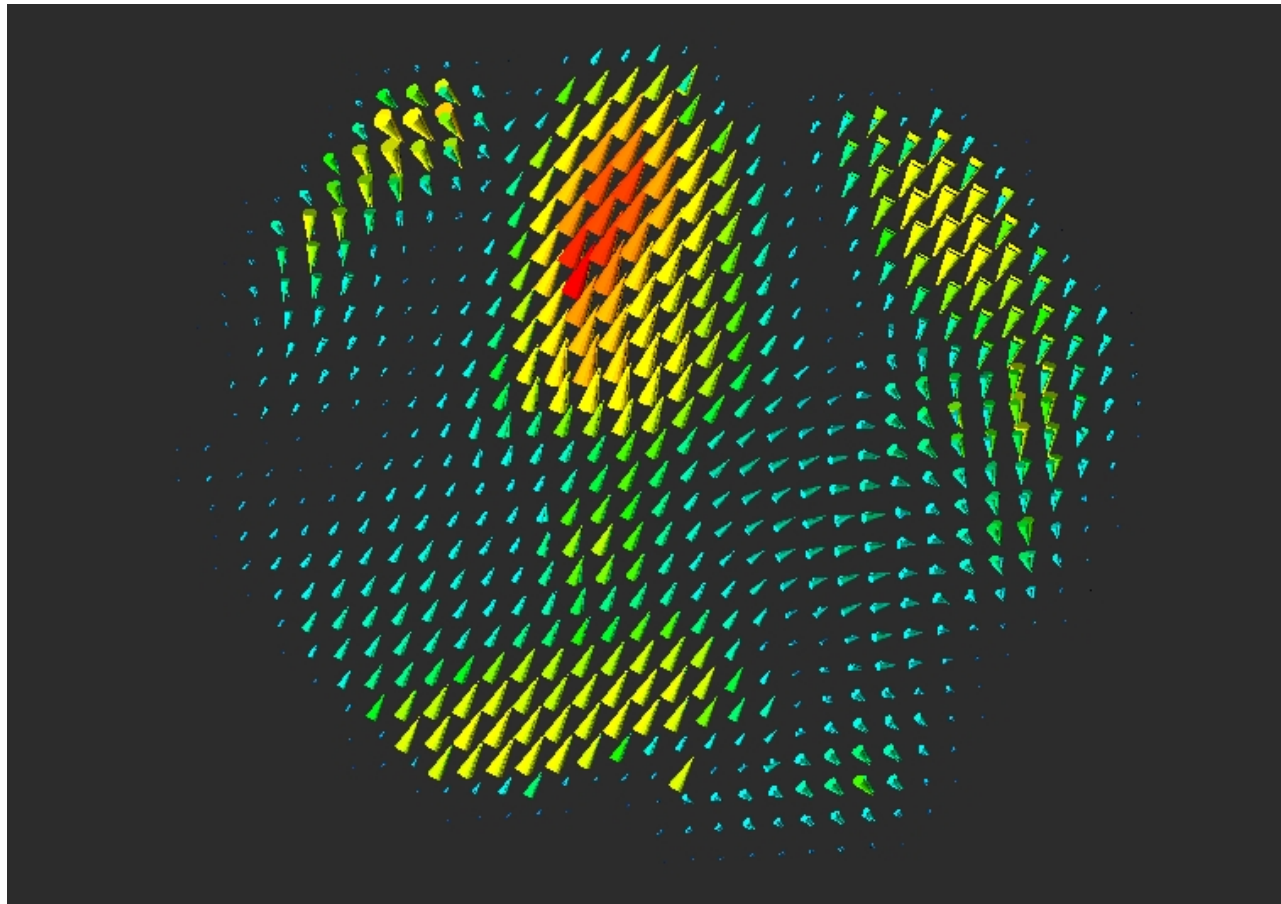


Typical displacement field

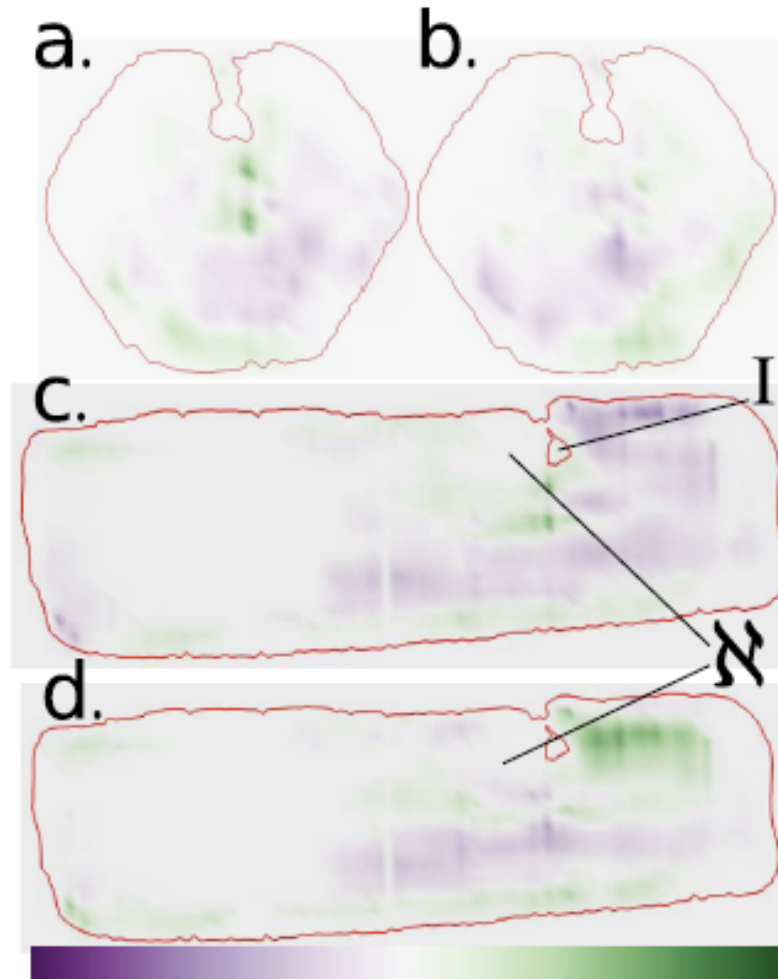
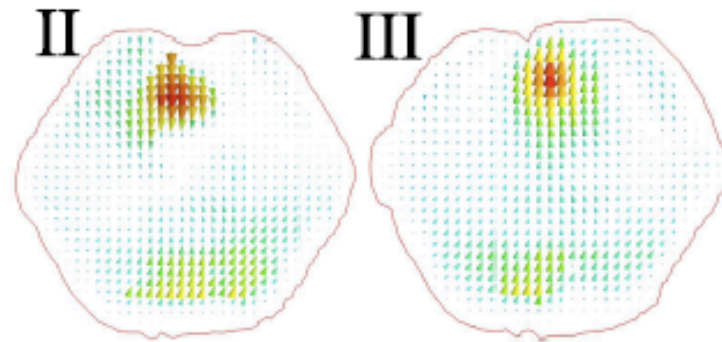
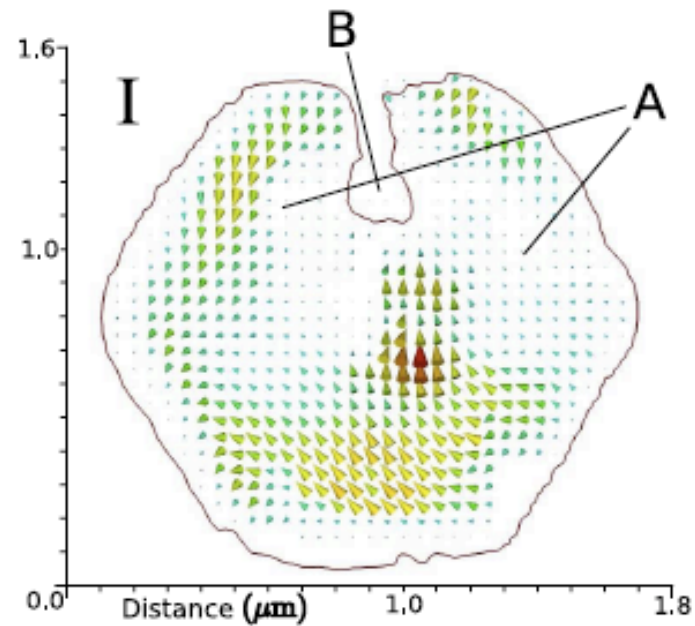


2D vector field of displacements

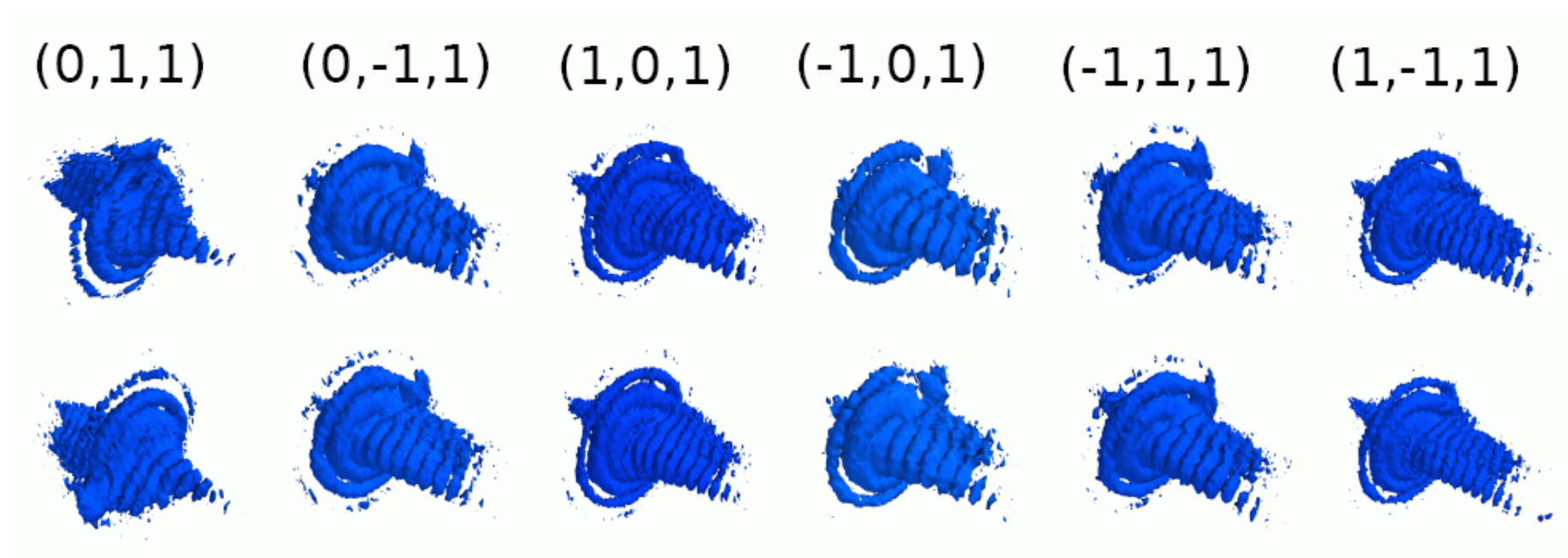
Marcus Newton, UCL, Jan 2009



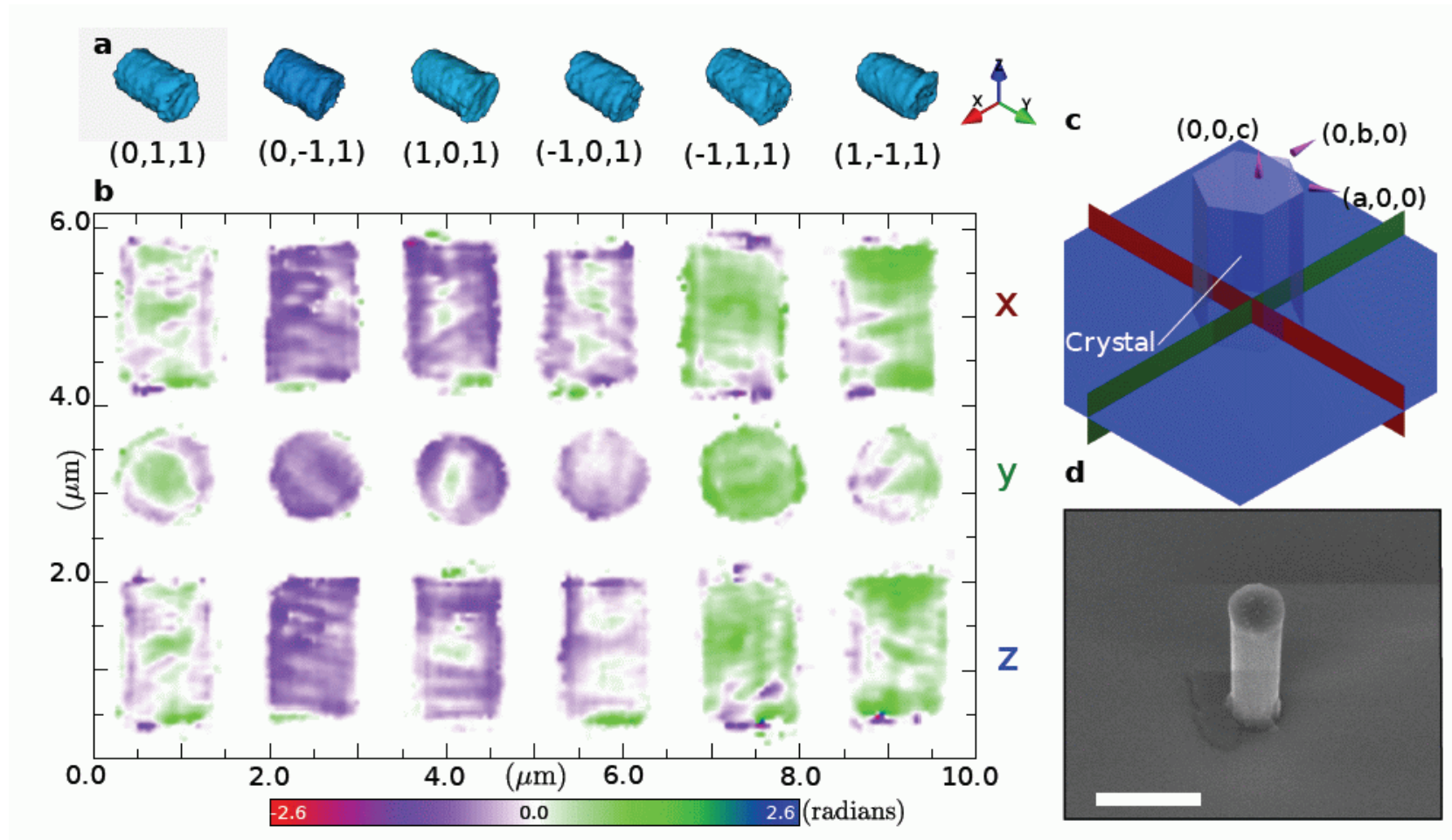
Strain and Rotation fields



Extension to 6 Bragg Peaks

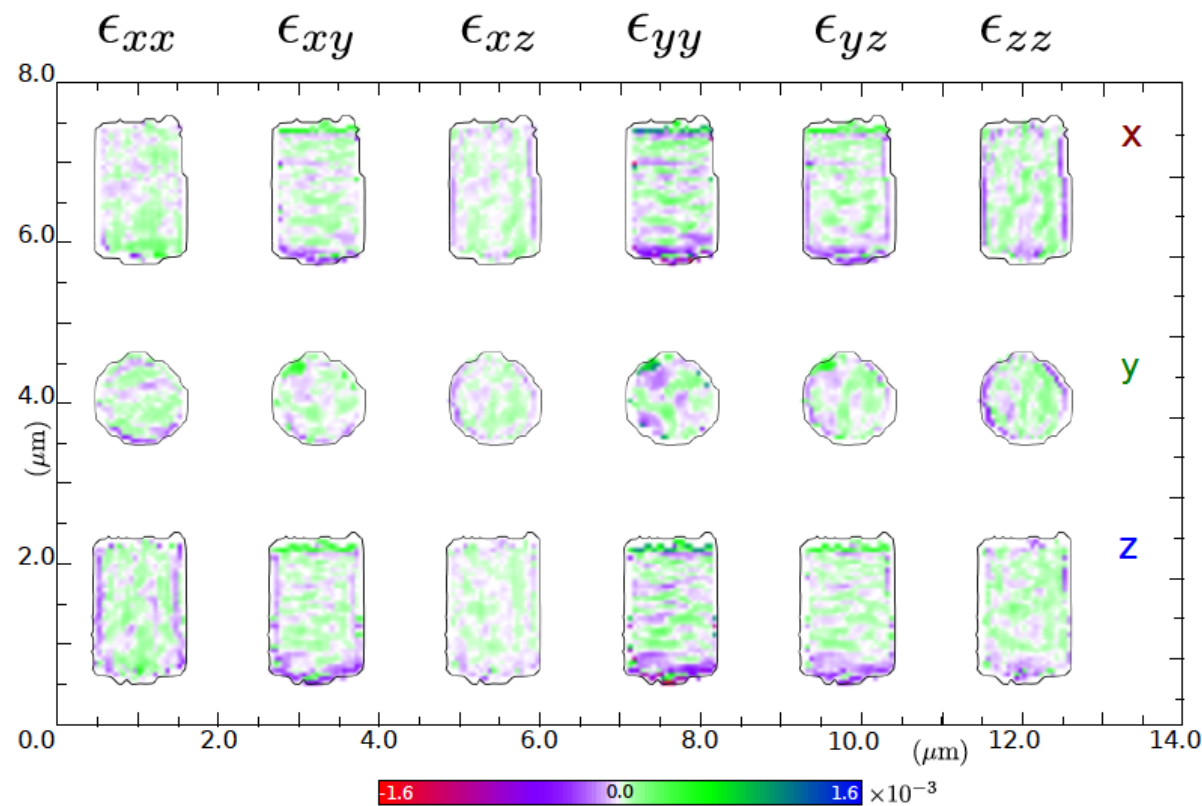


Extension to 6 Bragg Peaks

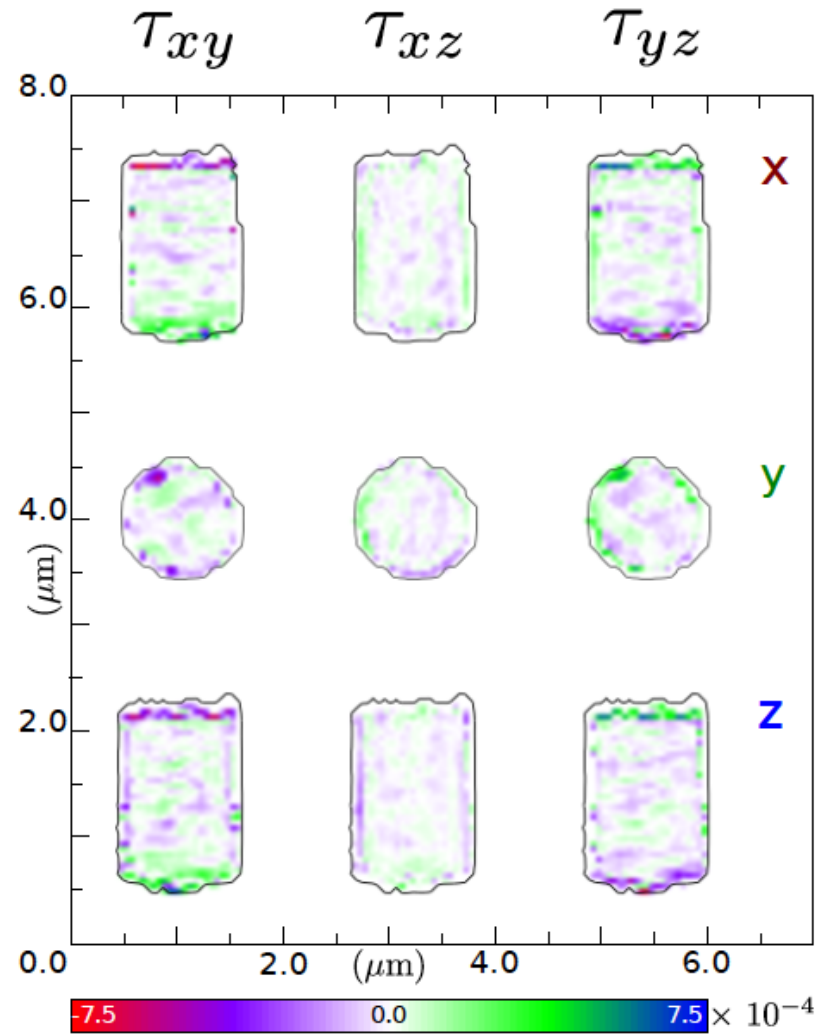


Full Strain Tensor

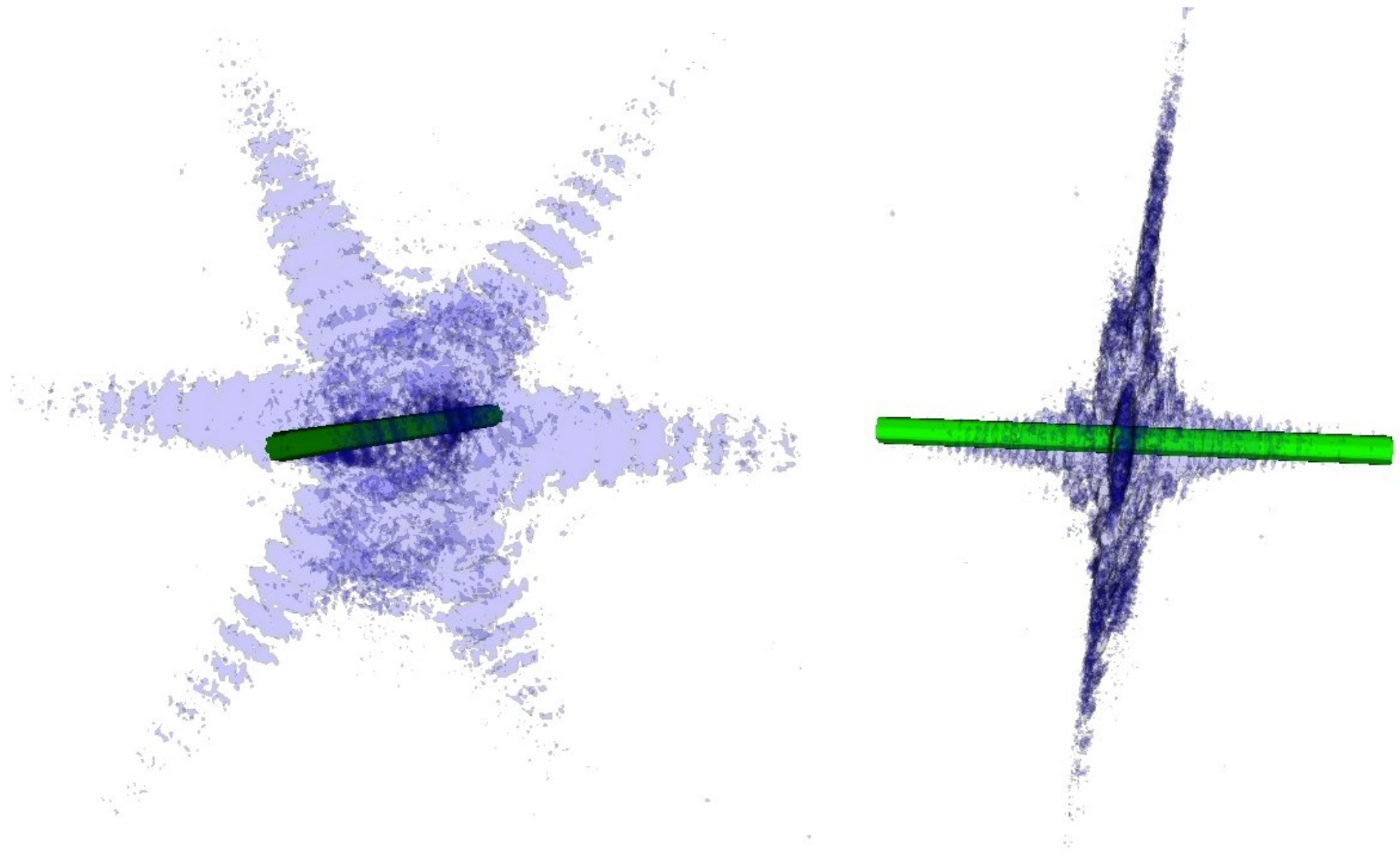
$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right), \quad \tau_{ij} = \left(\frac{\partial u_j}{\partial x_i} - \frac{\partial u_i}{\partial x_j} \right)$$



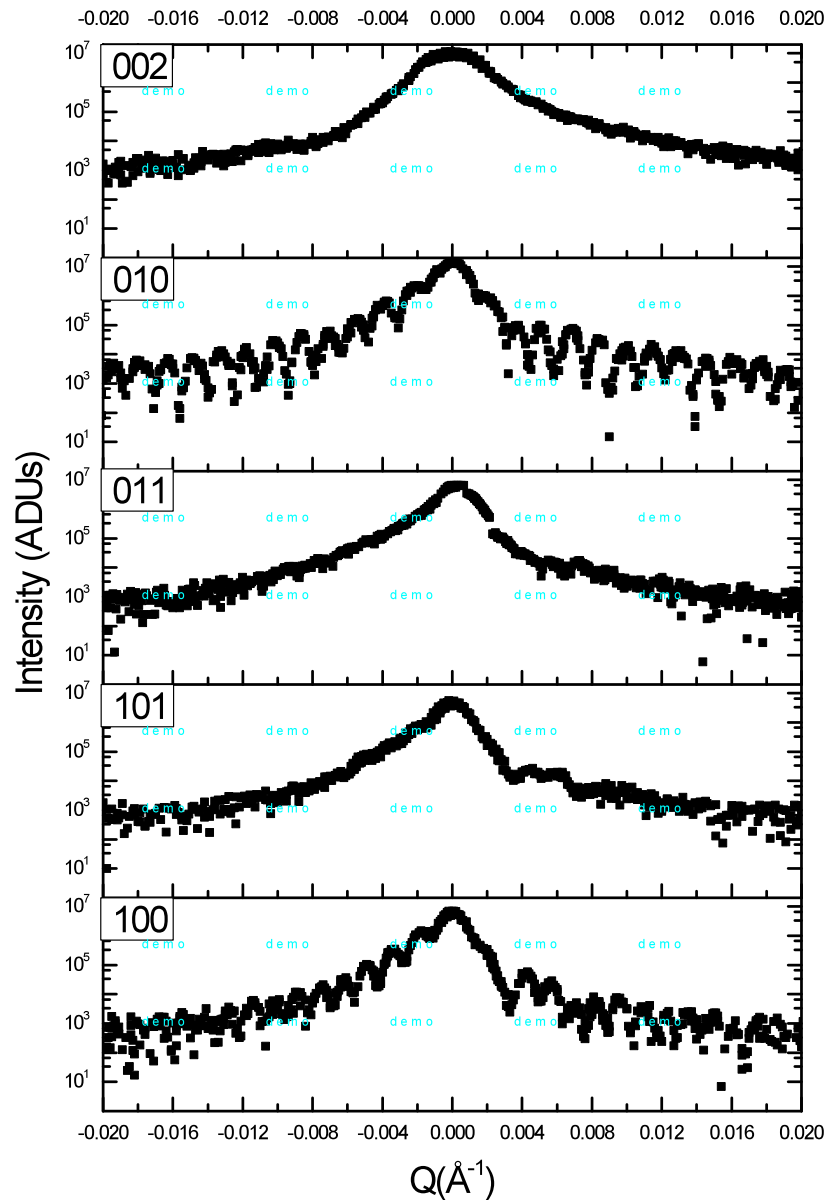
ZnO Rigid-body Rotations



How to extract the contrast data



Five Bragg peaks



002 no fringe visibility

010 & 100 good fringe visibility

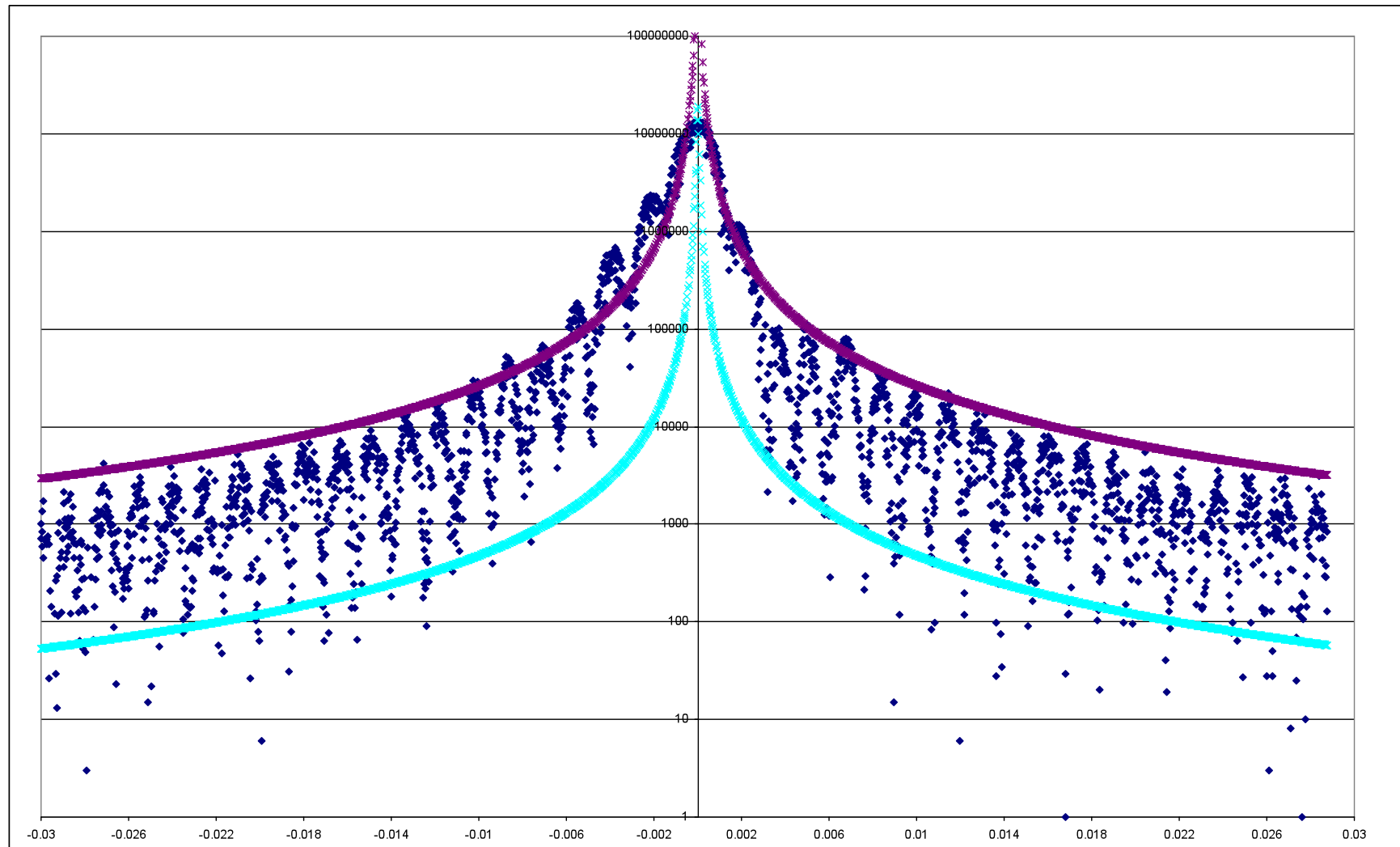
101 & 011 diminished fringe visibility
but fringes still evident

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

Error in coordinate transform ruled out

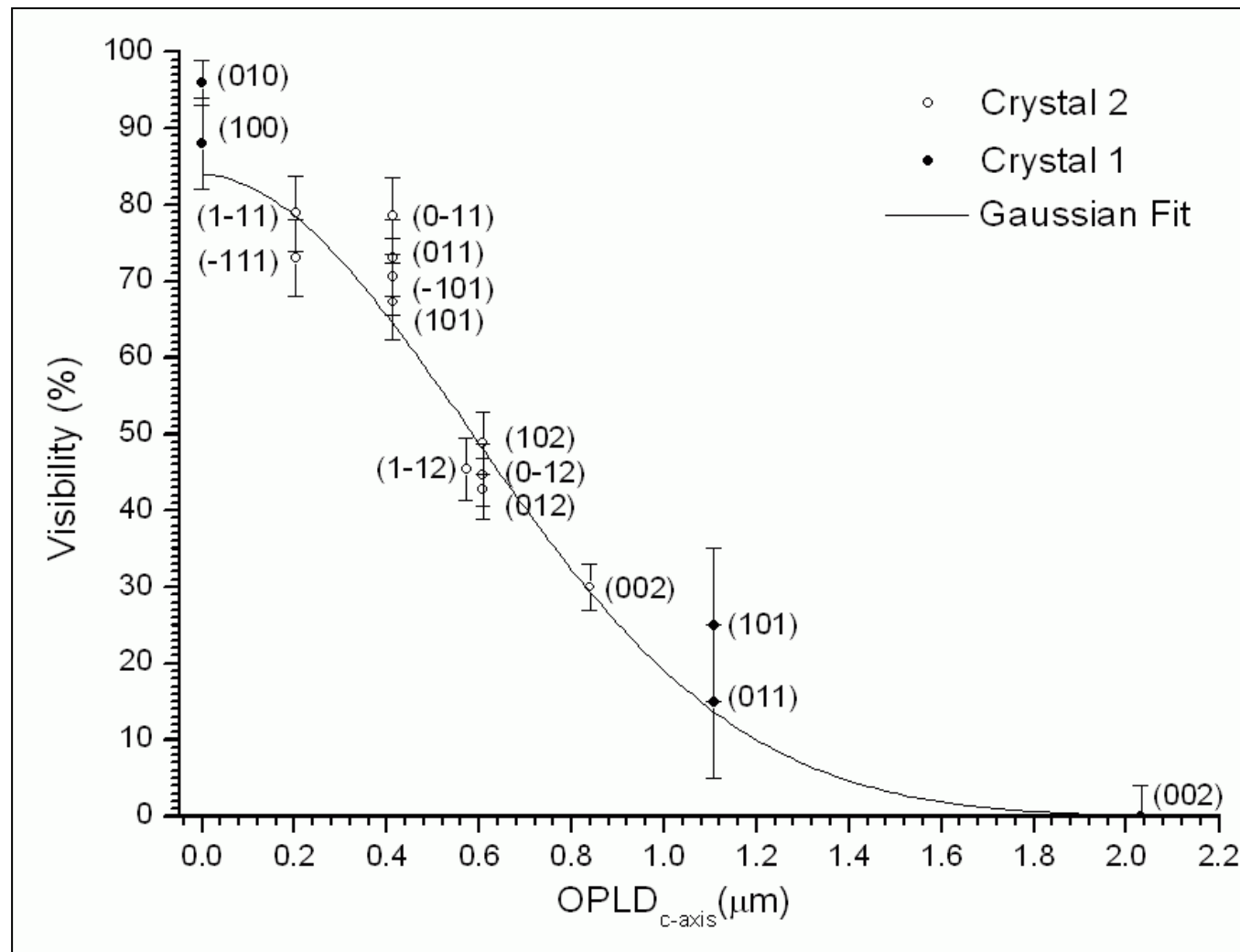
010 and 100 reflections fringe spacing
difference $\sim 20\%$

Fringe Visibility $96\pm 2\%$ @010



Measured Longitudinal Coherence

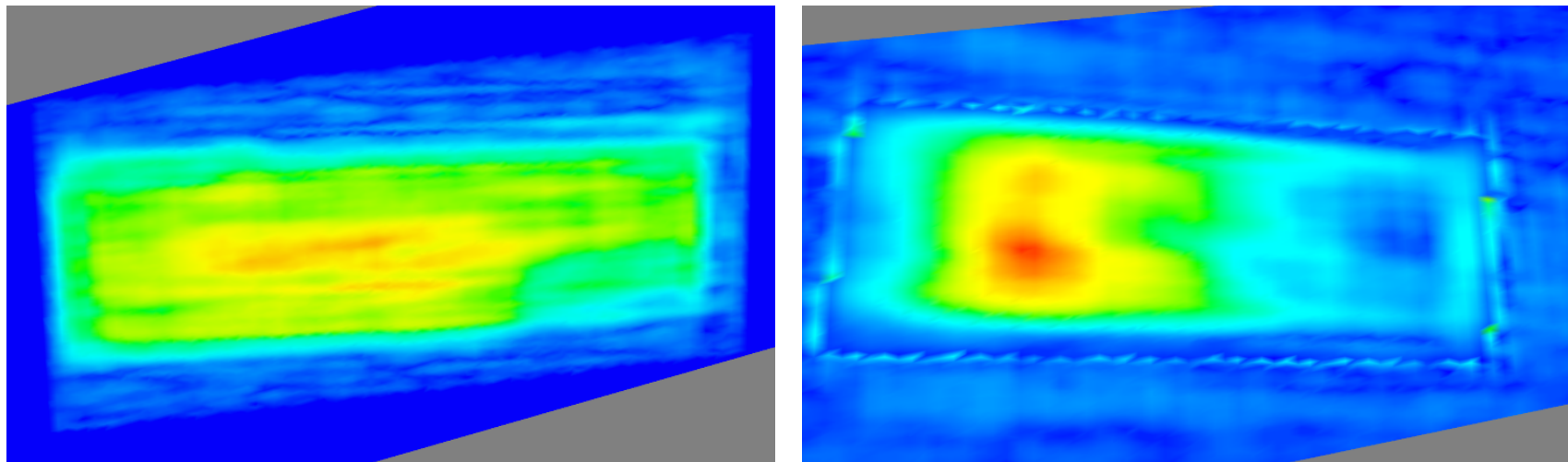
Steven Leake, Optics Express 17 15853 (2009)



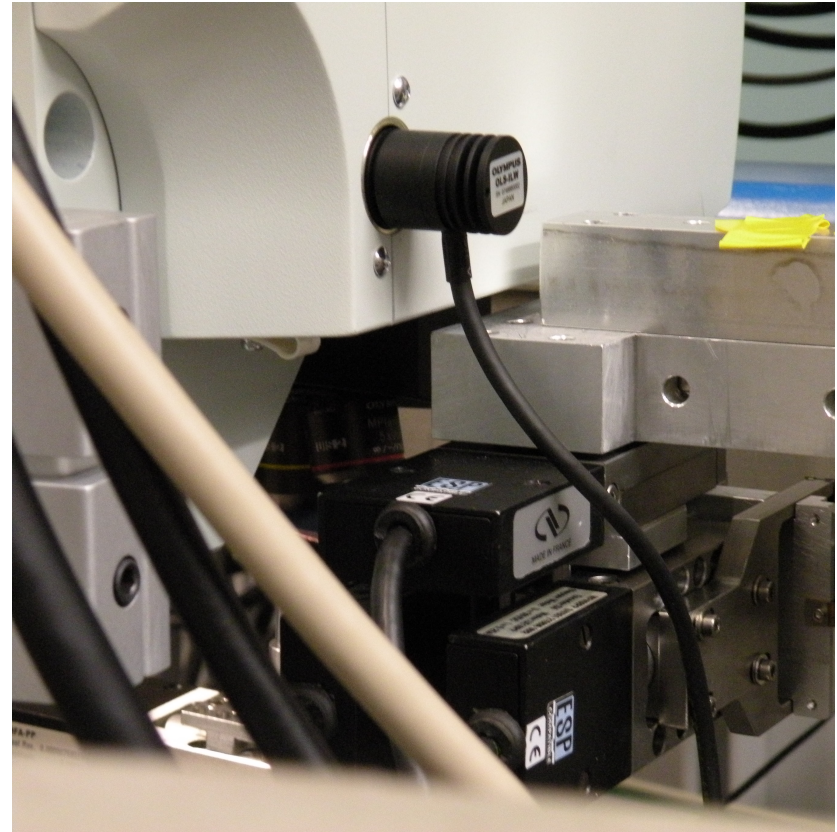
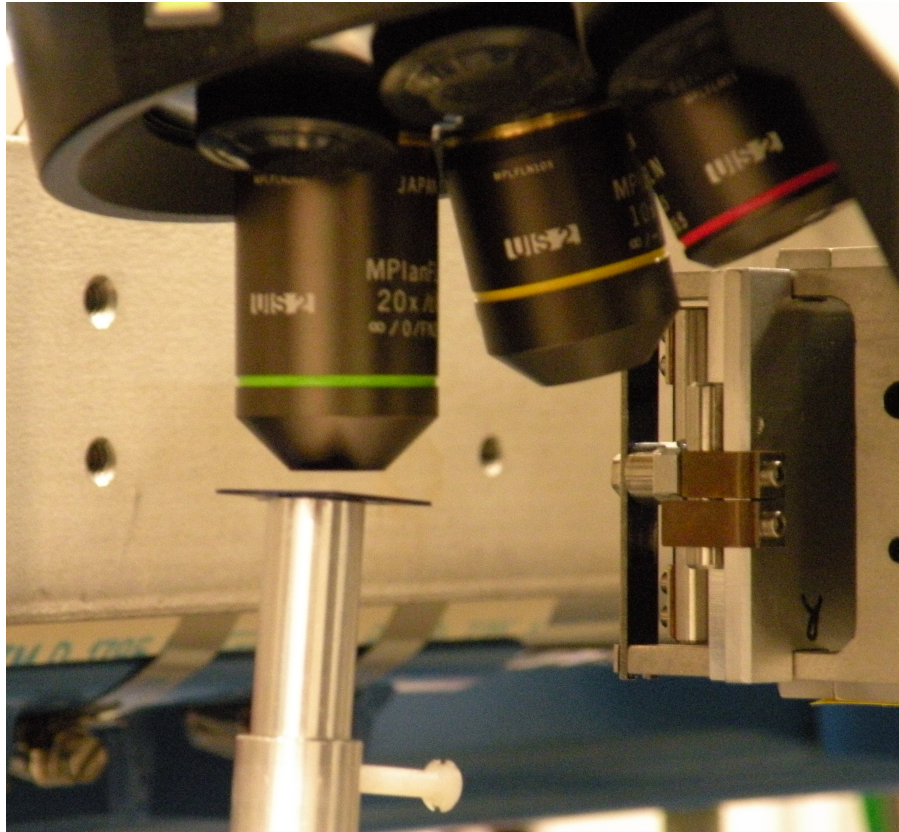
I. K. Robinson, Soleil 2009

Density Section of Reconstruction using 100 and 101 reflections

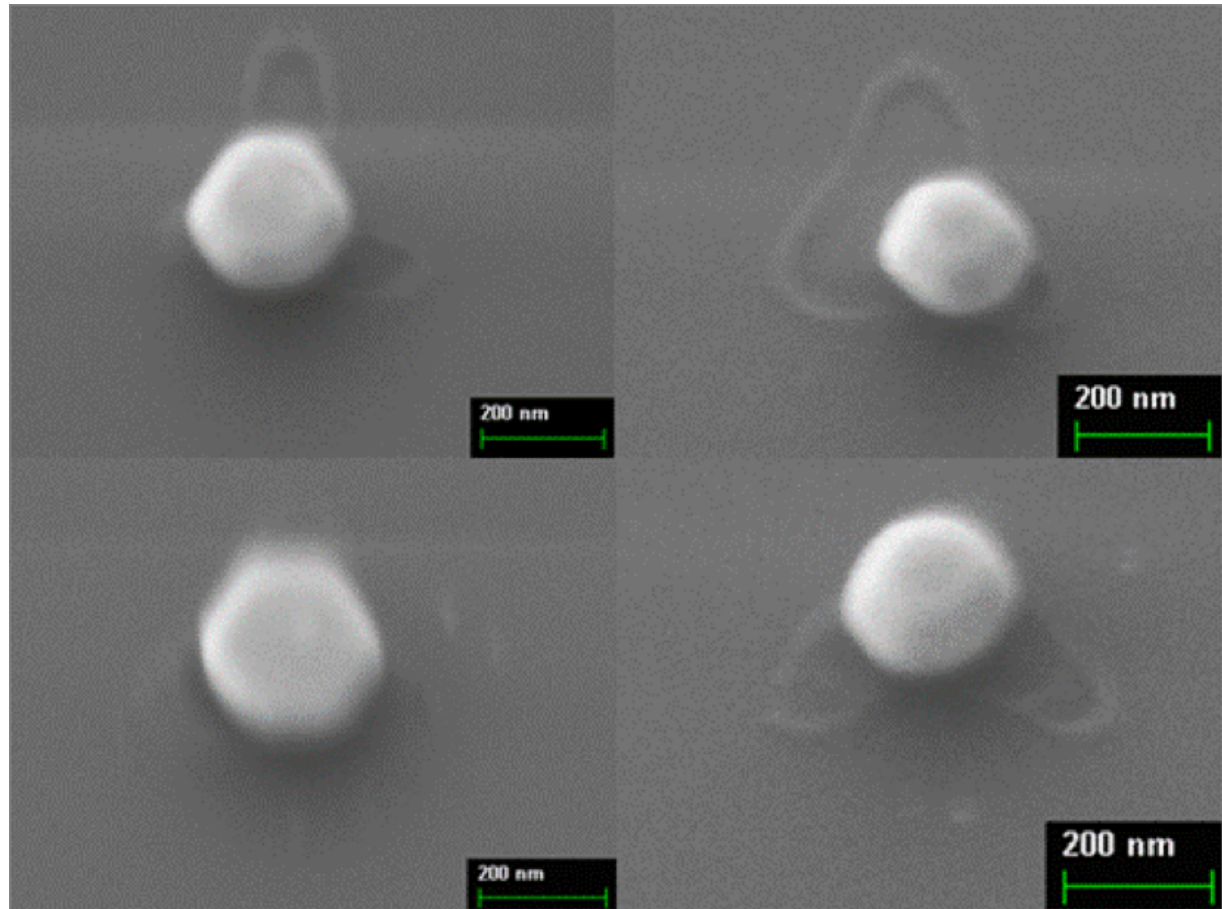
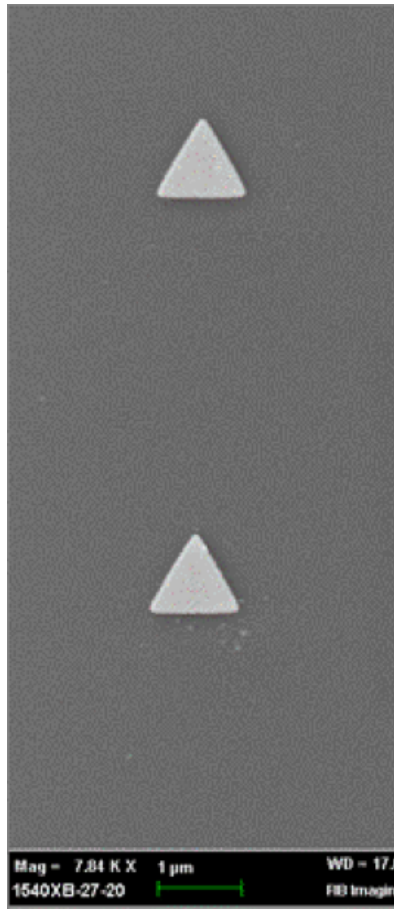
“hot spot” more developed for limited coherence
Steven Leake, Optics Express 17 15853 (2009)



Confocal Alignment Microscope

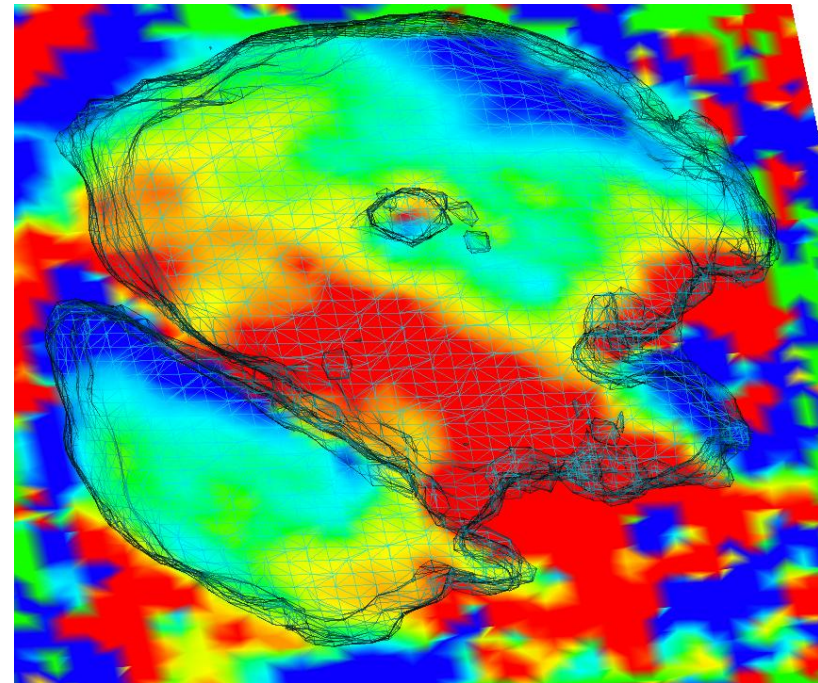
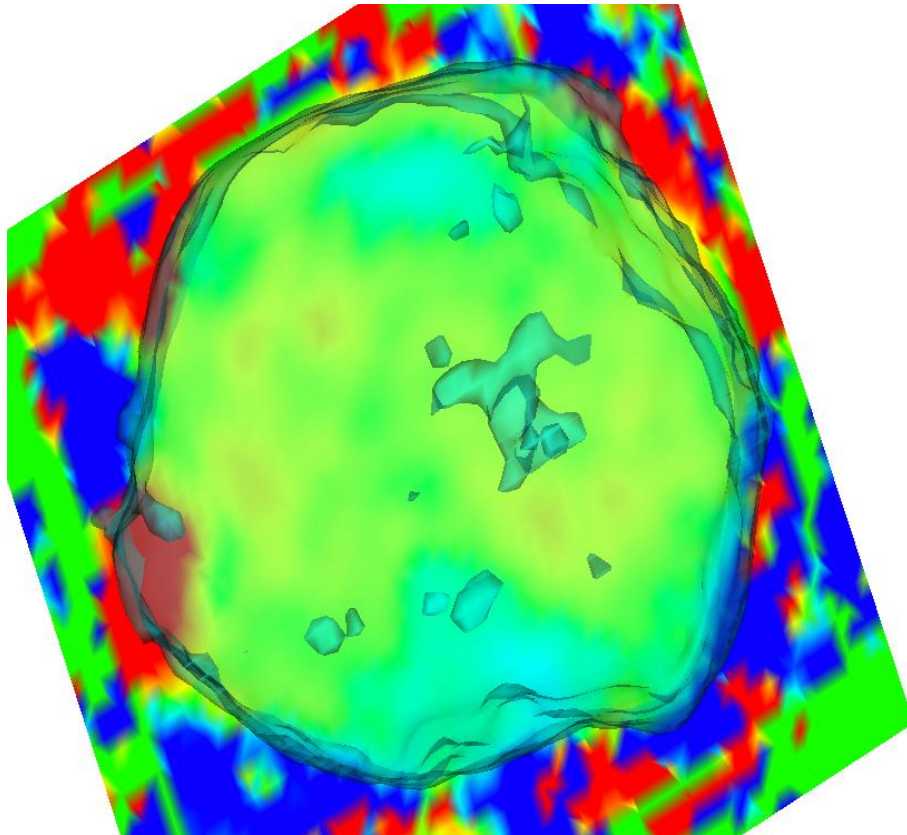


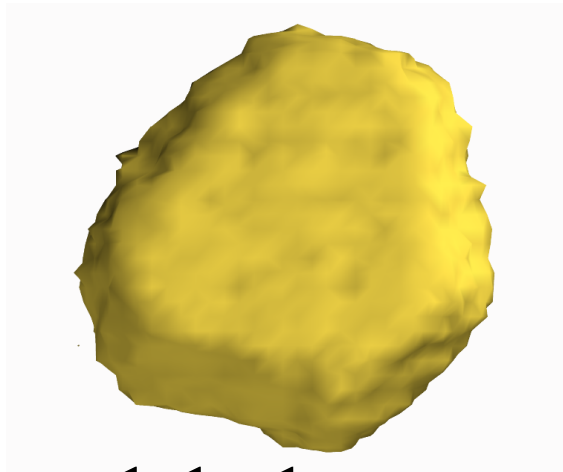
Single Au nanocrystal synthesis



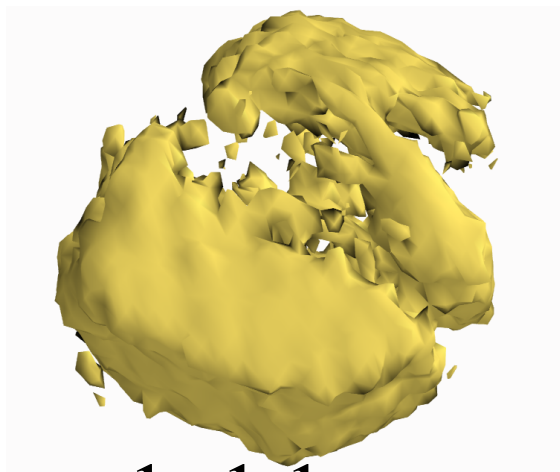
Two views of strain in Au NC

Au409B-52 (11-1) and Au409B-60 (200)

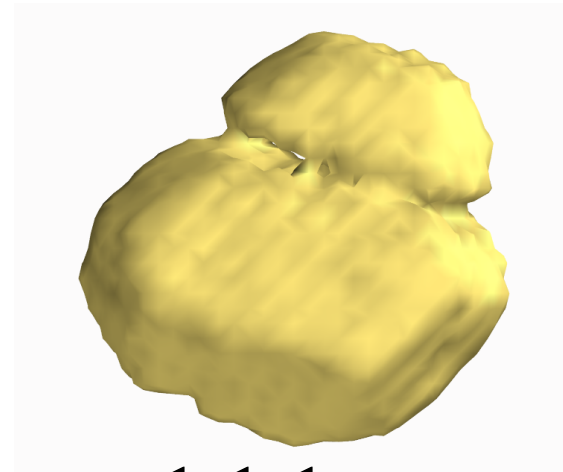




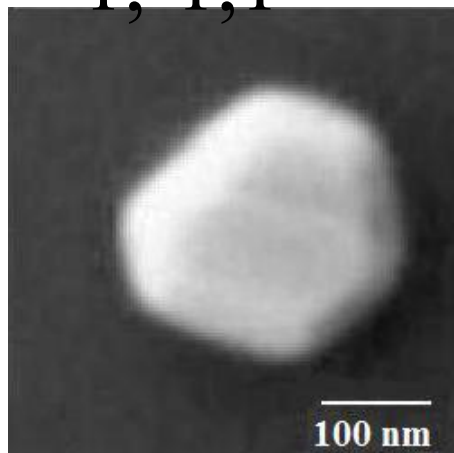
1,1,-1



1,-1,1

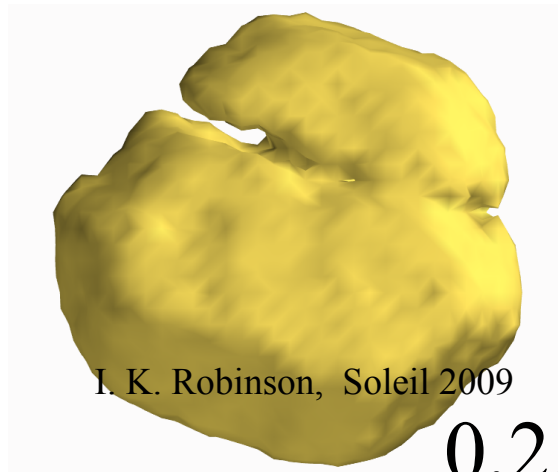
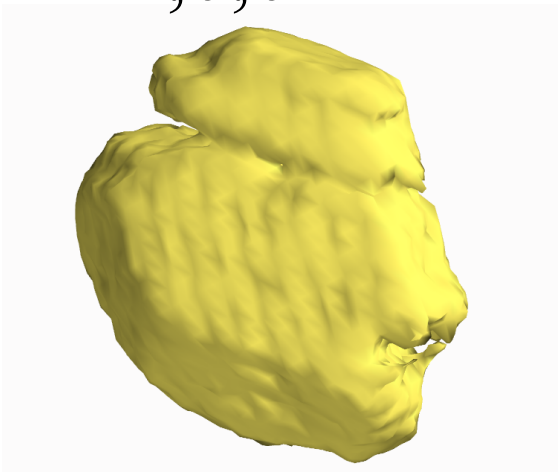


-1,1,1

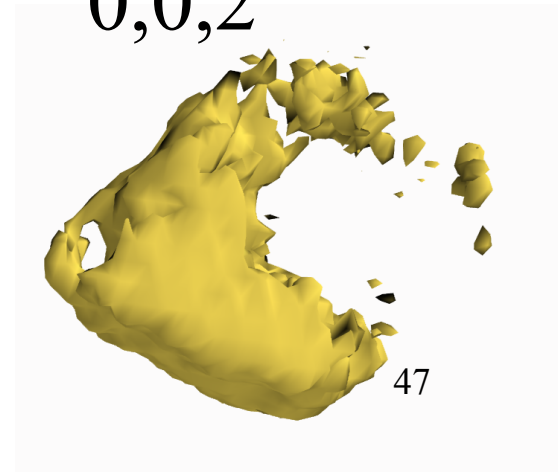


100 nm

2,0,0



0,2,0

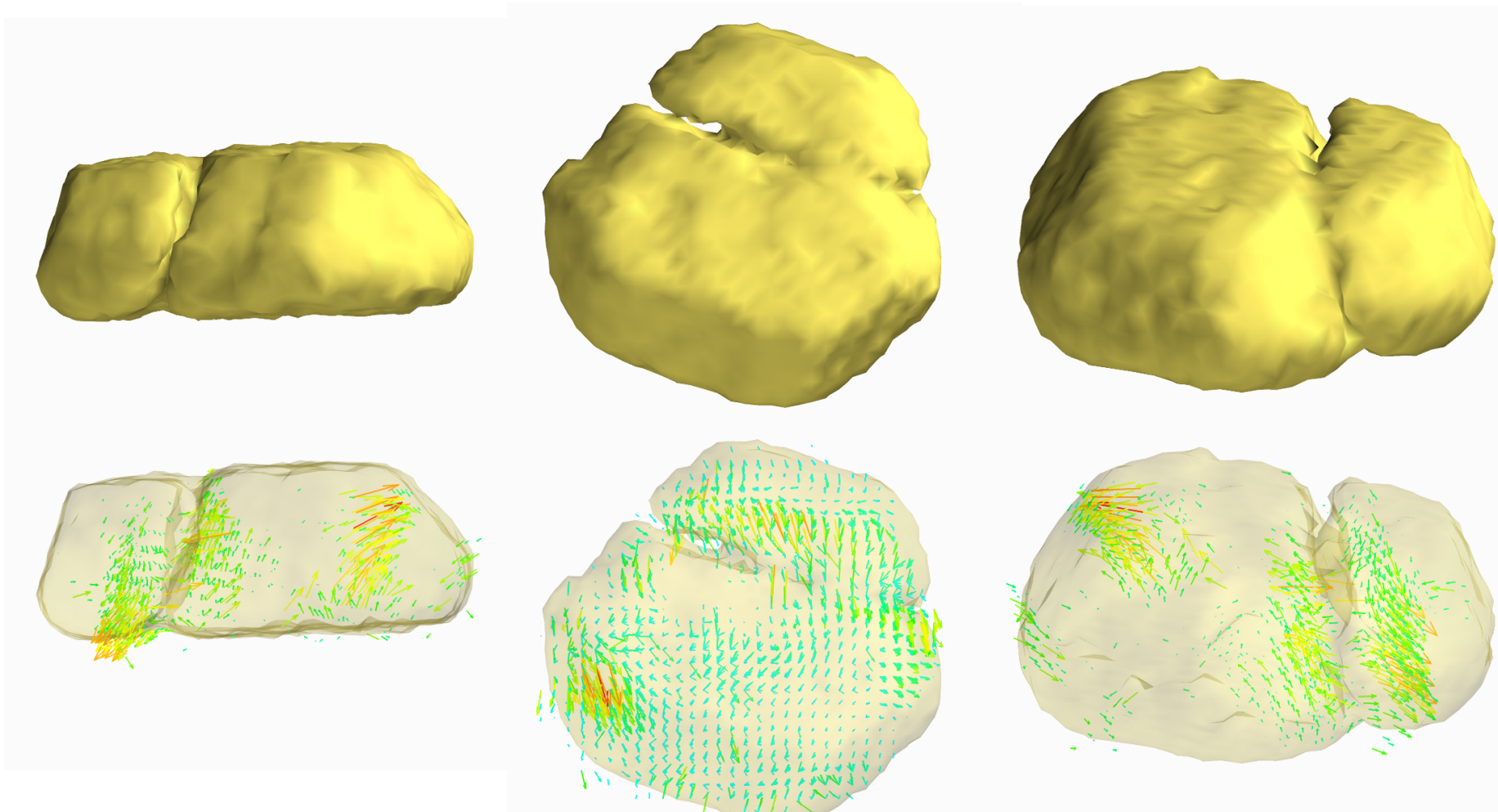


0,0,2

I. K. Robinson, Soleil 2009

Vector displacement field

Merged reconstructions from (11-1) (020) and (-111)



Conclusions

- Internal structure of Nanocrystals
- Phasing by computation instead of lens
- Strain fields imaged from asymmetric patterns
- Contact Forces and Surface Strains
- Full Strain Tensor accessible
- Partial Coherence affects Image Quality