

Materials Science on the Nanoscale using Coherent X-ray Diffraction

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London Centre for Nanotechnology

Diamond Light Source

SLS Colloquium,

Paul Scherrer Institut, Dec 14 2007

Outline

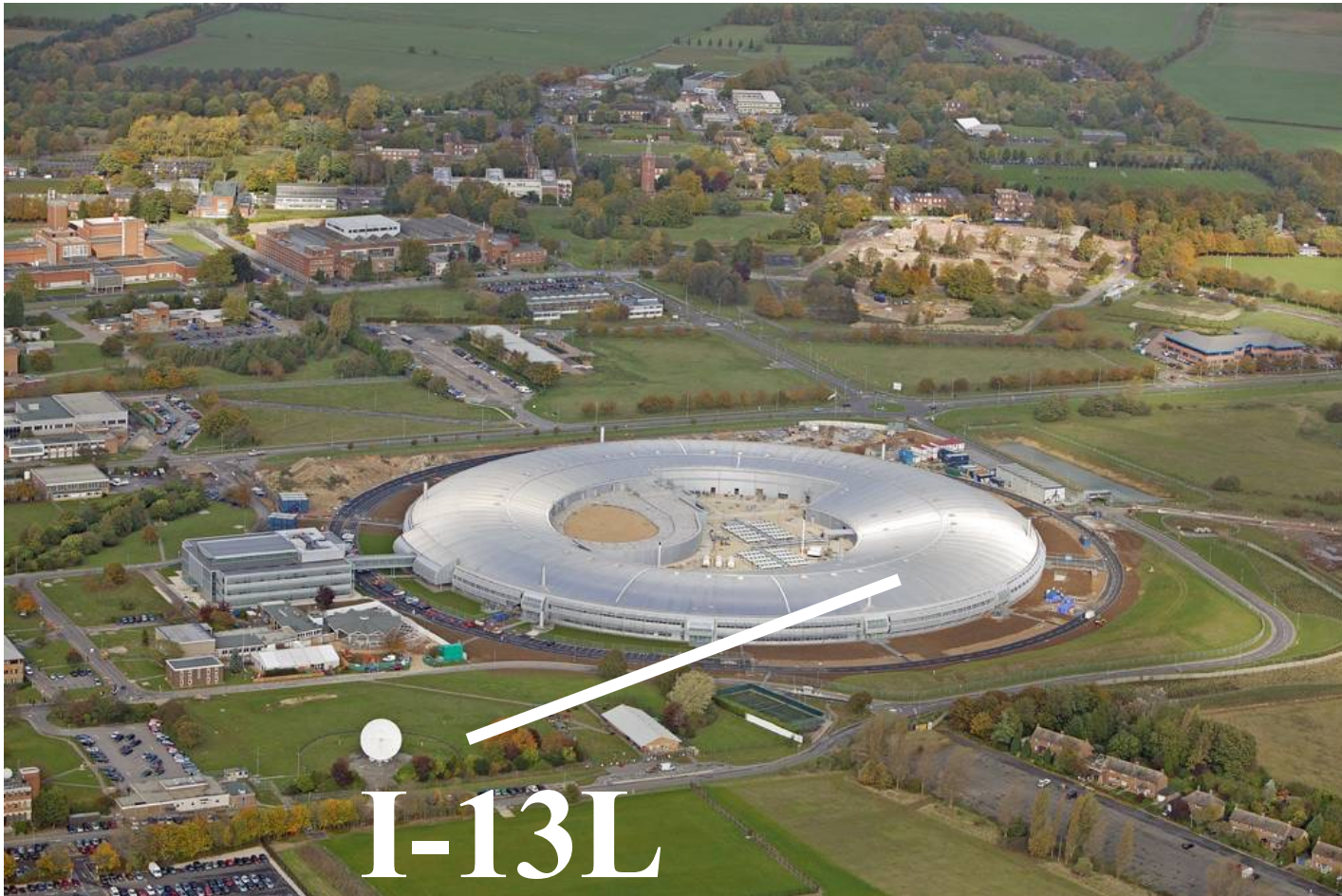
- Coherent x-ray diffraction
- CXD can solve the **phase** problem
- Nanocrystal structures
- Extension to **phase** objects
- Exploration of crystal strain
- Nanowire structures

London Centre for Nanotechnology

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

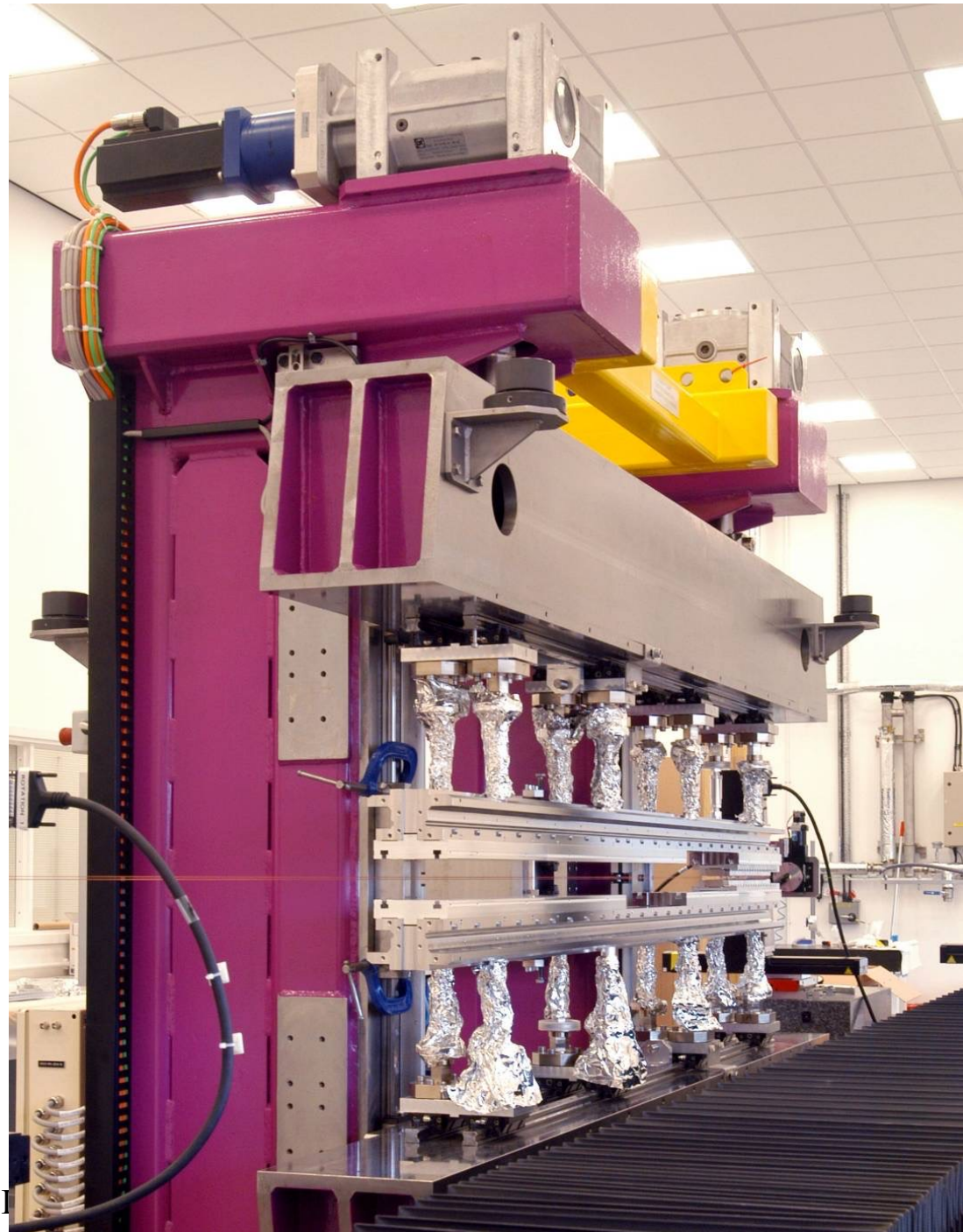


Diamond Light Source (RAL)

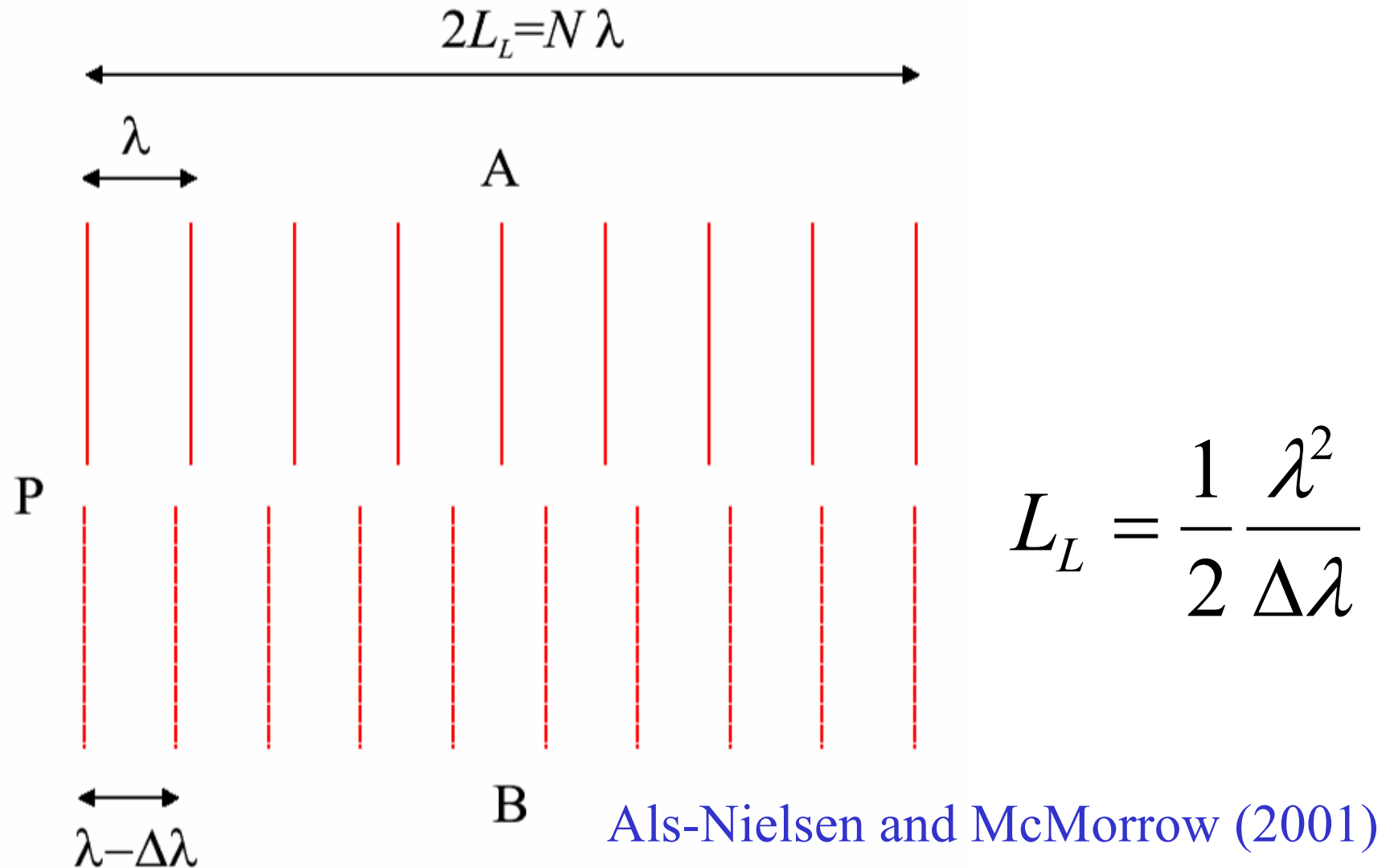


I. K. Robinson, SLS Dec 2007

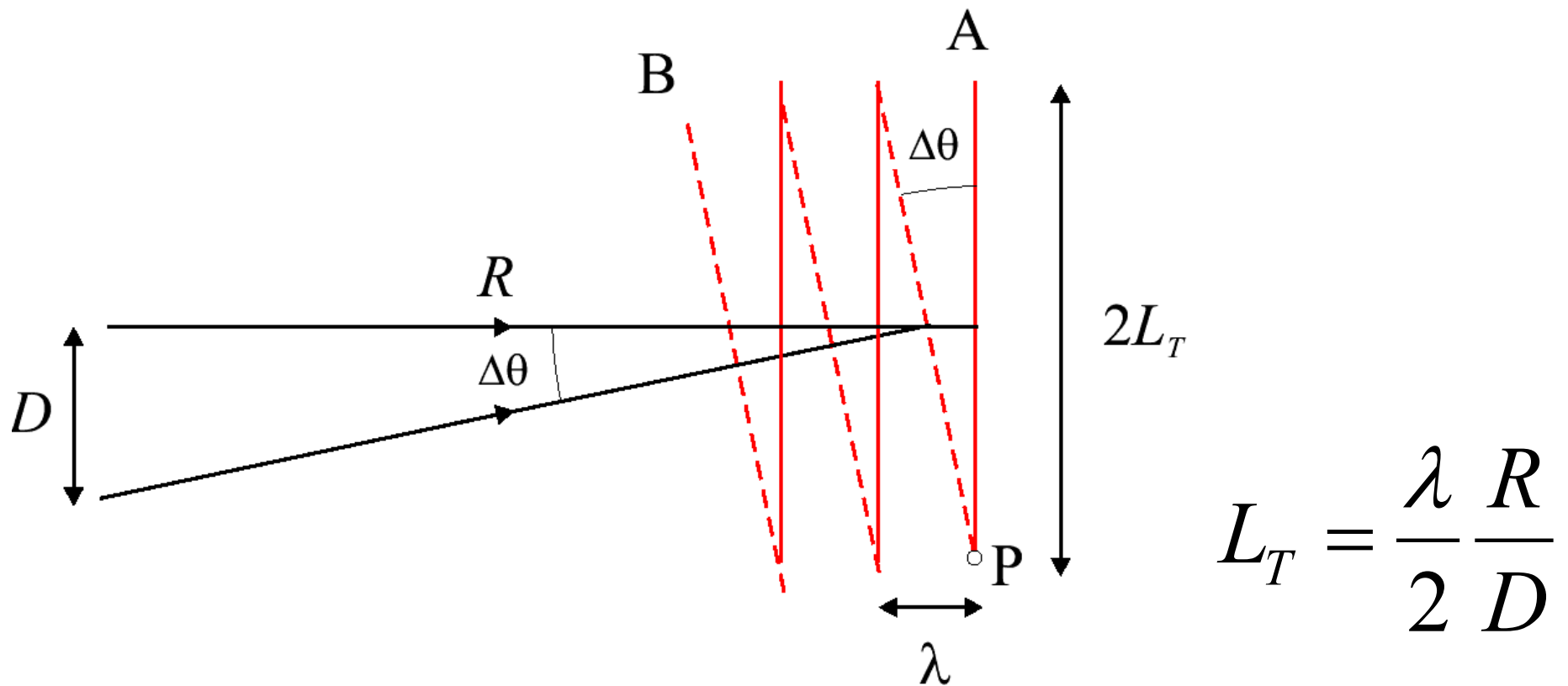
Diamond
in-vacuum
X-ray
Undulator



Longitudinal Coherence



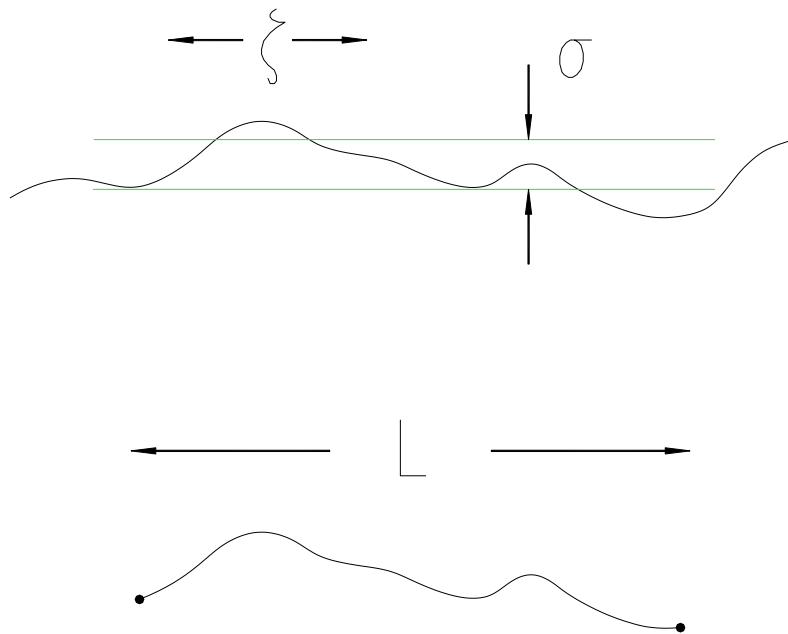
Lateral (Transverse) Coherence



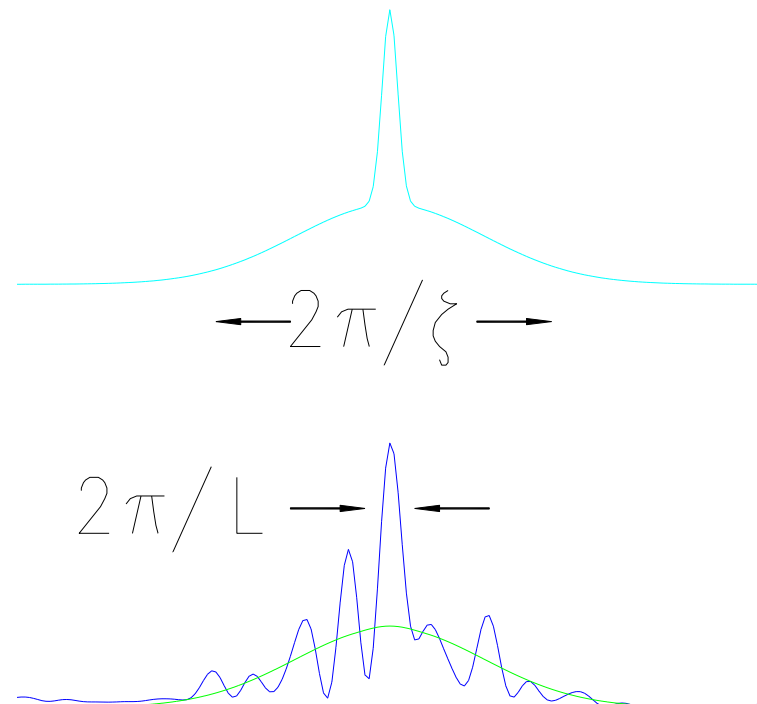
Als-Nielsen and McMorrow (2001)

Diffuse Scattering acquires fine structure with a Coherent Beam

Real Space

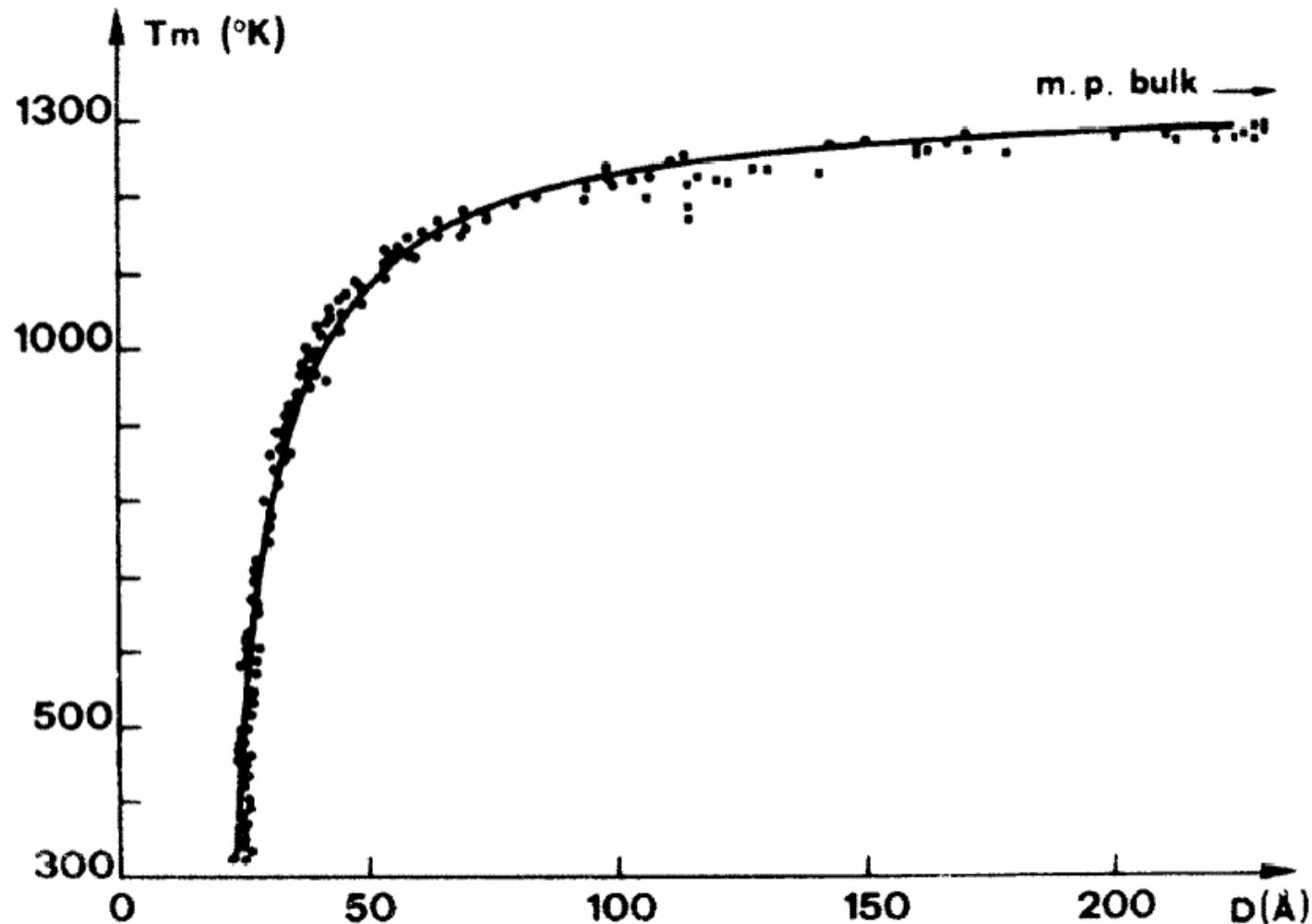


Reciprocal Space

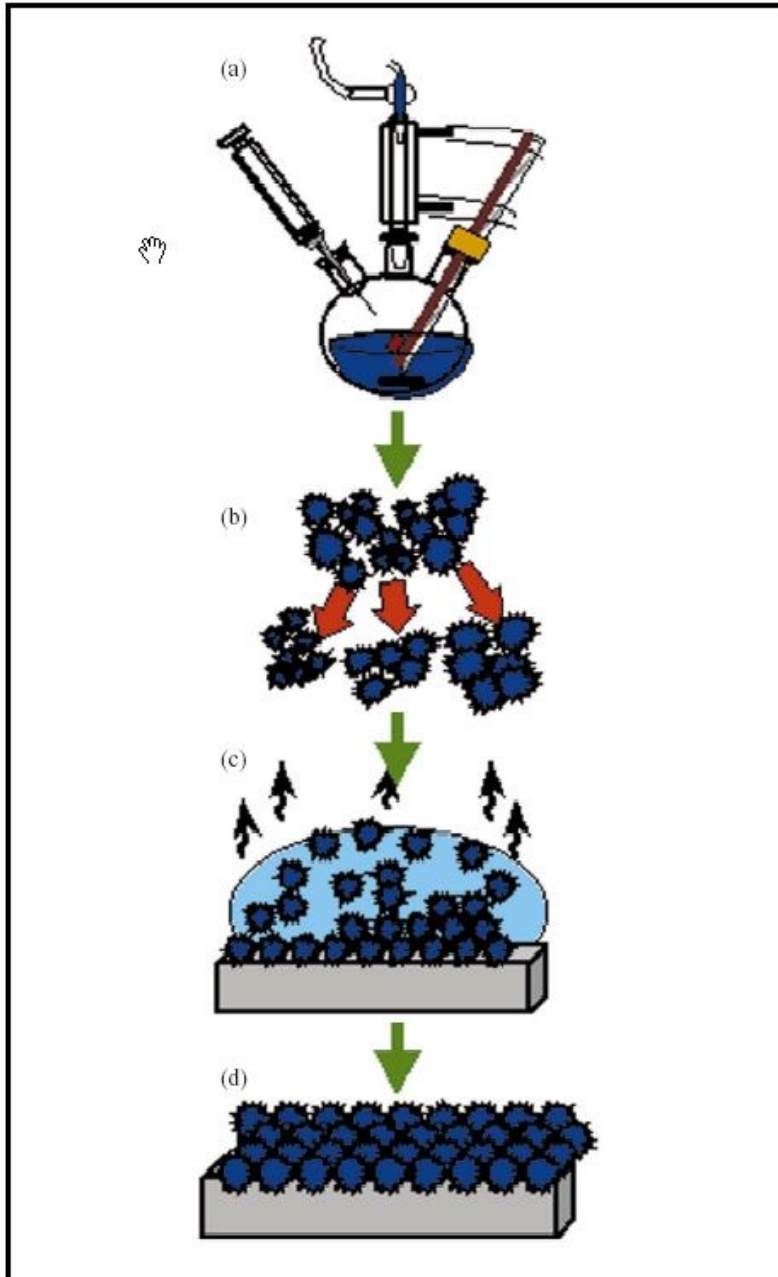


Size-dependent Melting of Au Particles

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

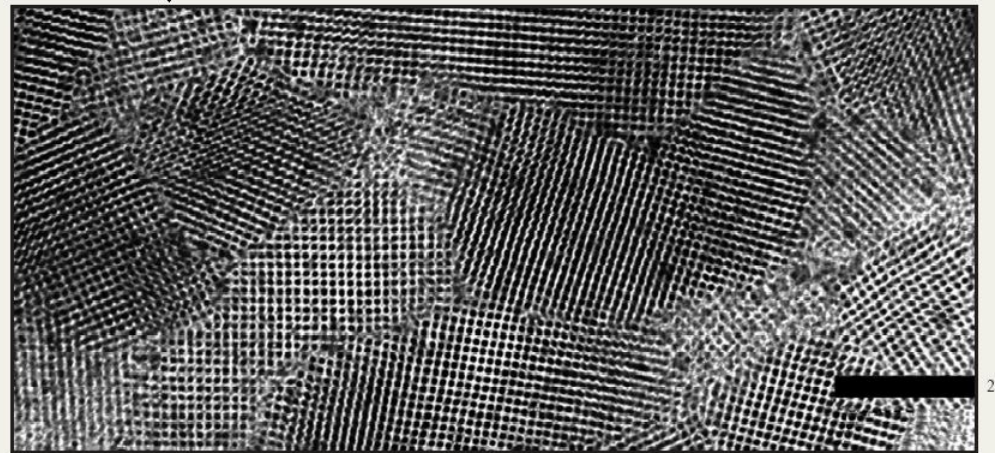


Chemical Synthesis of Nanocrystals

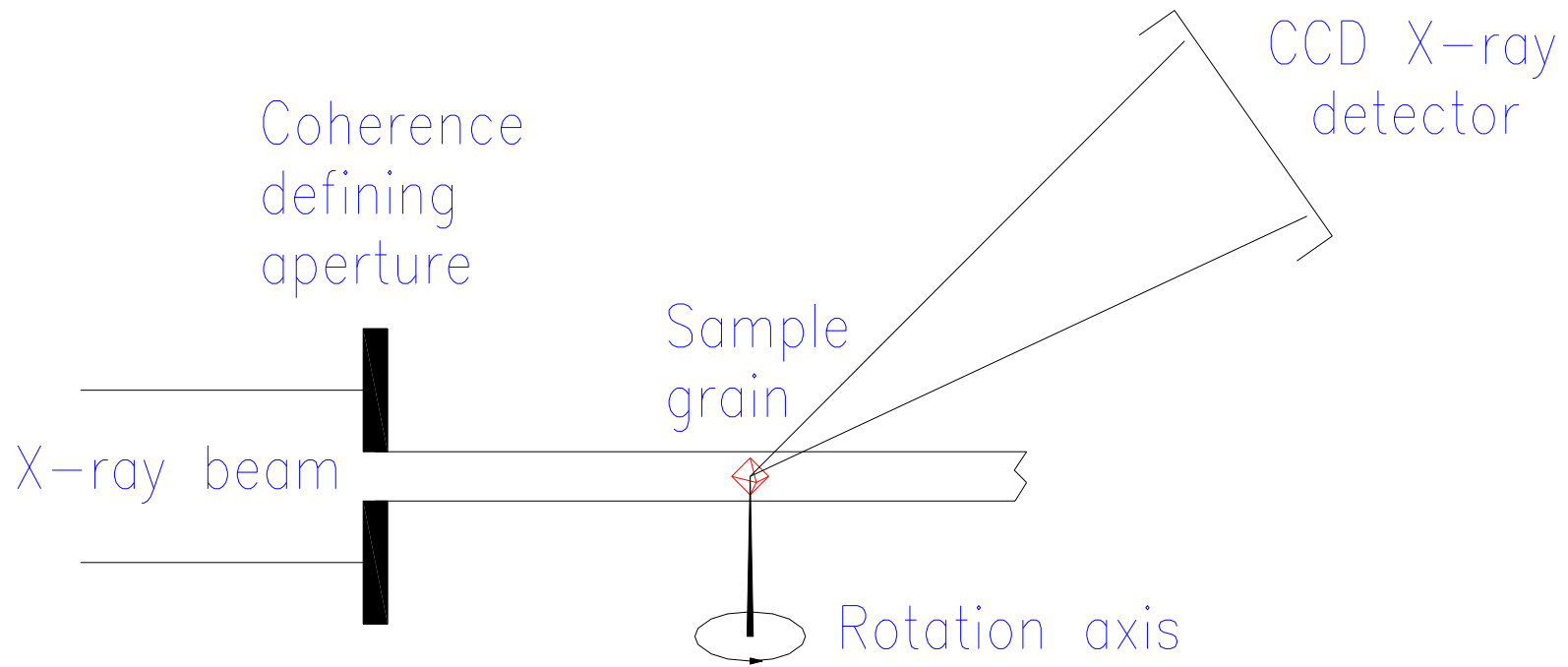


- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

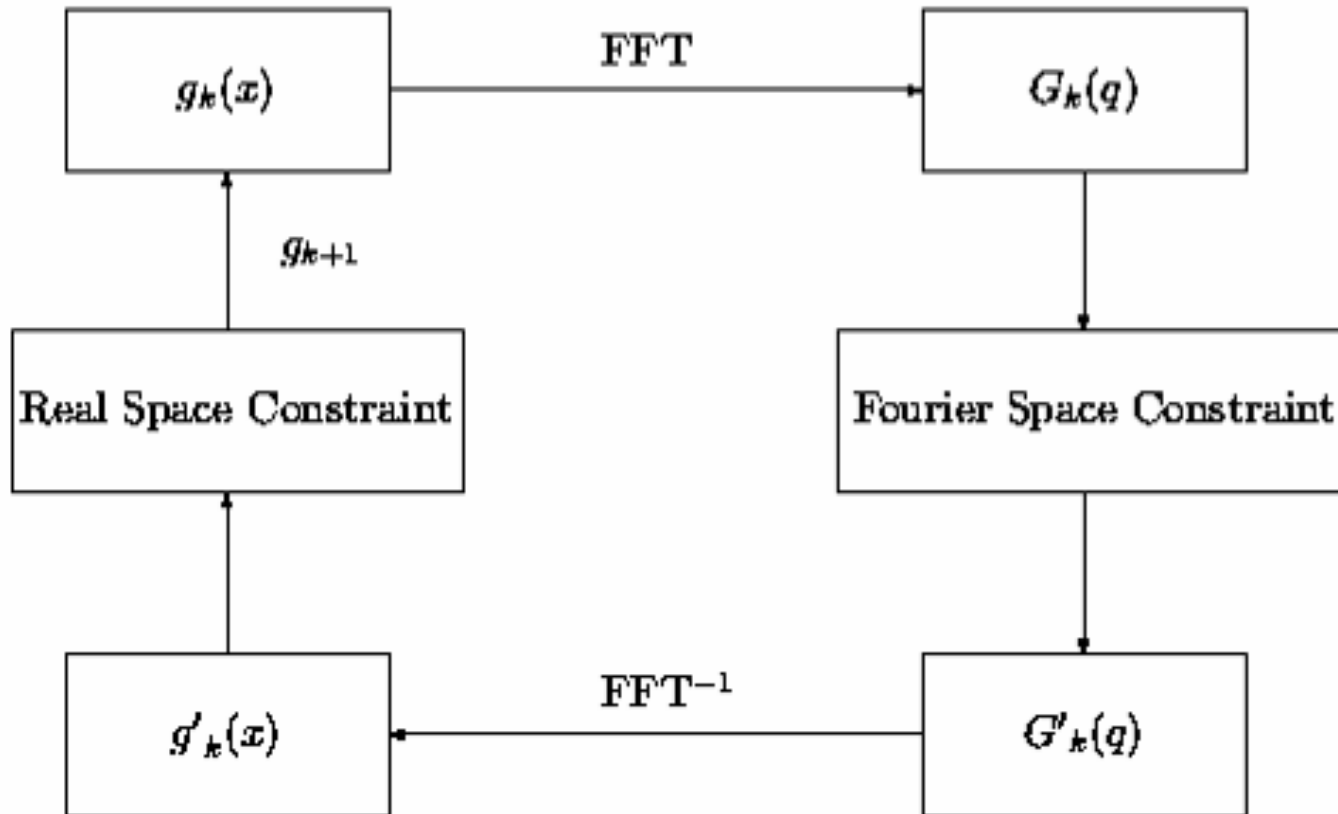
C. B. Murray, IBM J. Res. & Dev. **45**
47 (2001)



Lensless X-ray Microscope

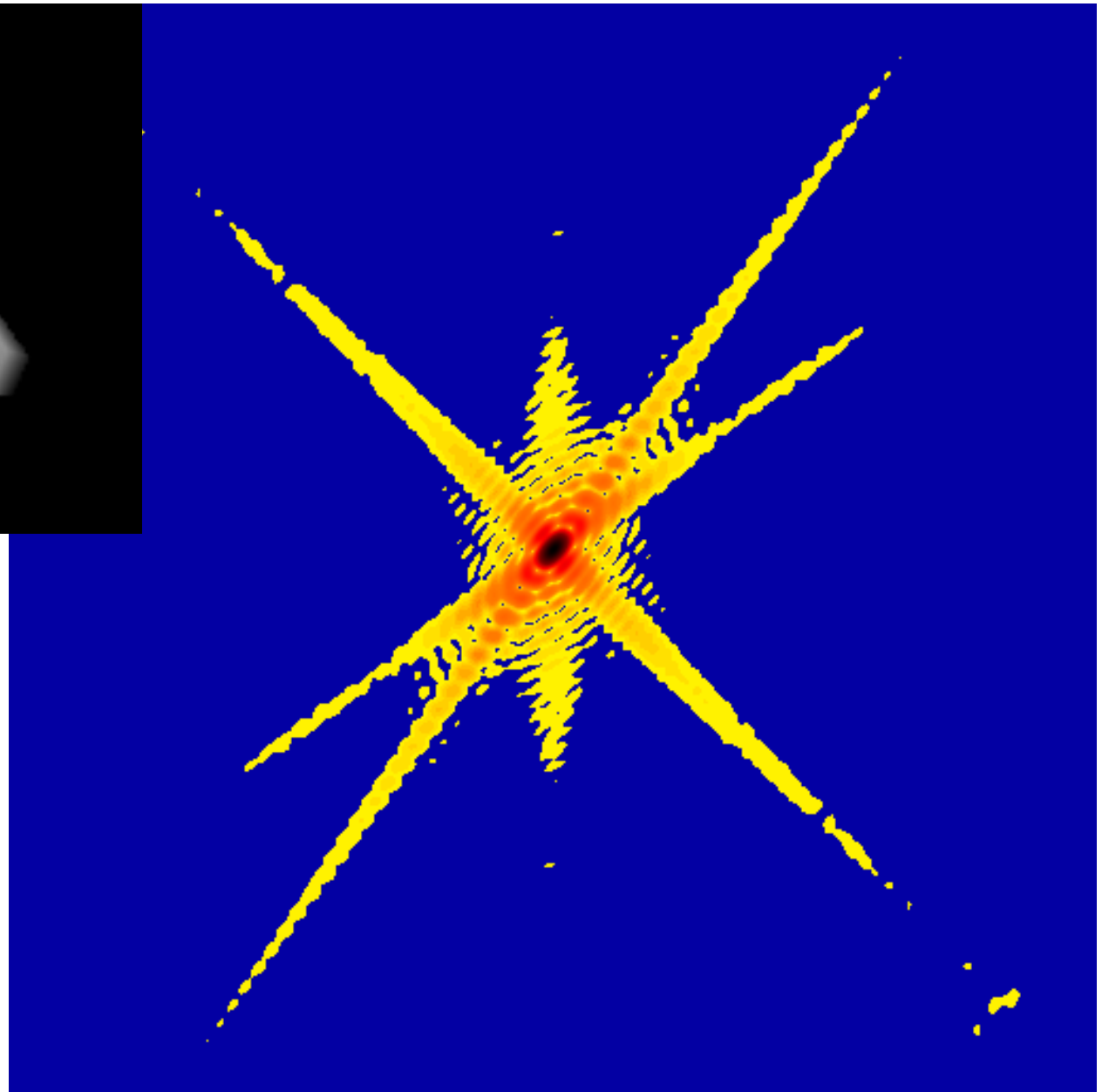
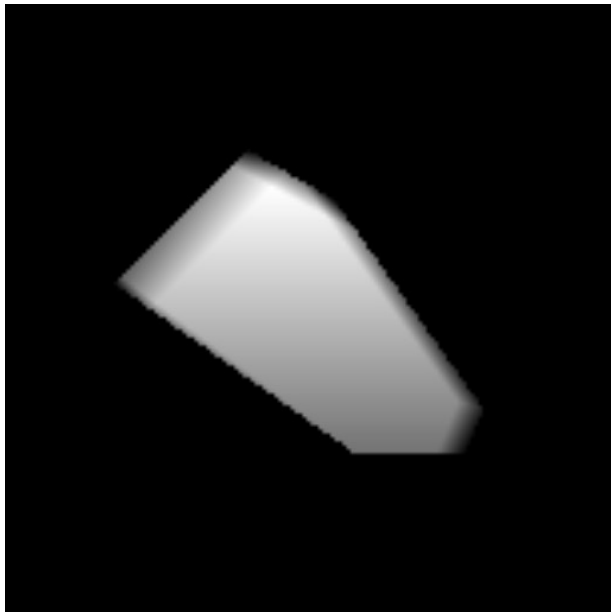


Generic “Error Reduction” method

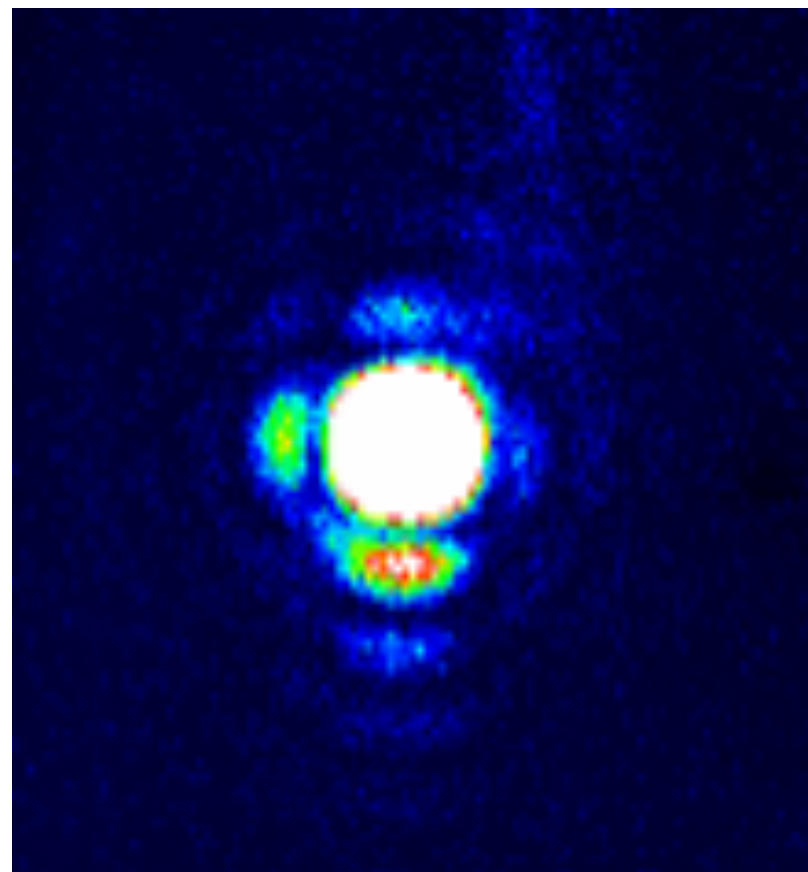
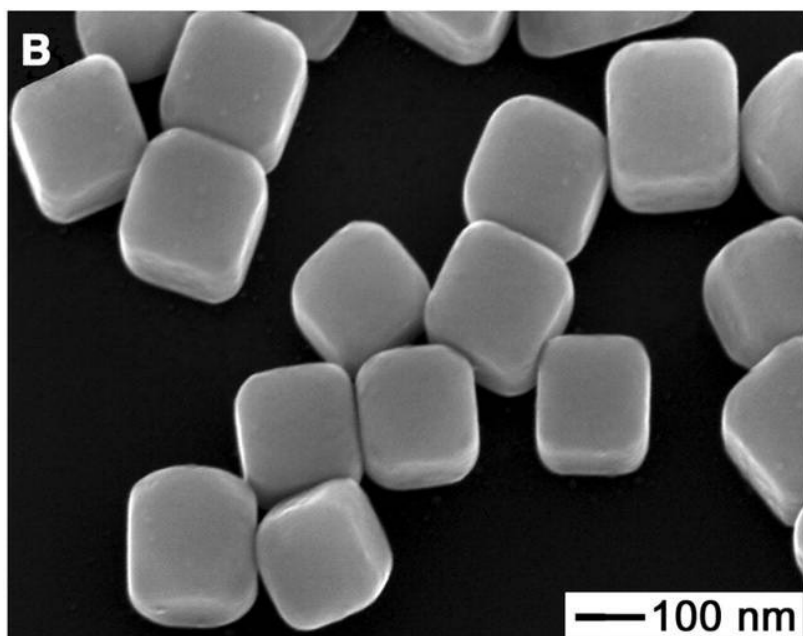


J. R. Fienup *Appl. Opt.* 21 2758 (1982)

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

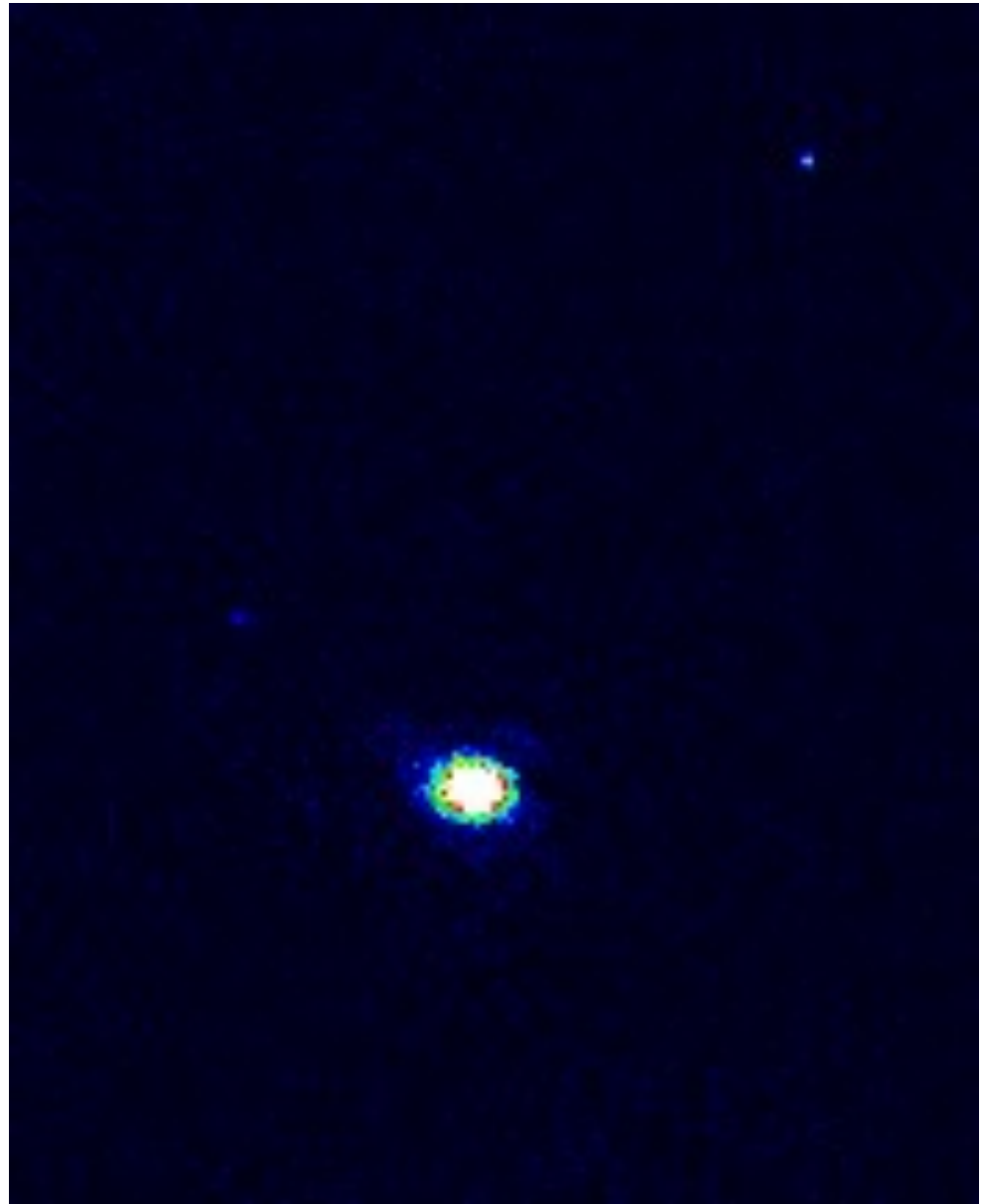


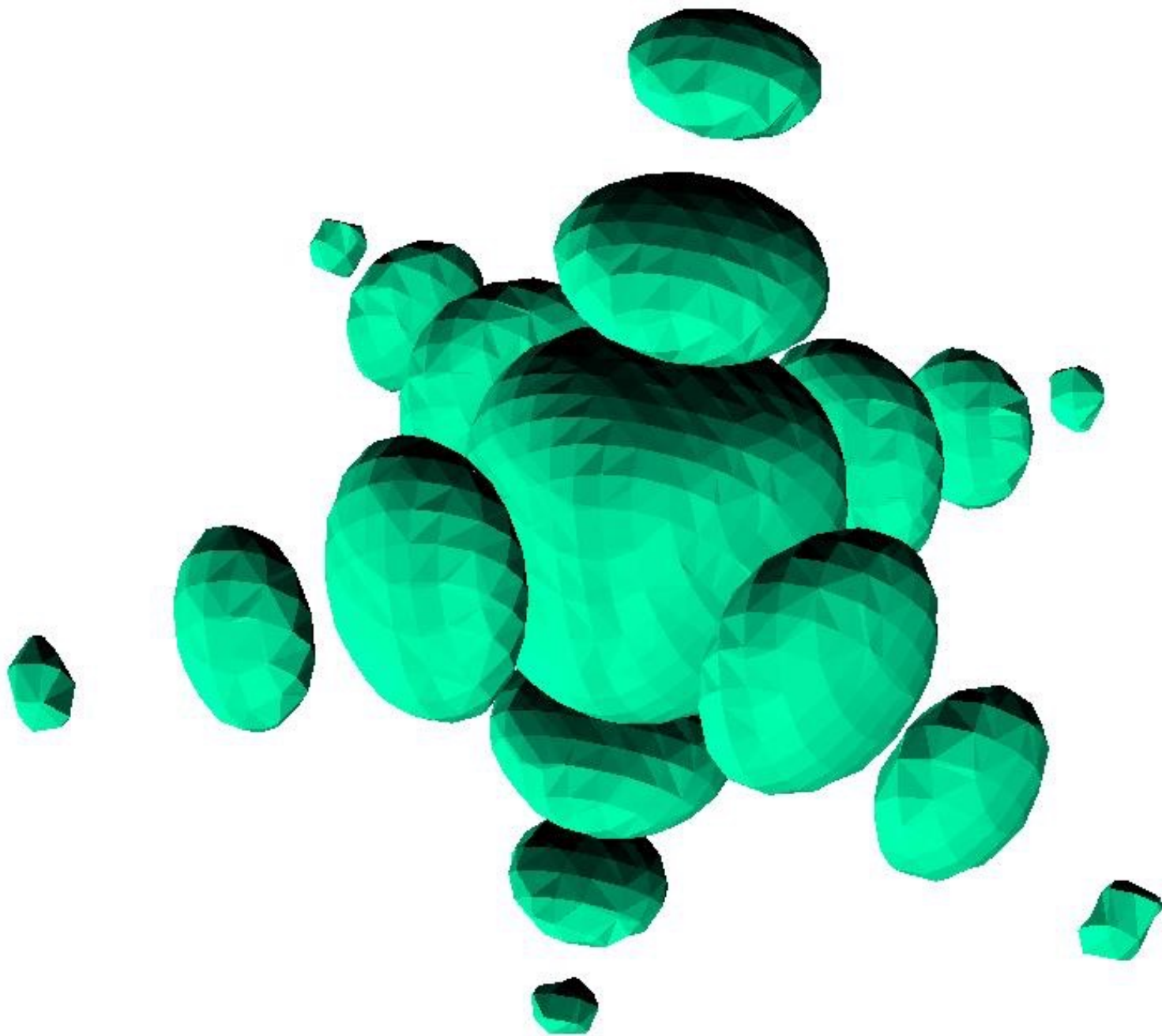
Chemically Synthesized Silver Nanocubes

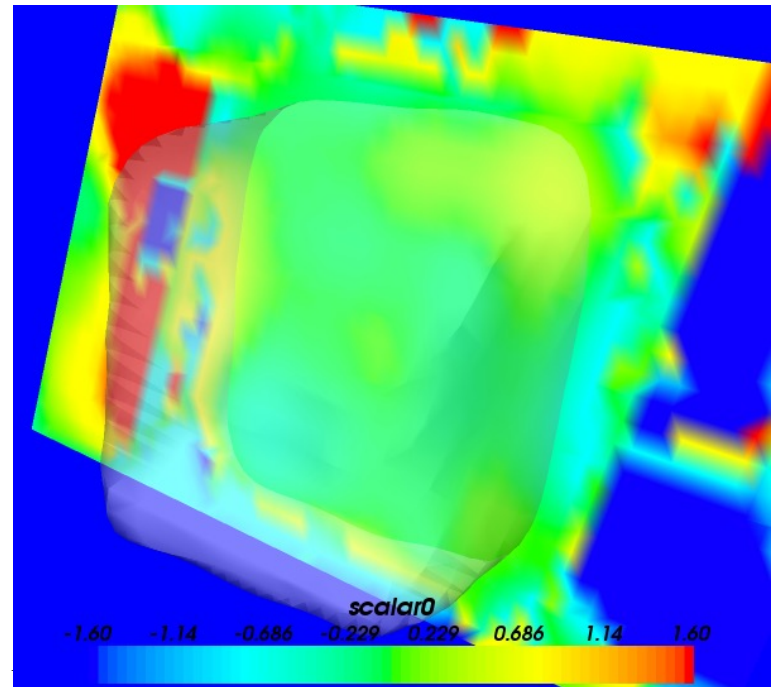
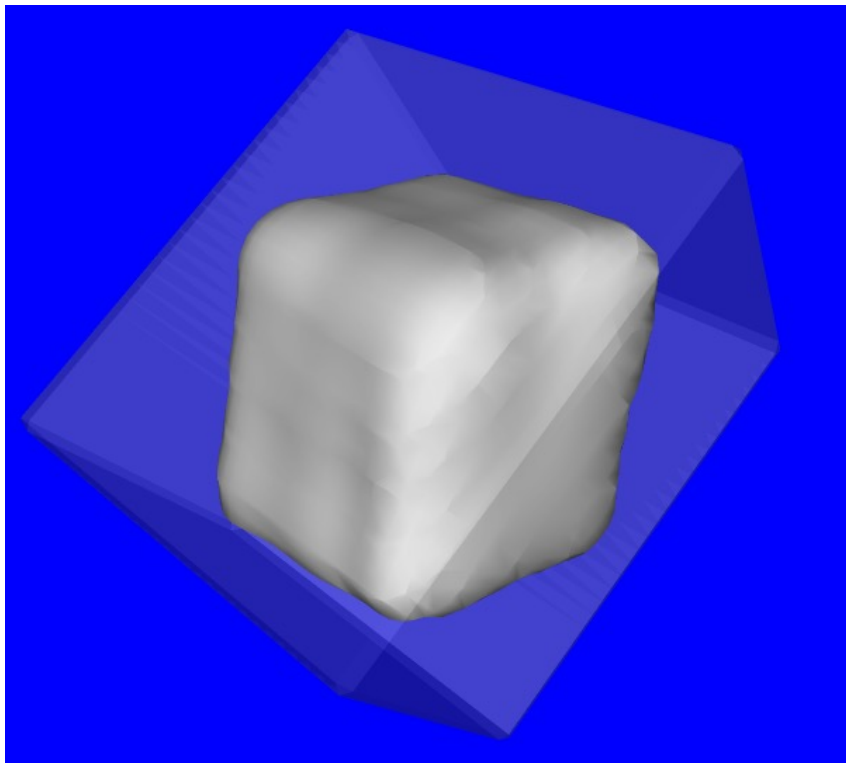
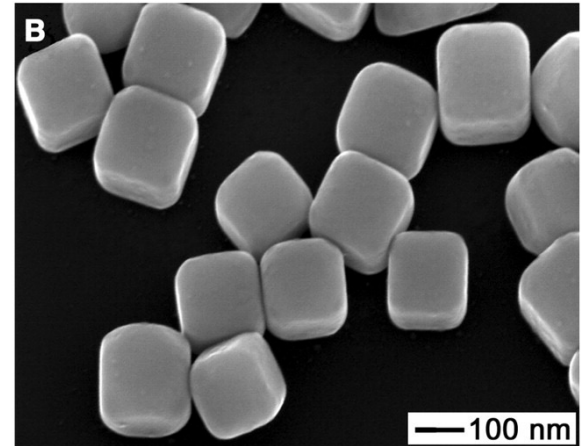
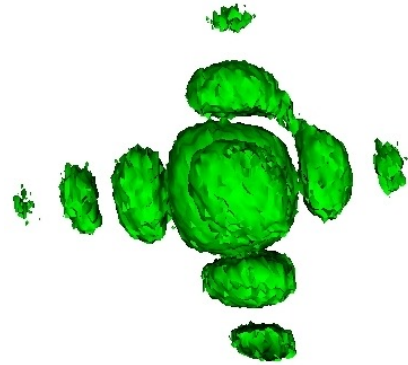
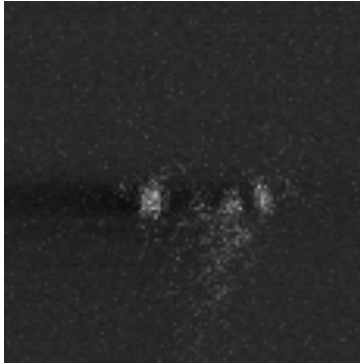


Yugang Sun and Younan Xia,
Science 298 2177 (2003)

Rocking
scan of Ag
cubes with
 0.01° steps

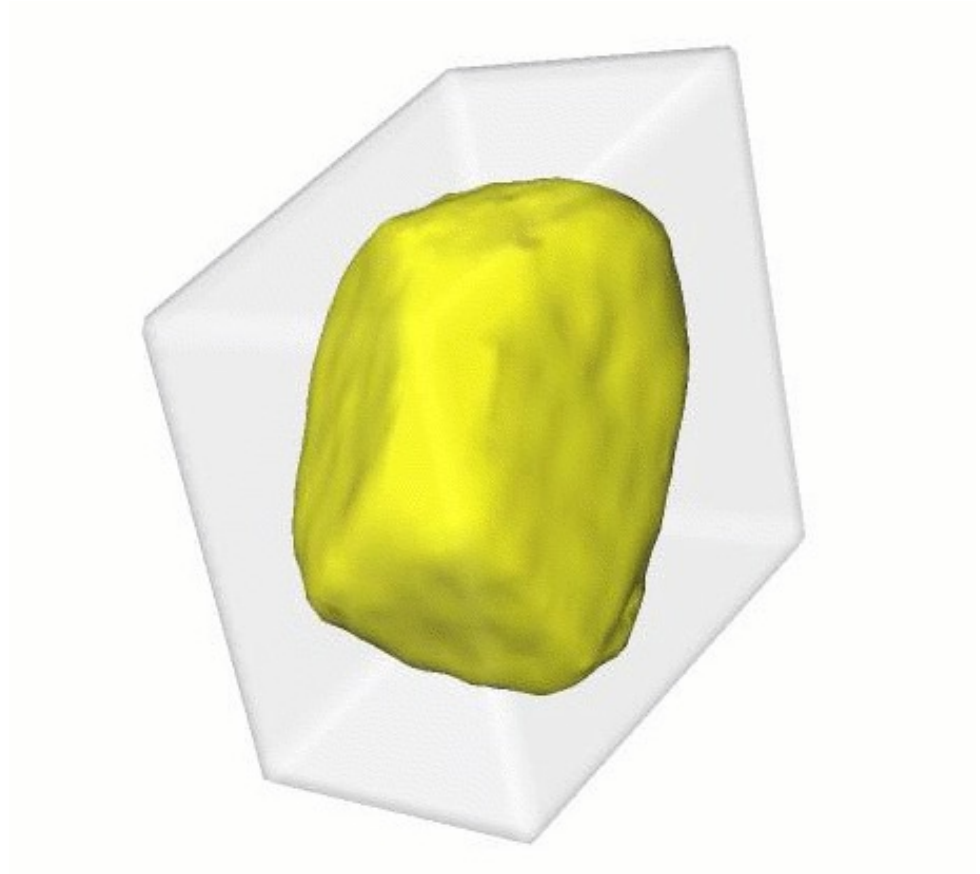
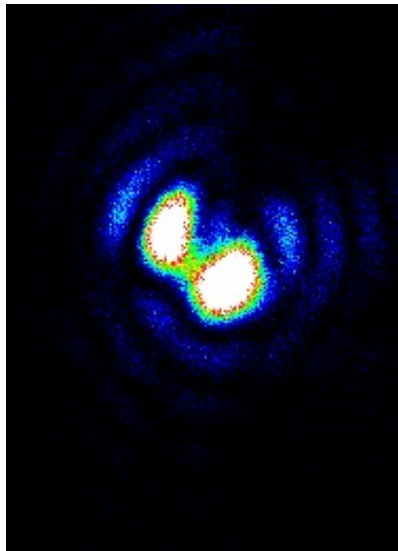




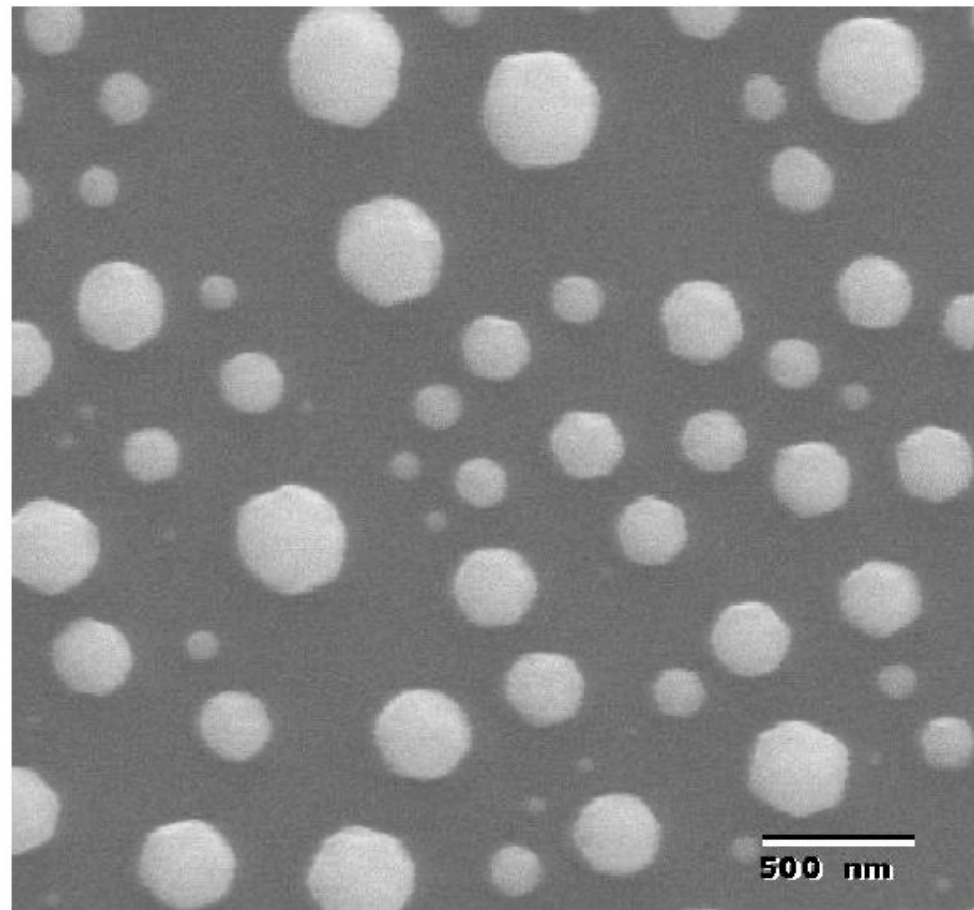
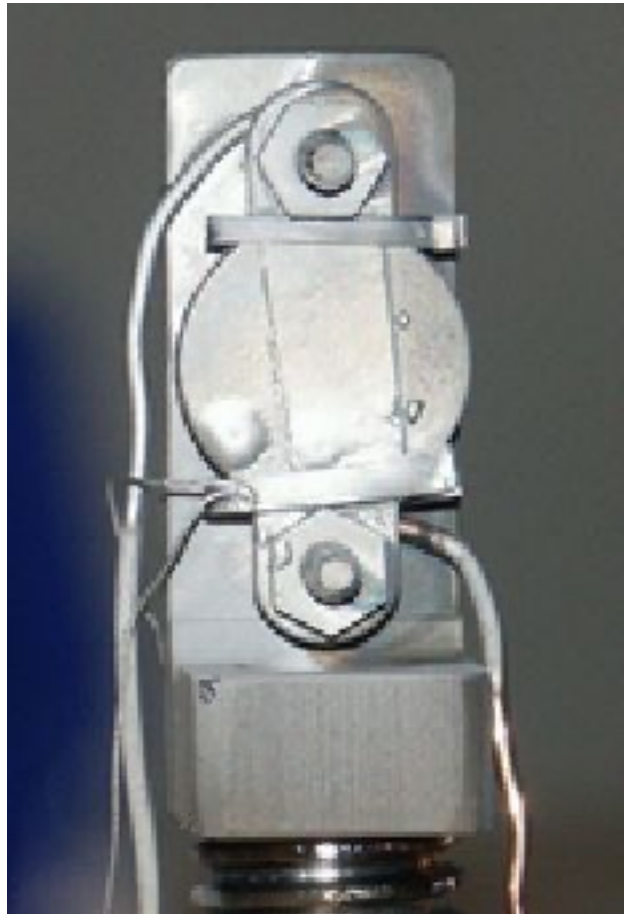


Gold nanocrystal reconstruction

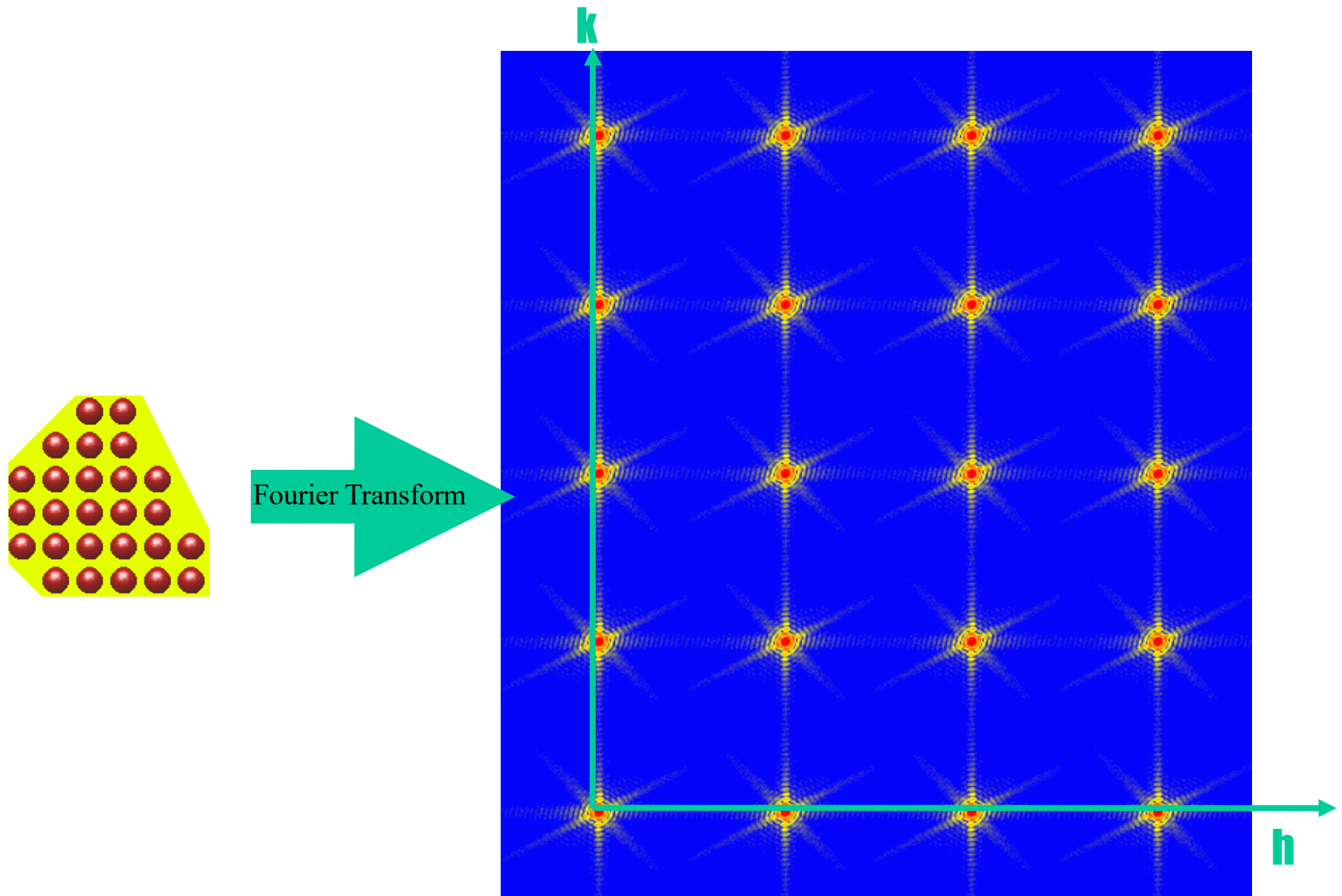
showing support used for 20 HIO followed by 10 ER



In situ growth of Pb crystals



Coherent Diffraction from Crystals

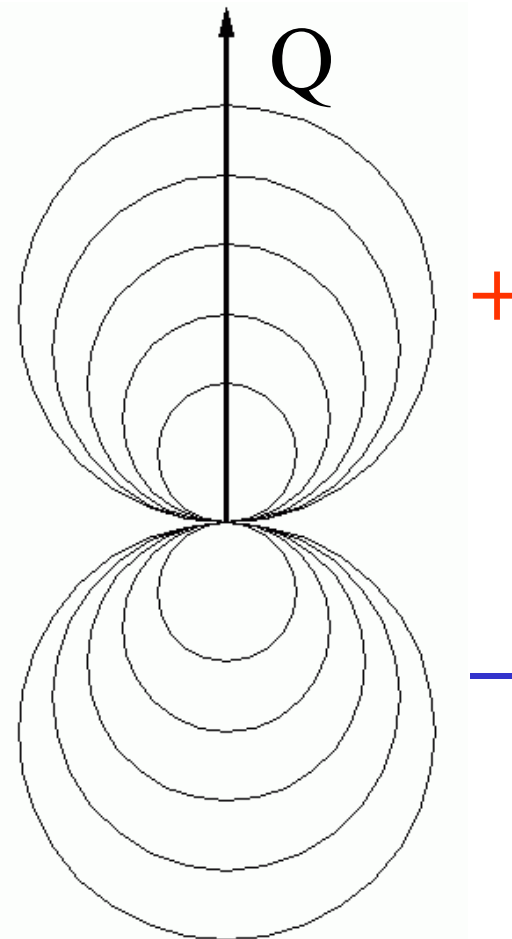
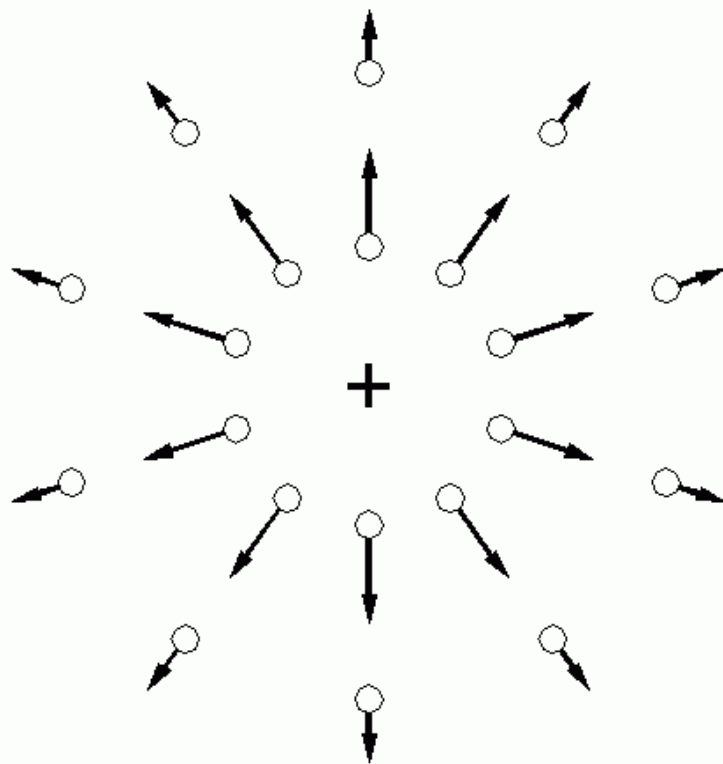


Diffraction by Strain of Point Defect

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

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

Imaginary density



Good statistics, 3D diffraction data

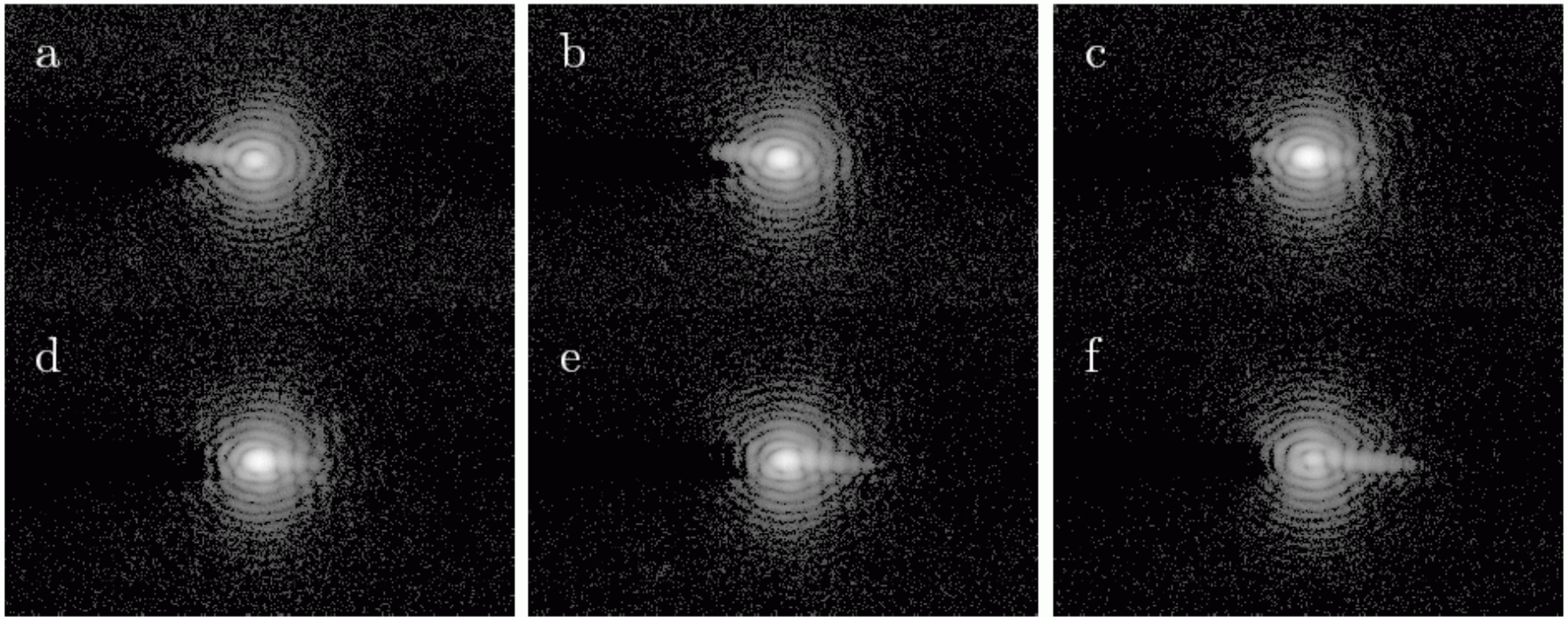
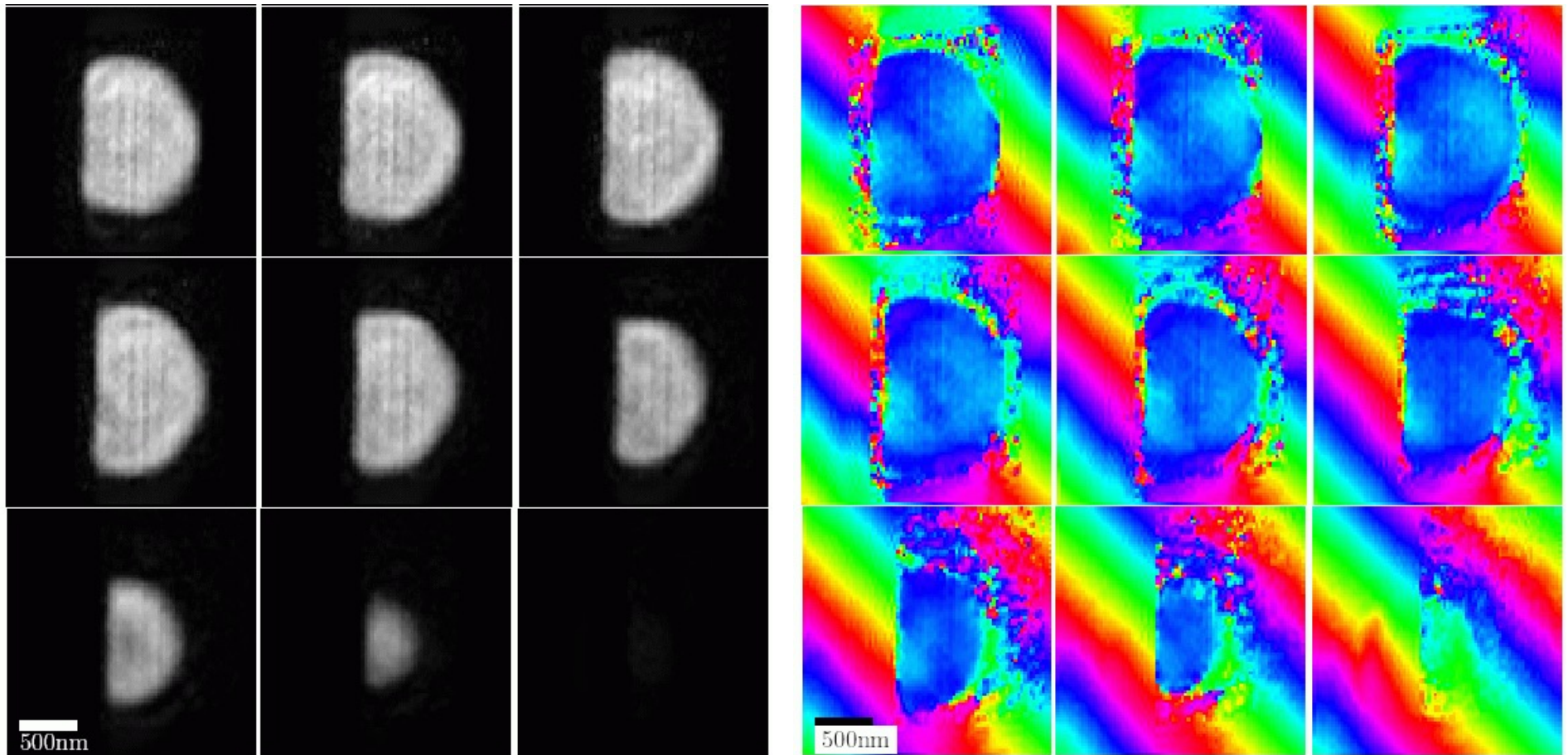
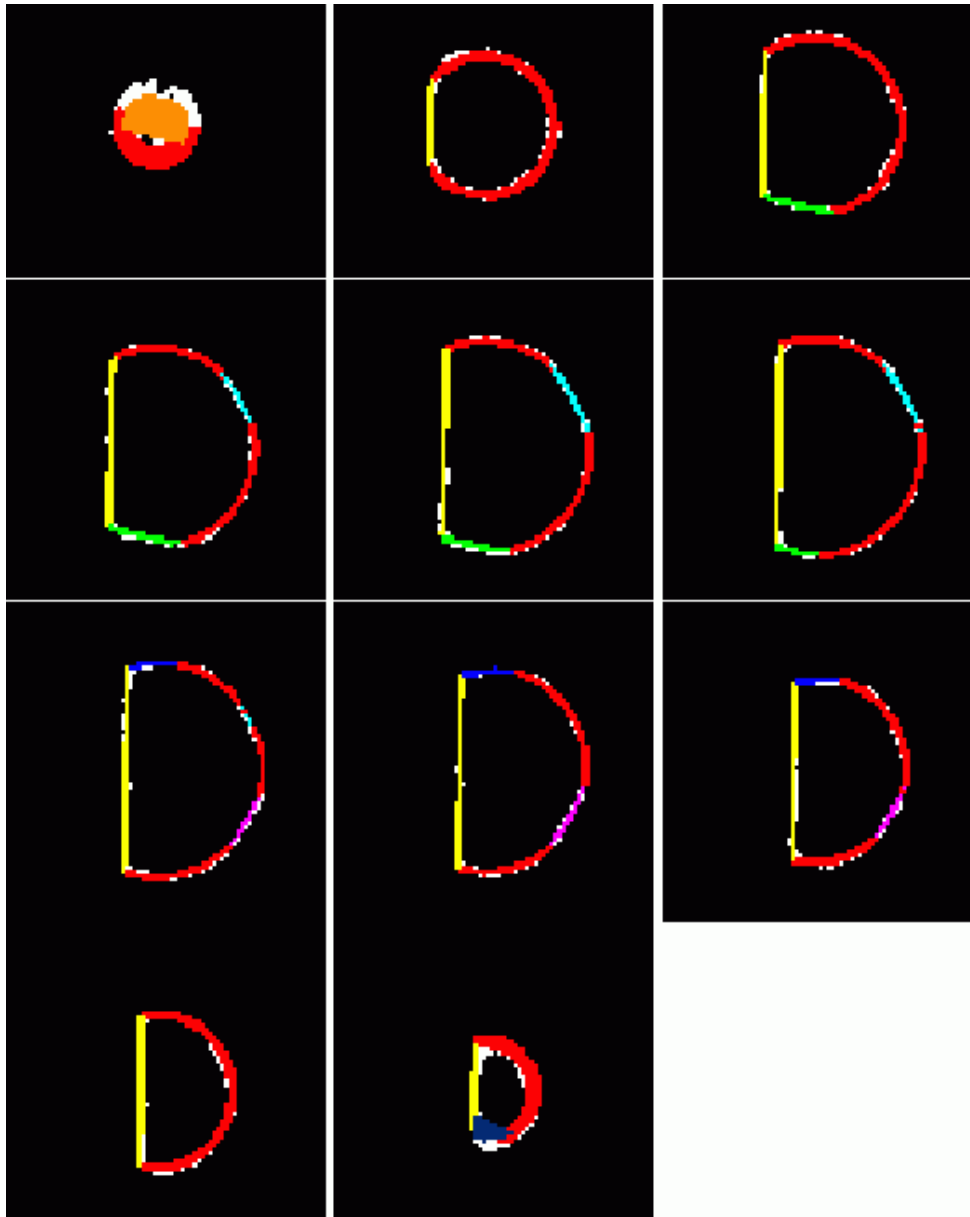









Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

Complex Density (amplitude *and* phase)

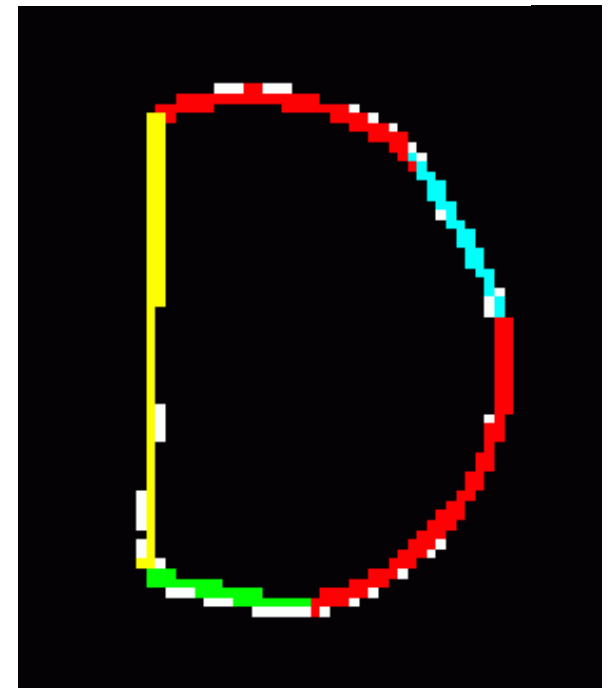


Fitting to faceted shape

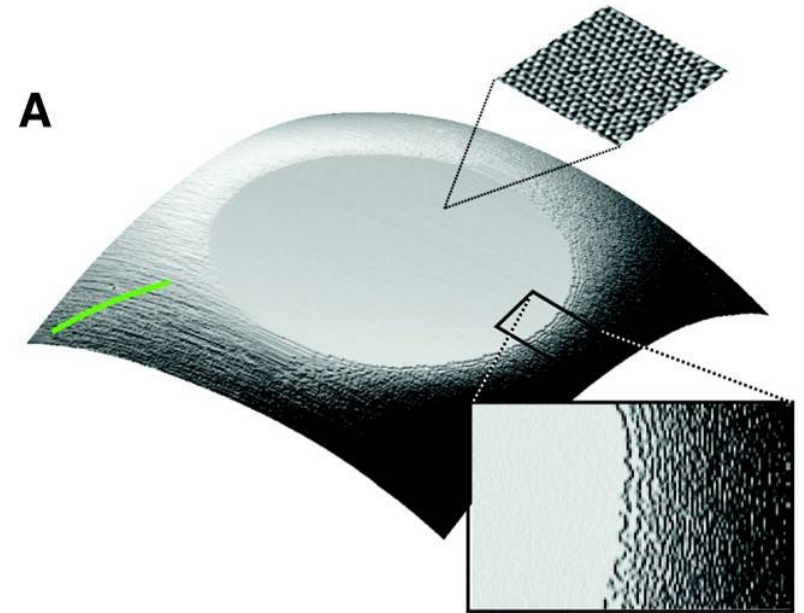
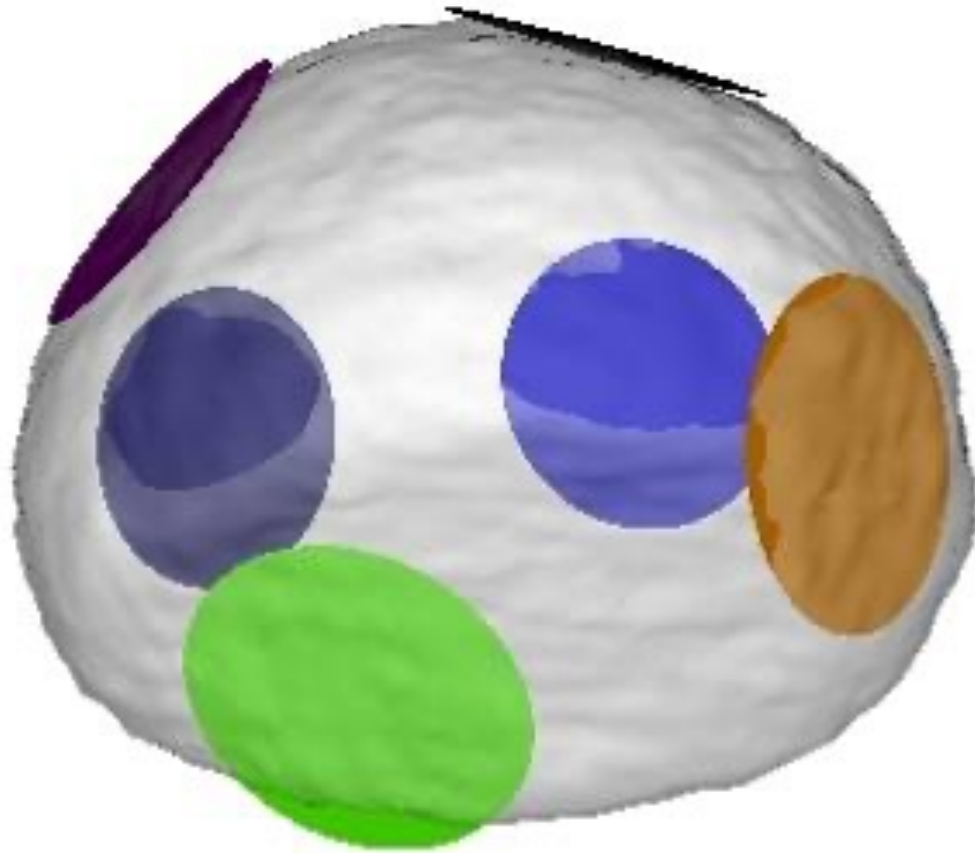


	$ R $		P0	P1	P2	P3	P4	P5	P6
	9.4	P0	0	85	149	79	134	106	71
	25.7	P1		0	123	164	83	76	102
	25.1	P2			0	72	67	74	110
	25.9	P3				0	111	106	76
	25.4	P4					0	113	68
	25.4	P5						0	176
	26.0	P6							0 0

Angles between facets

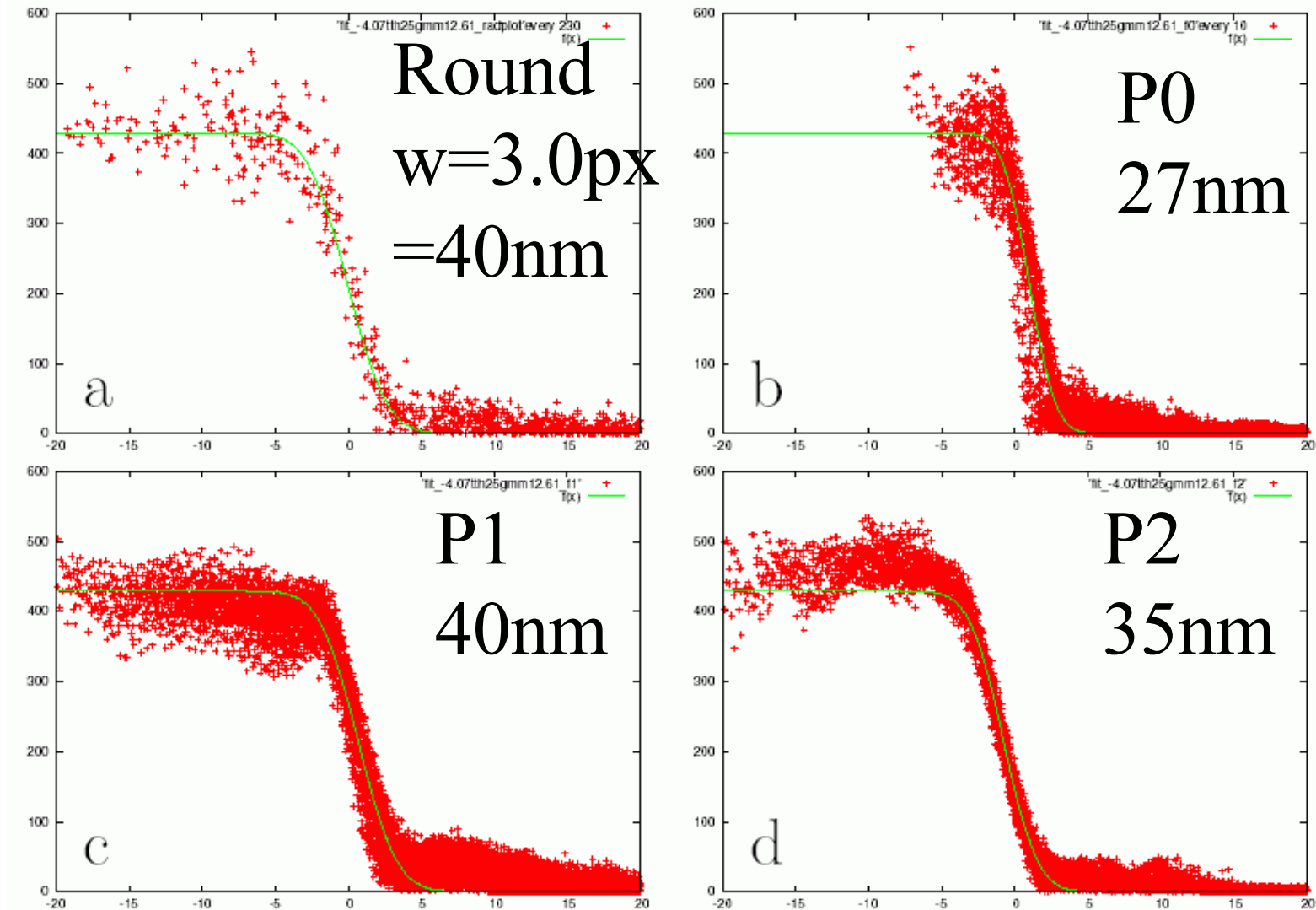


Facets of Equilibrium Crystal Shape

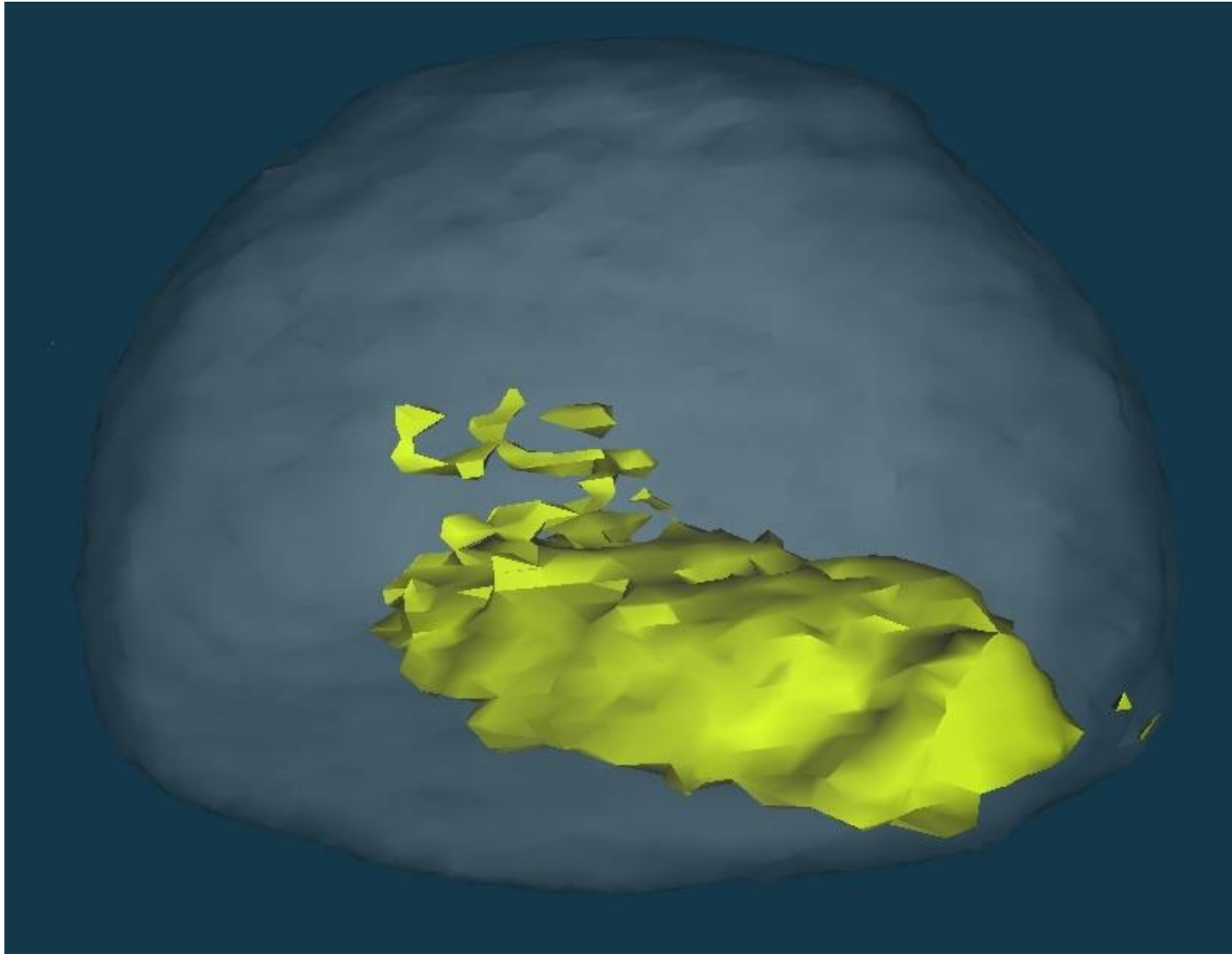


Thurmer K, Williams E, Reutt-Robey J
Science **297** 2033 (2002)

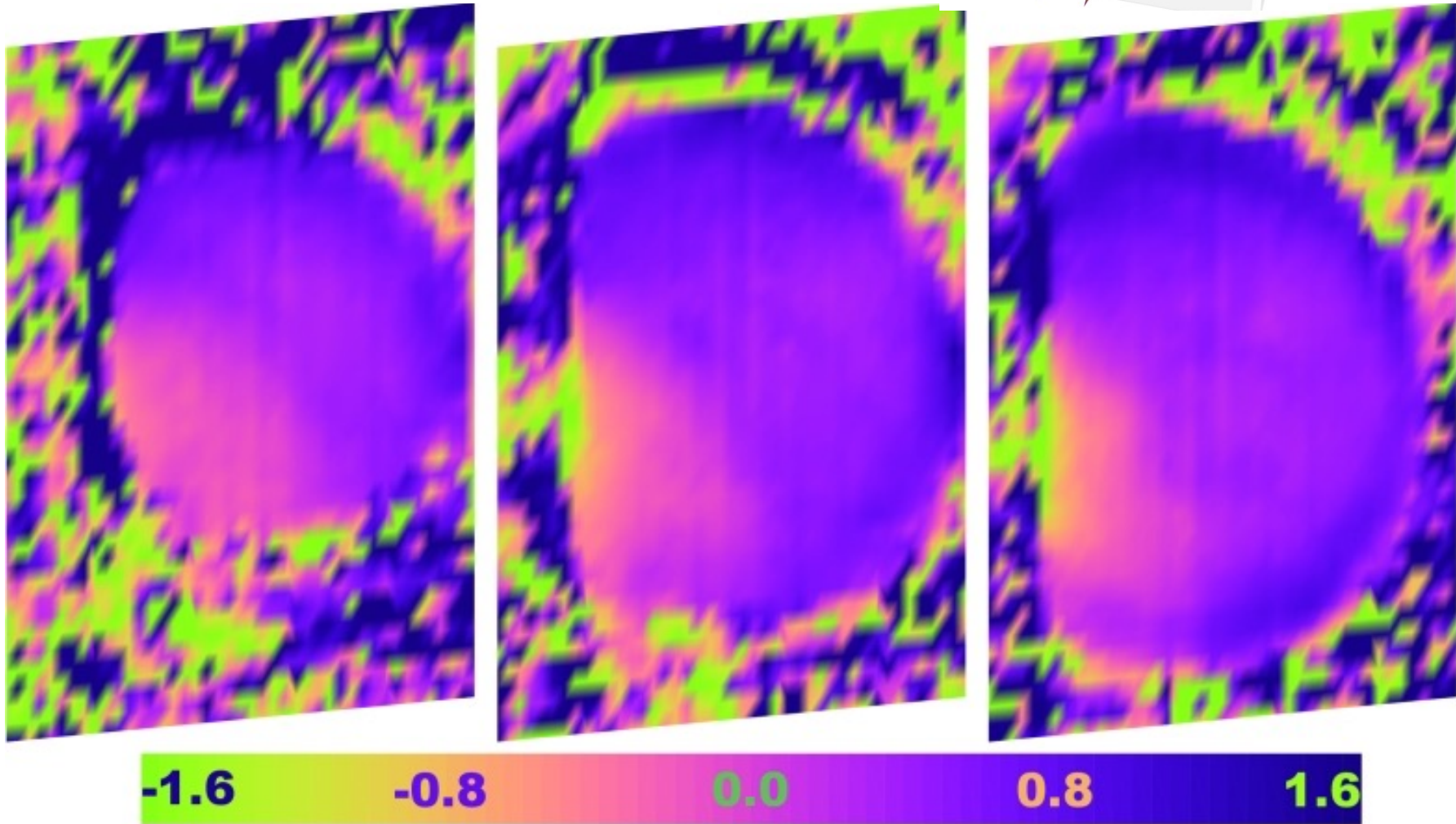
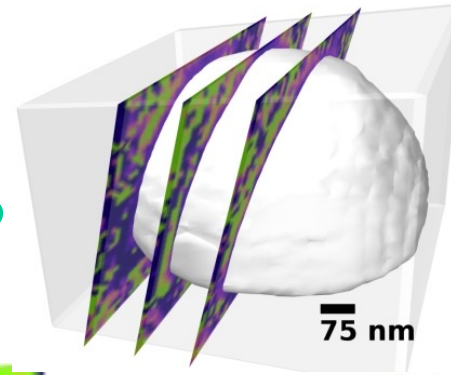
Density distribution across surface



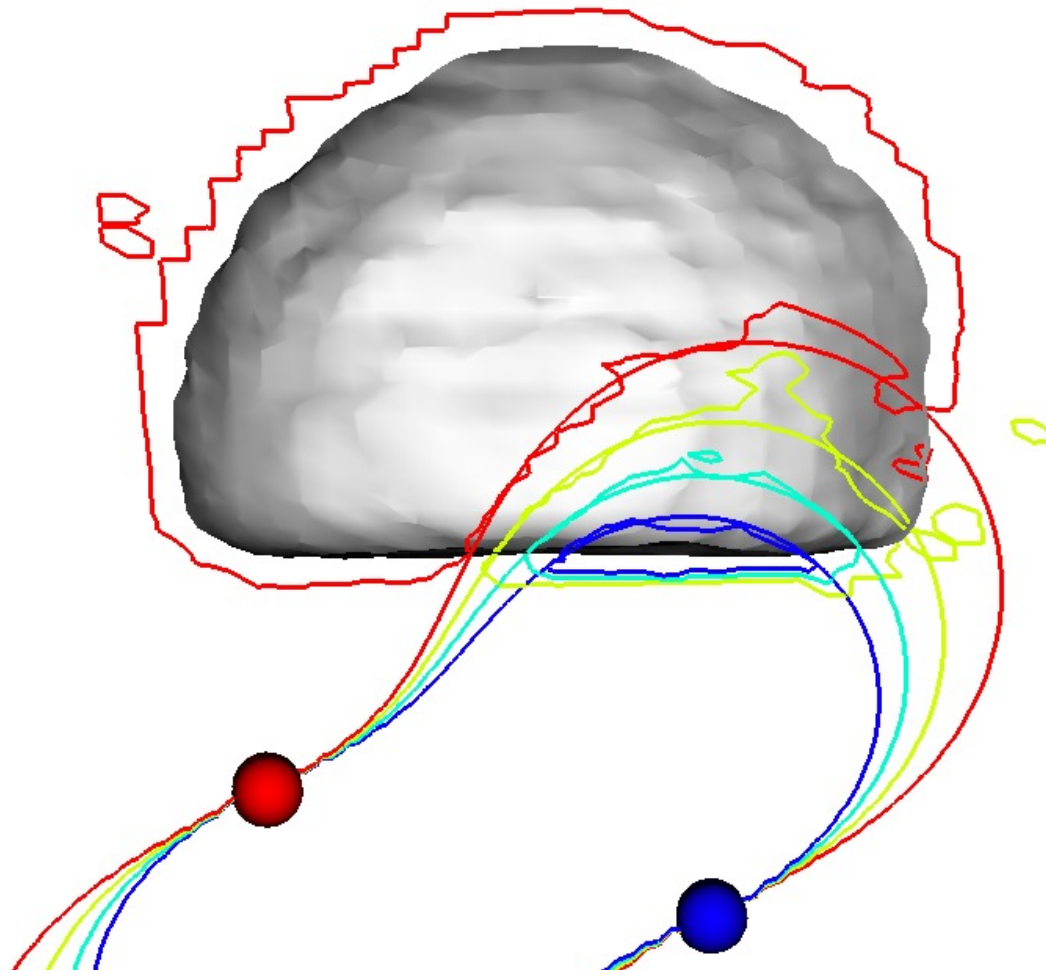
Modeling of 3D Phase Bump



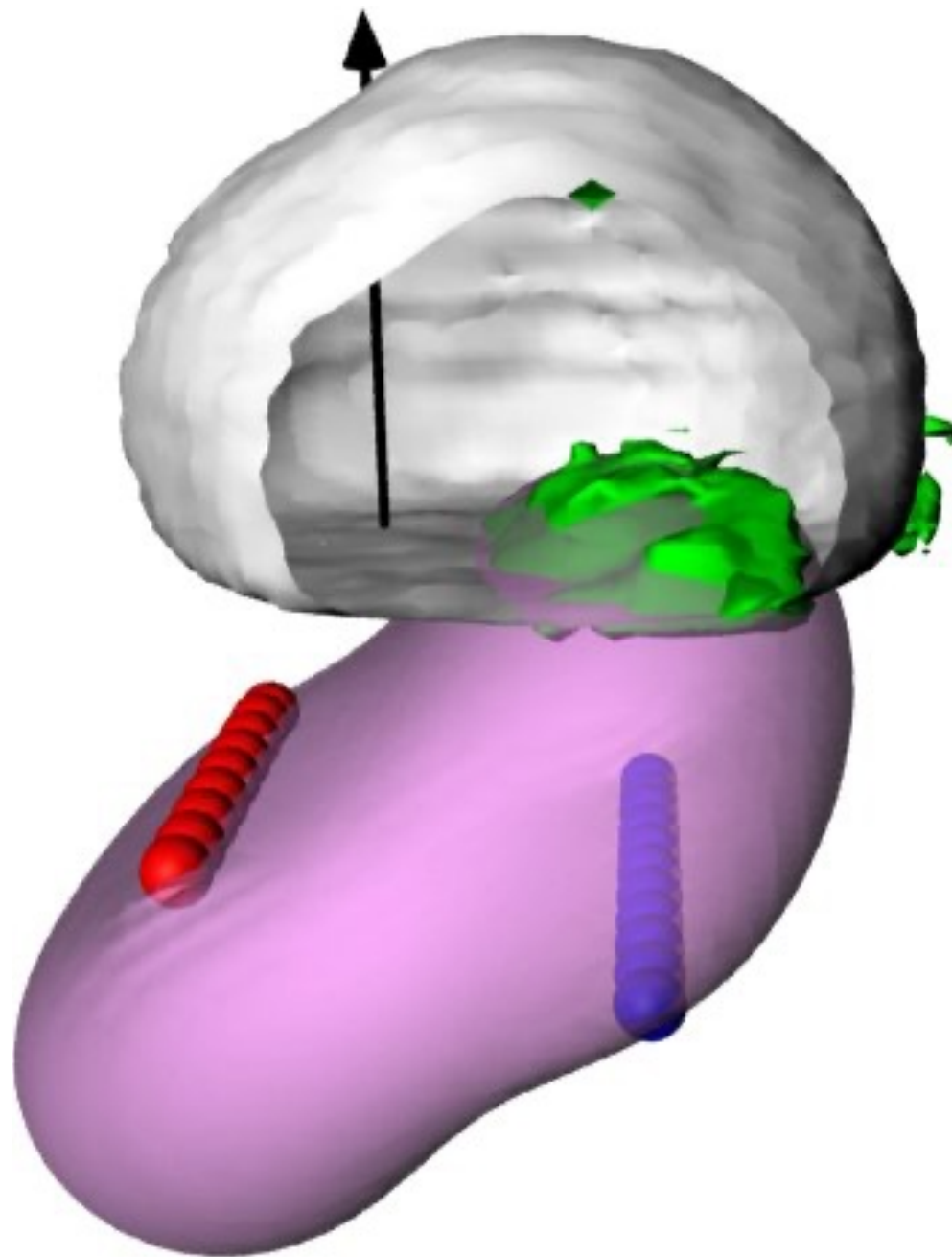
3D phase map sections



Field lines of “Point Charges”

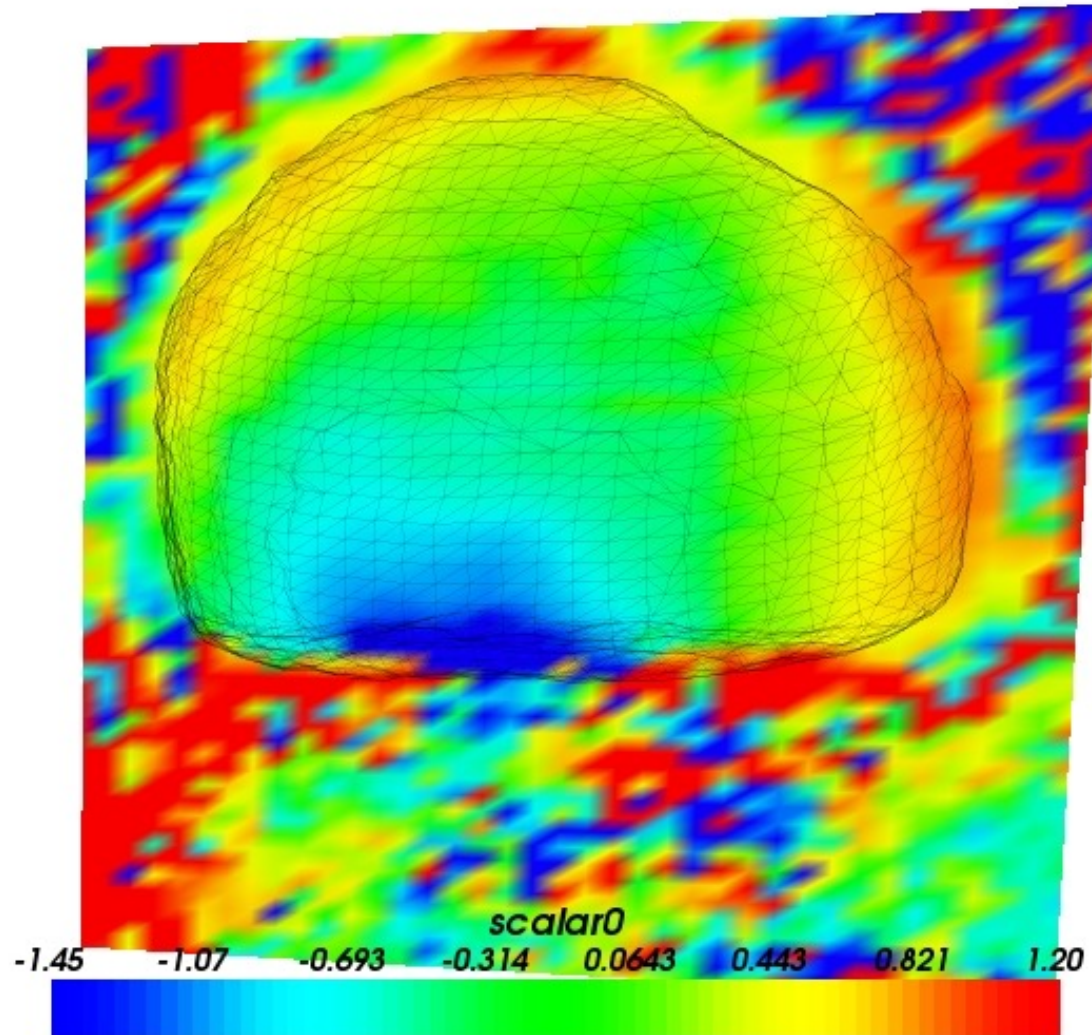


I. K. Robinson, SLS Dec 2007



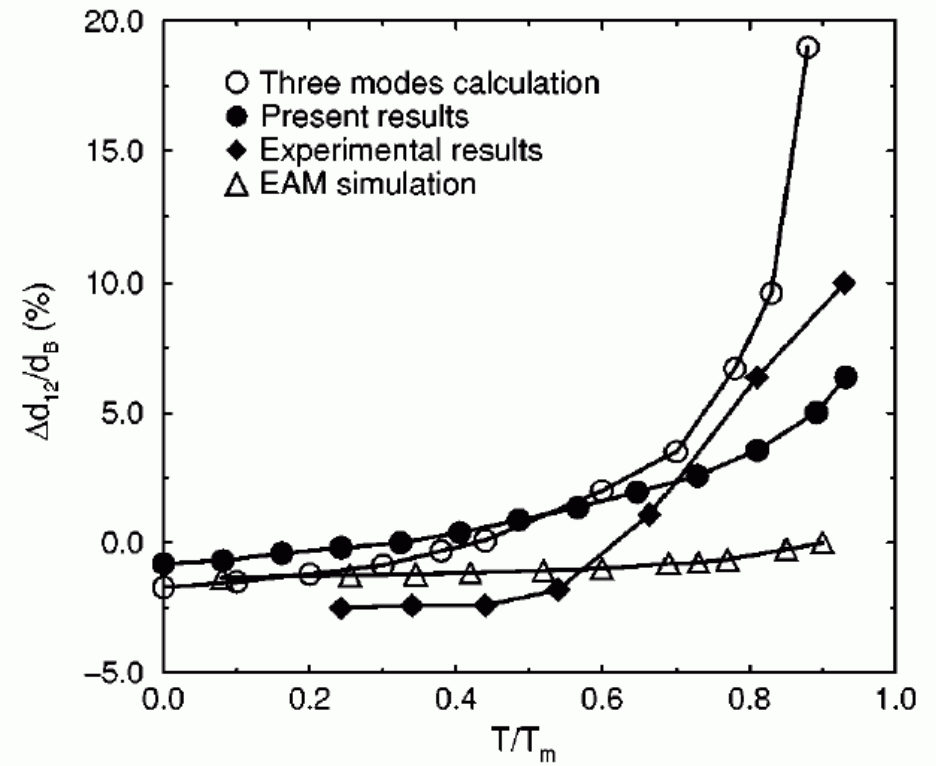
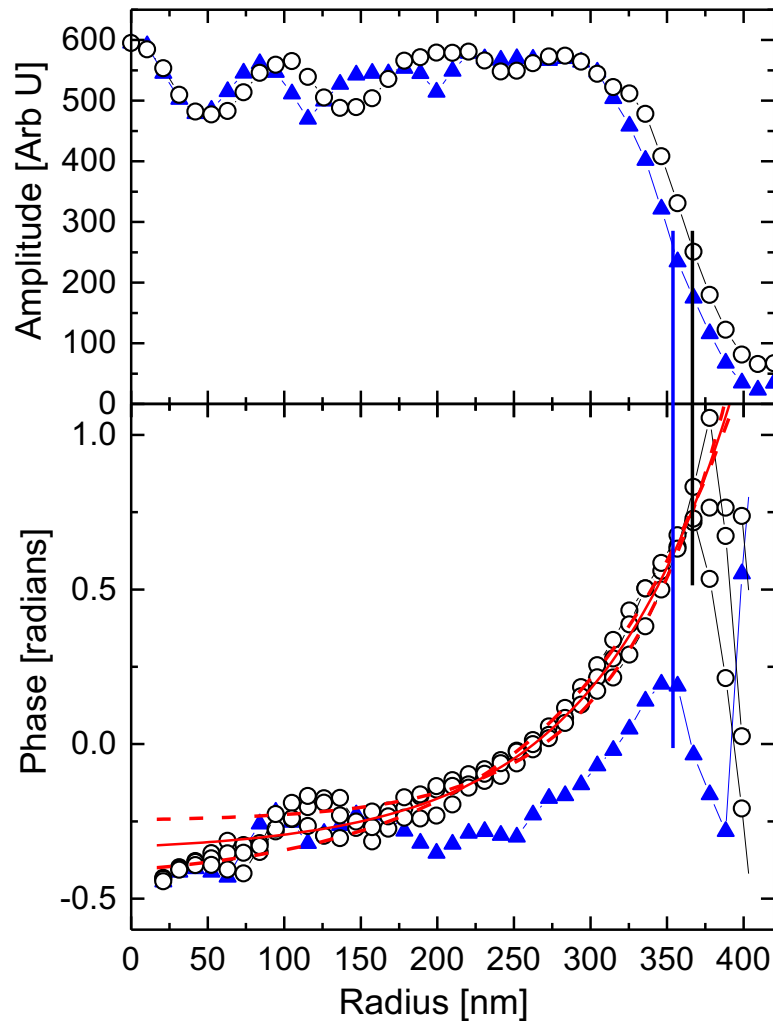
Contours showing Positive Phase

including correction for refraction by crystal



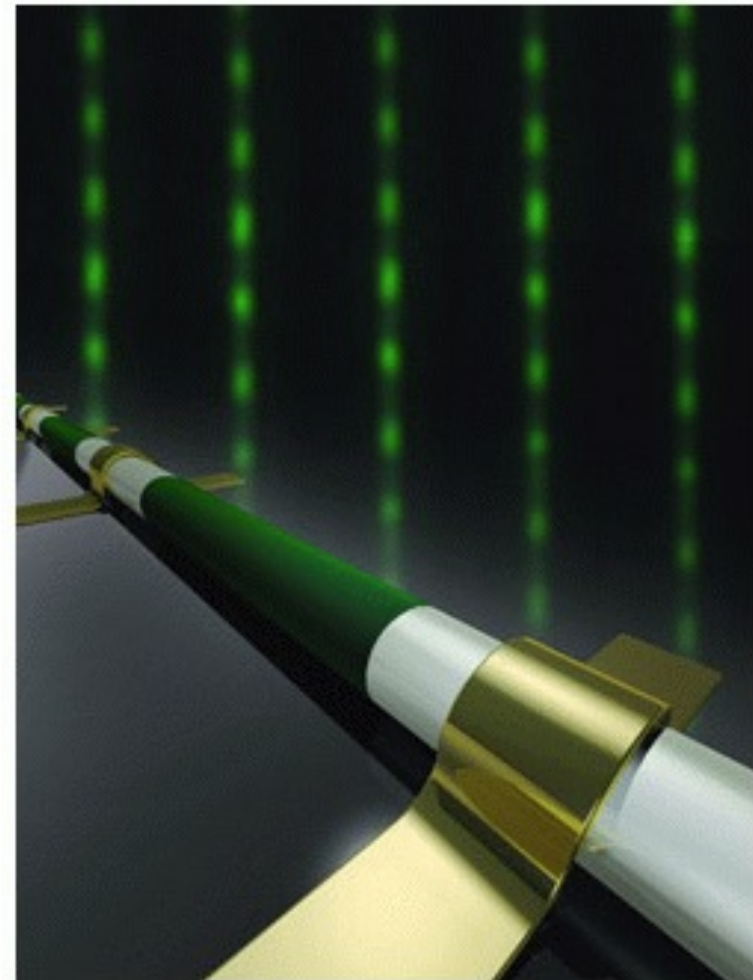
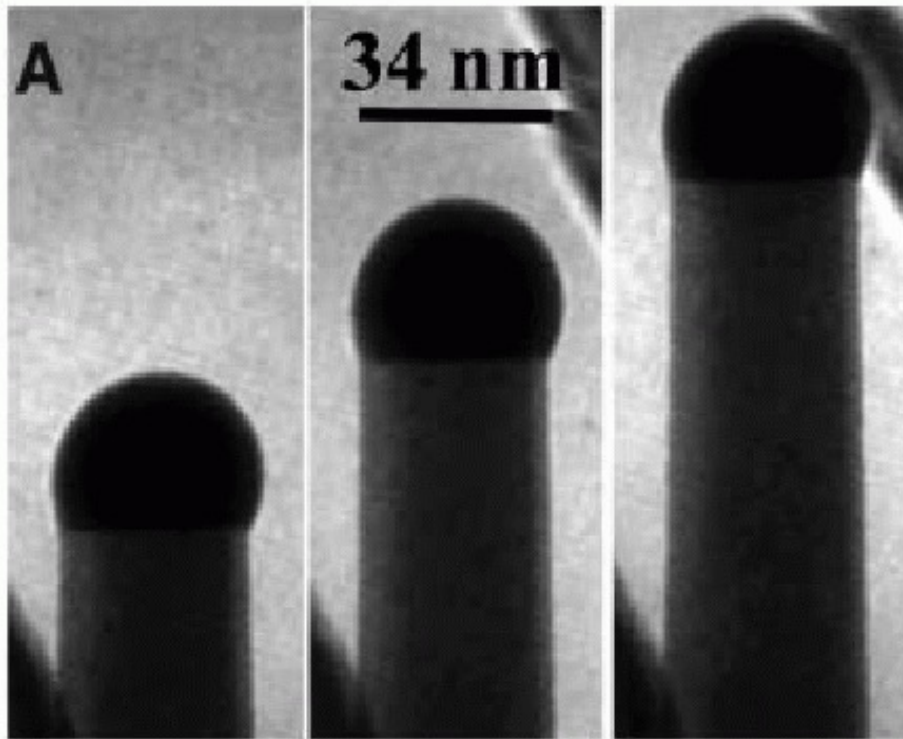
Surface Thermal Expansion

Ag(111): Scheffler et al PRB 59 970 (1999)



VLS growth of nanowires

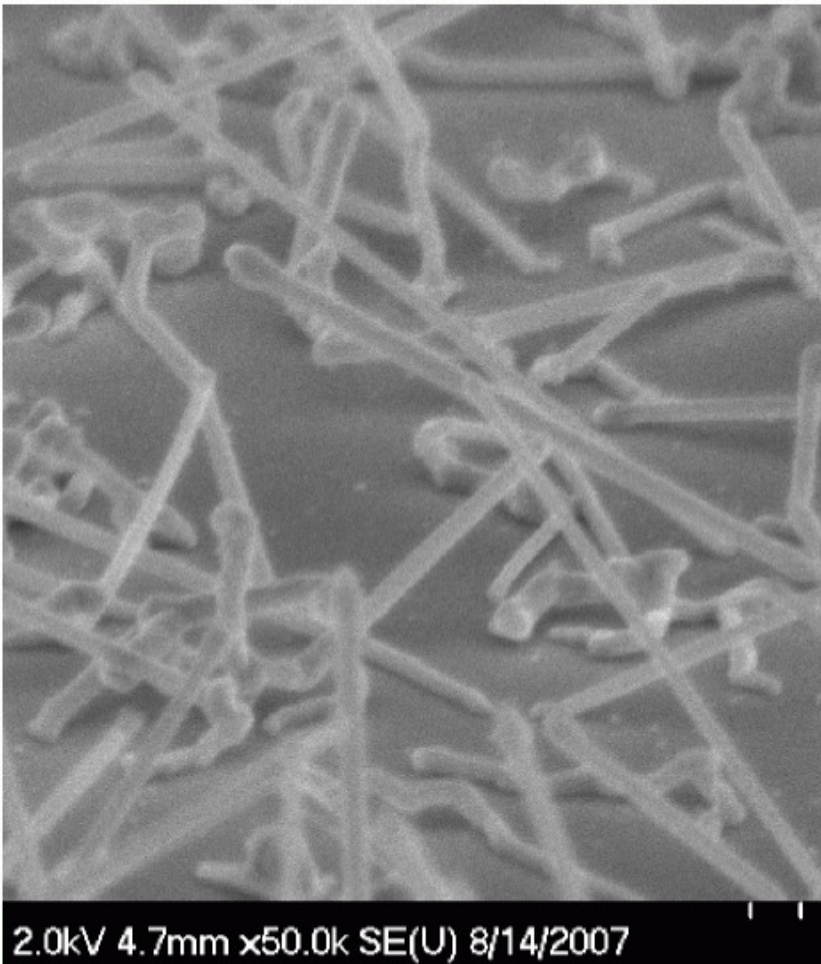
S. Kodambaka et al., *Science* 316 729 (2007)



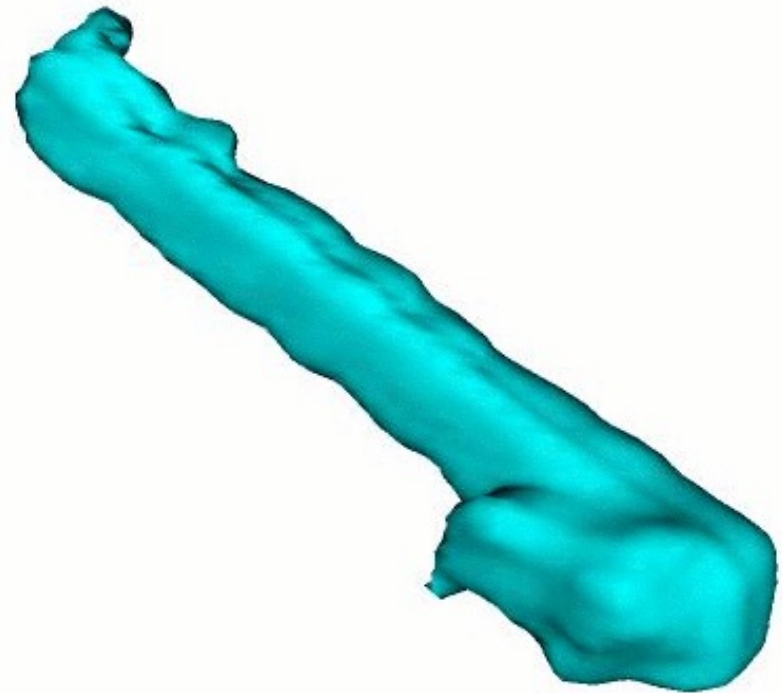
I. K. Robinson, SLS D NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

Reconstruction of InP nanowire

CVD on Si, Suneel Kodambaka, UCLA

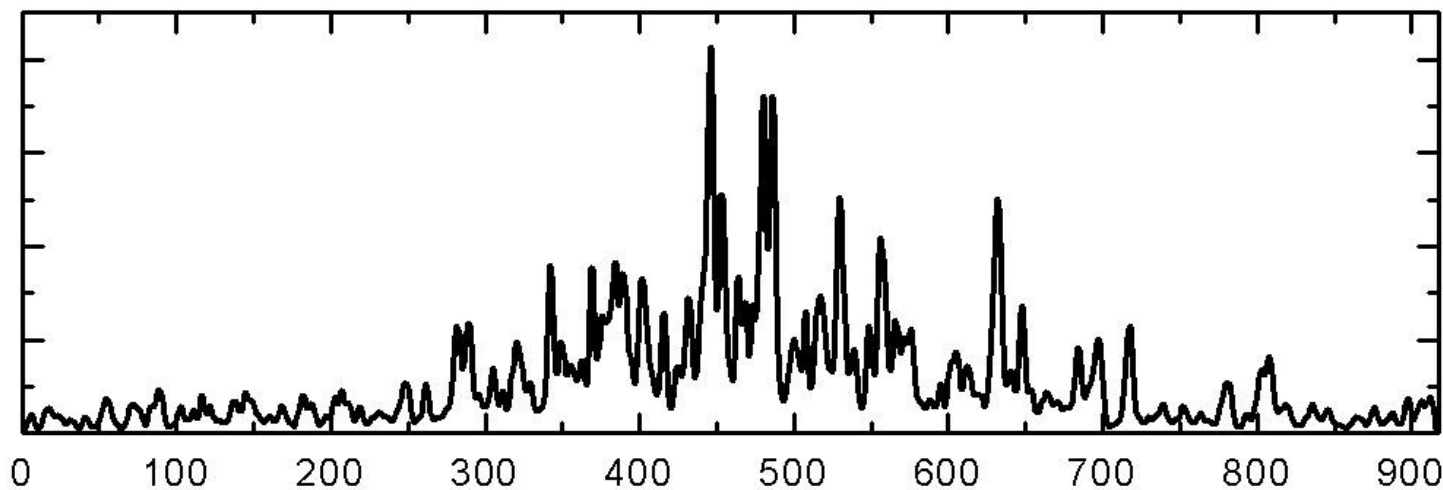
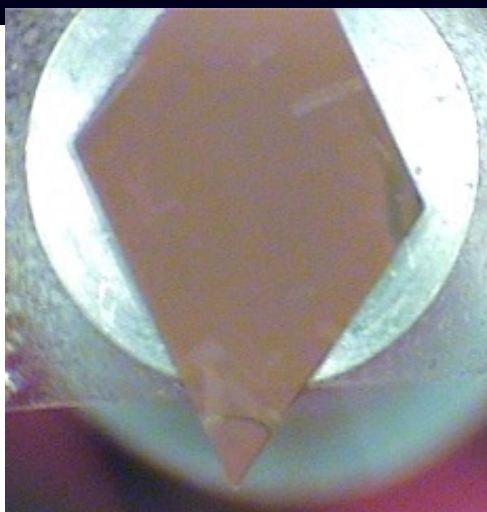
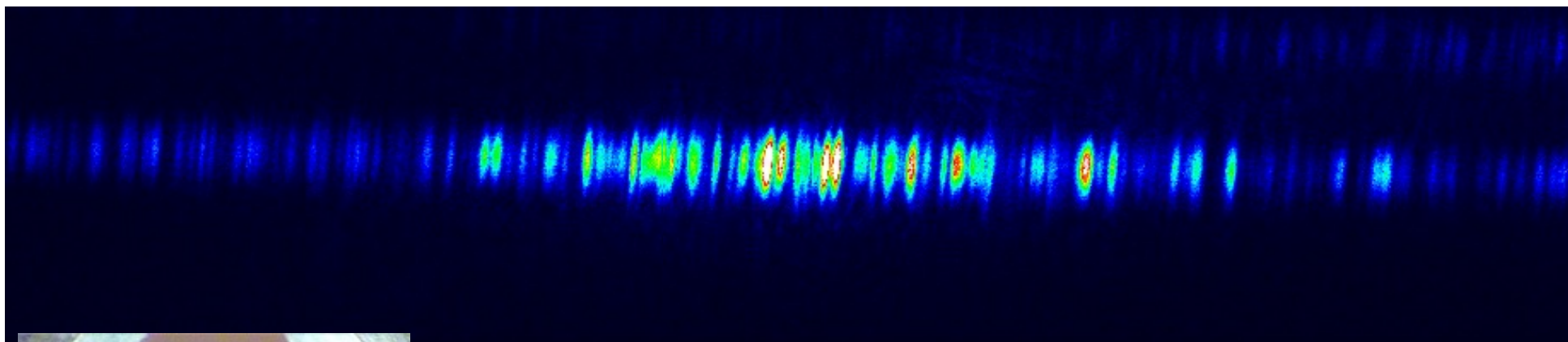


InP nanowires grown on Si (111)



GaAs Nanowire “Barcode”

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

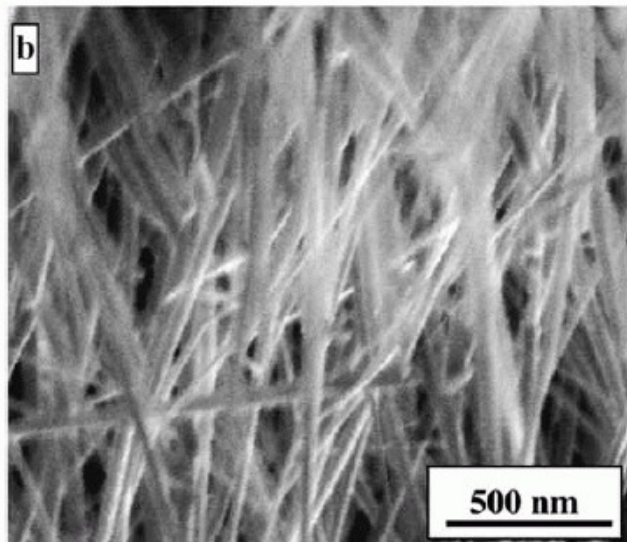
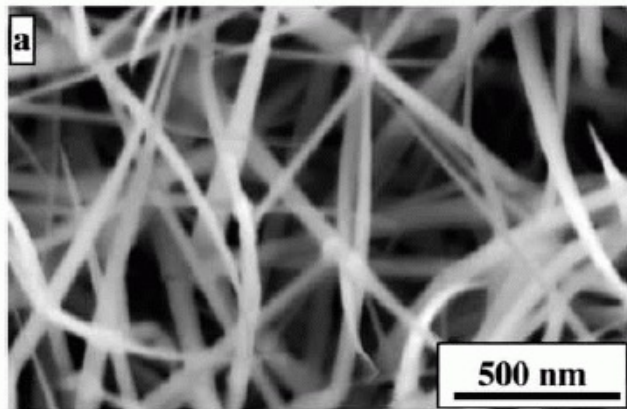


GaAsNW1106-22.spe
B9348 from Philips

Pixel number (22.5 micron)

Dark Field TEM of GaAs Nanowires

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

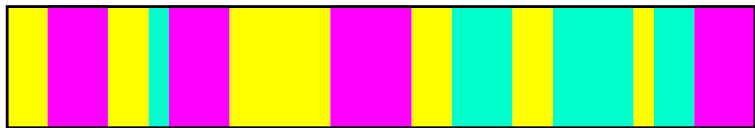


Models of Barcode Diffraction

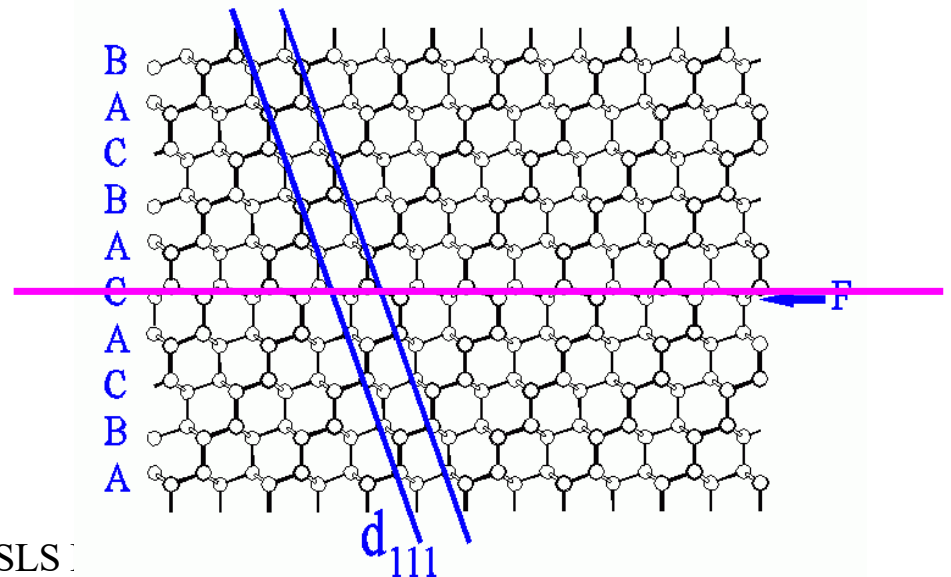
(111) wires at (11-1) reflection



- Twinned stacking sequence

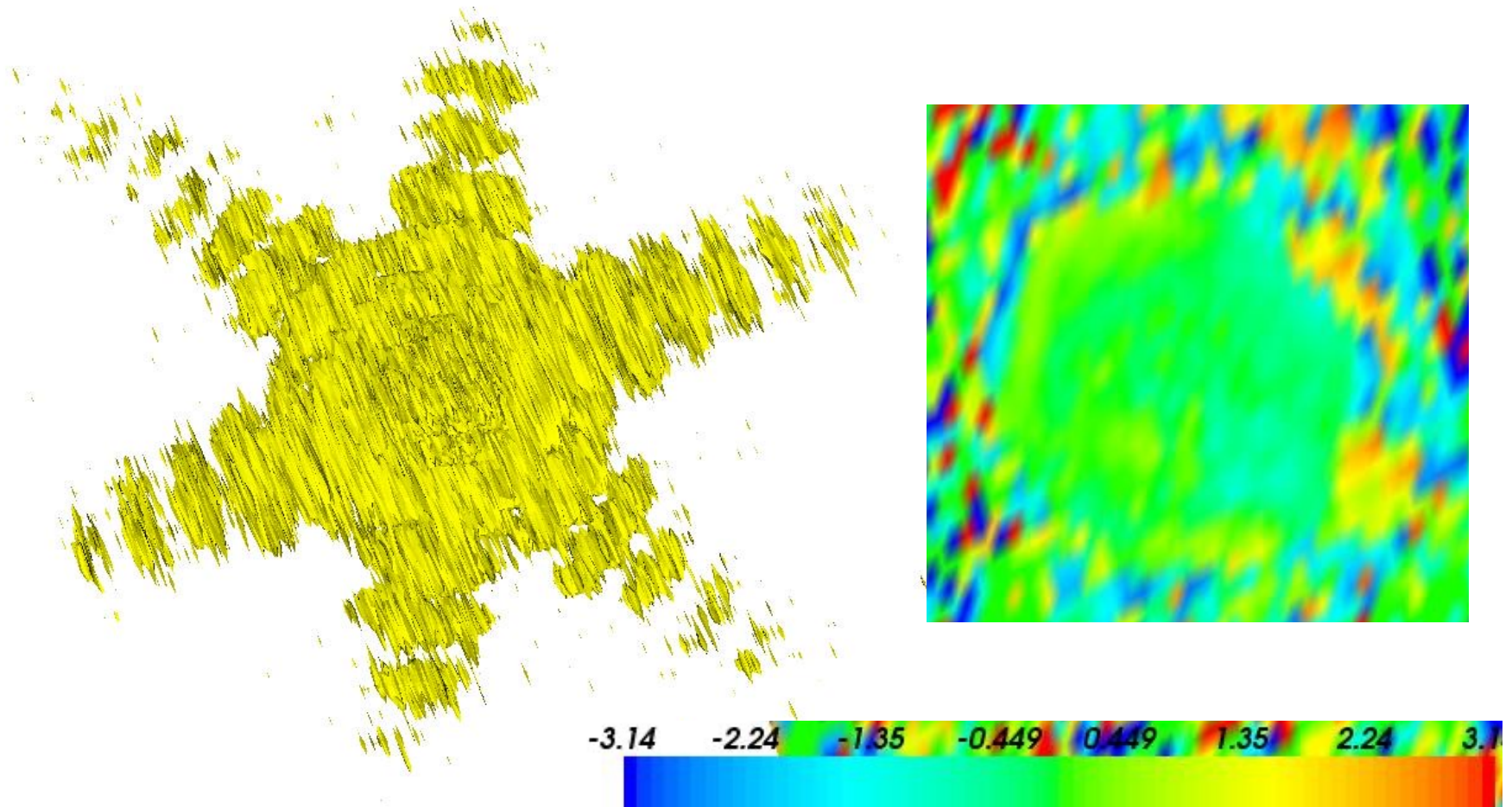


- Deformation faults

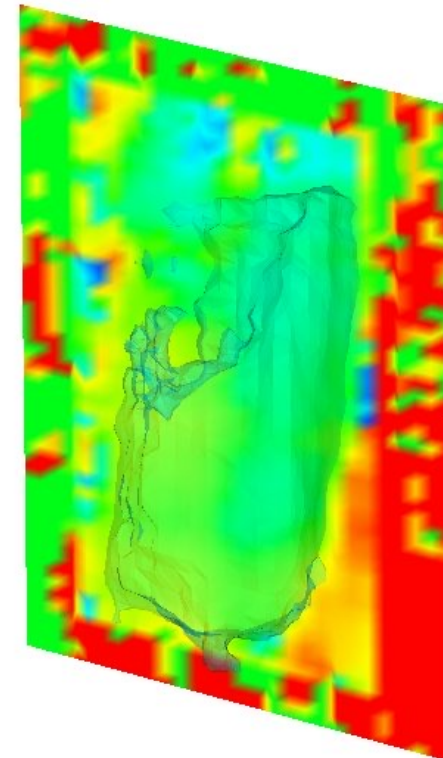
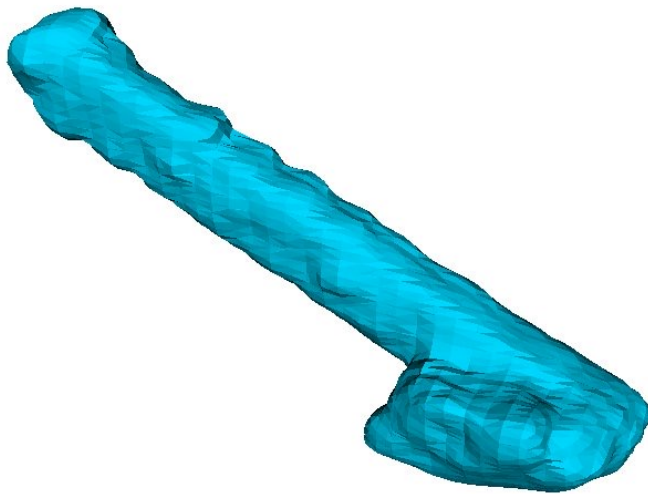
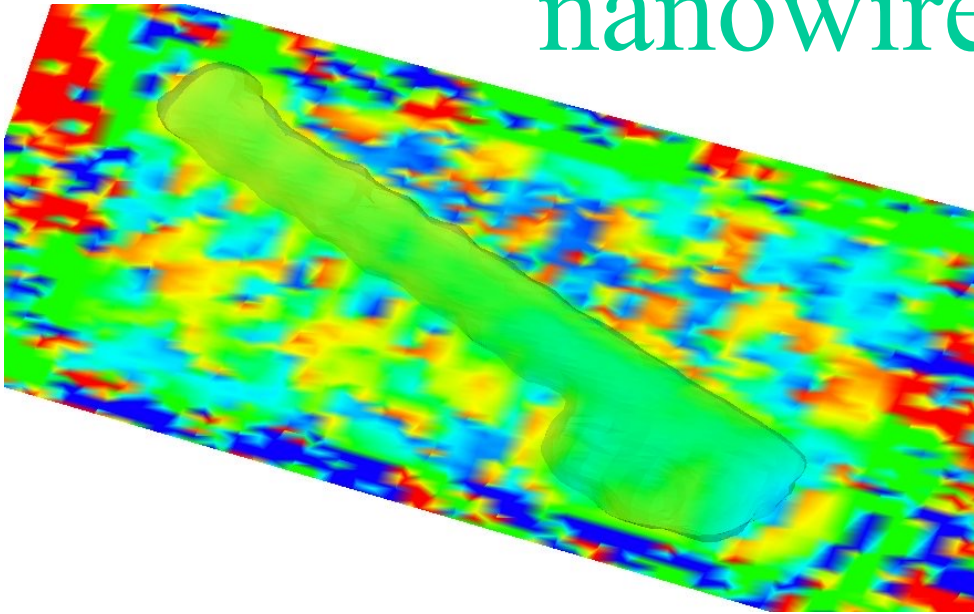


ZnO Nanowire Reconstruction

Ross Harder, Steven Leake, PhD project at UCL



Phase structure in nanowires



Dec 2007

Conclusions

- Internal structure of Ag and Pb Nanocrystals
- 3D imaging practical for nanocrystals
- Phasing by computation instead of lens
- Strain fields imaged from asymmetric patterns
- Contact Forces cause strain inside crystal
- Surface strain has orientation dependence