Stress in Nanoparticles

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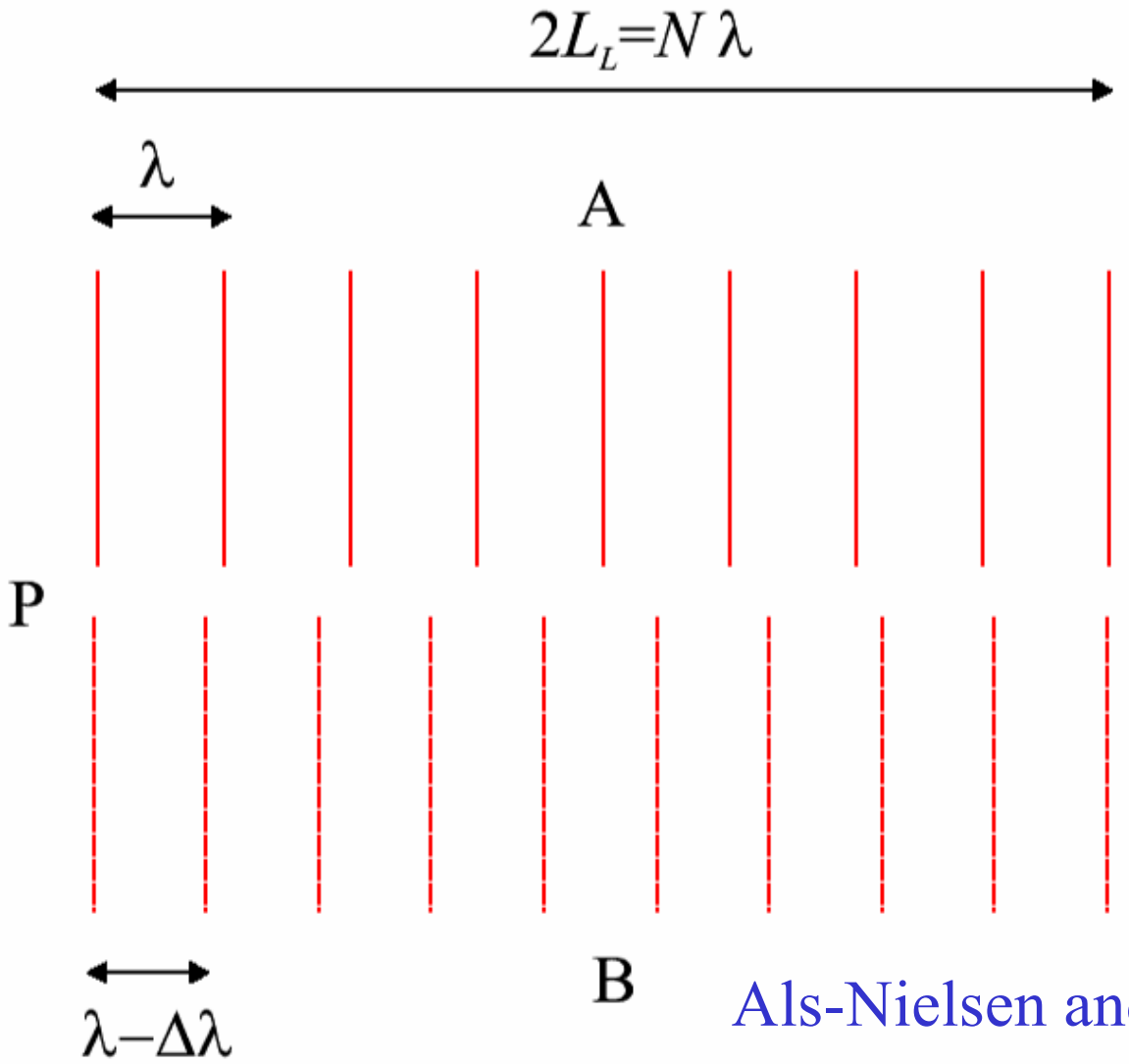
Outline

- Coherent x-ray diffraction
- CXD can solve the phase problem
- Extension to phase objects
- Nanocrystal structures
- Nanowire structures

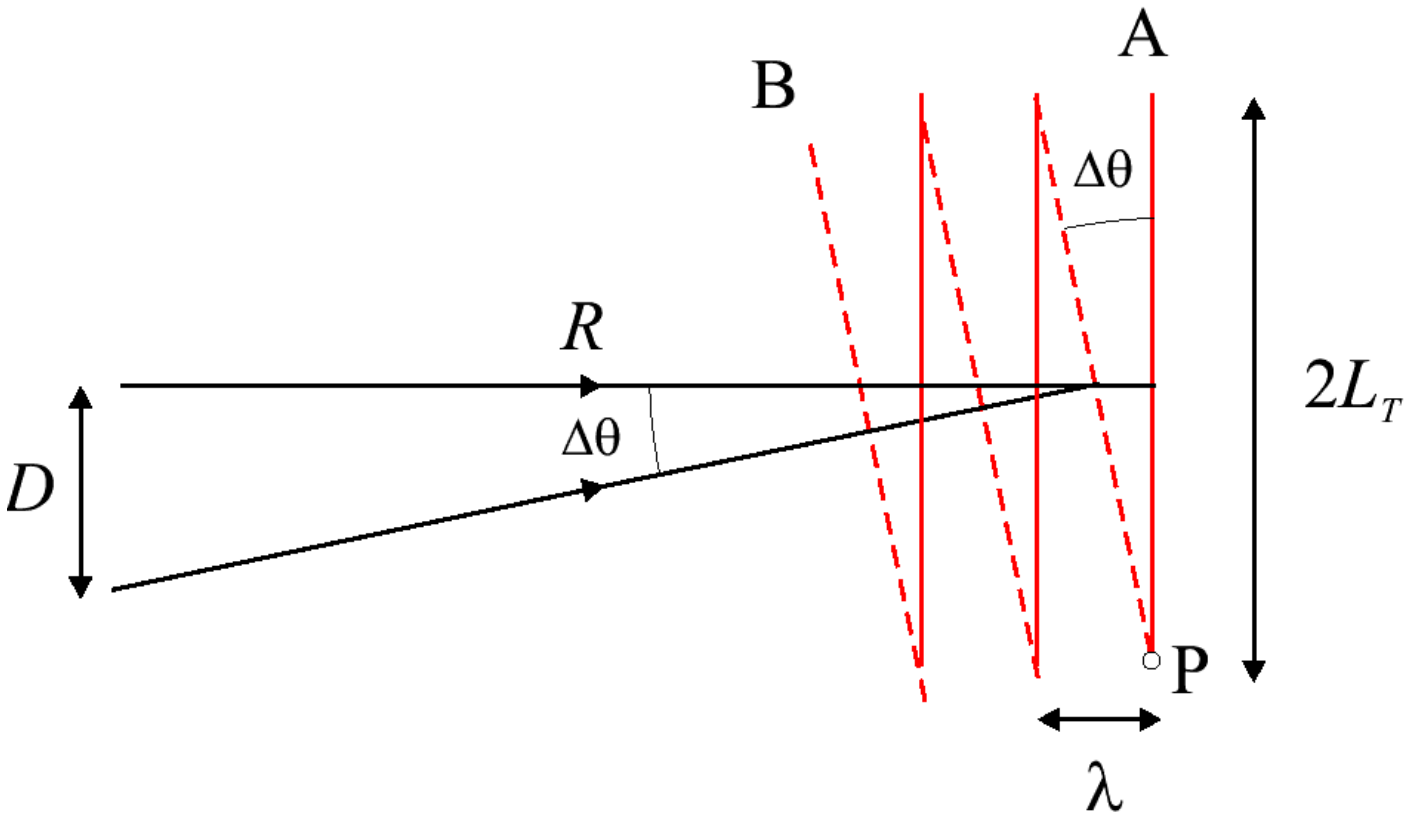
Longitudinal Coherence



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

Als-Nielsen and McMorrow (2001)

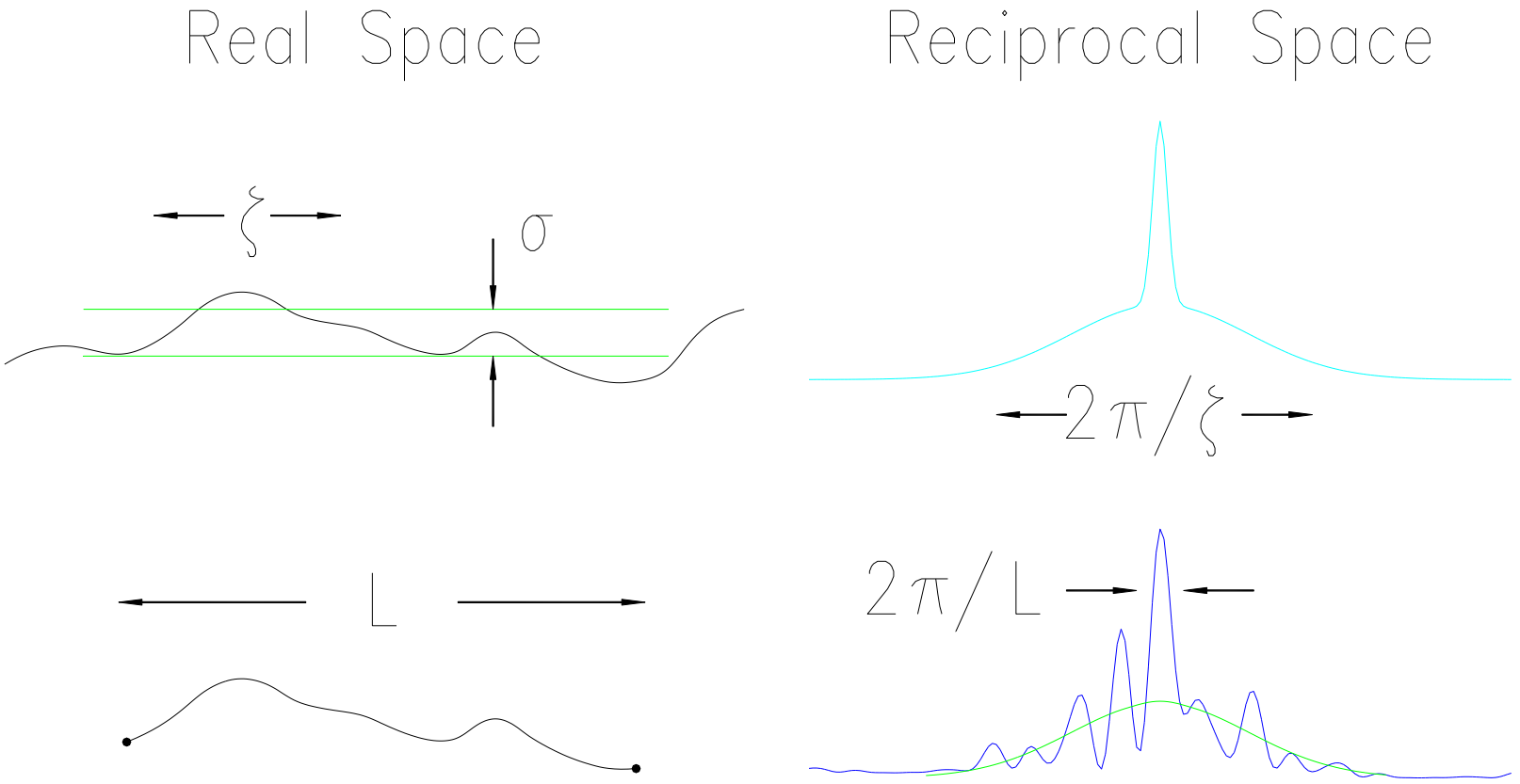
Lateral (Transverse) Coherence



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

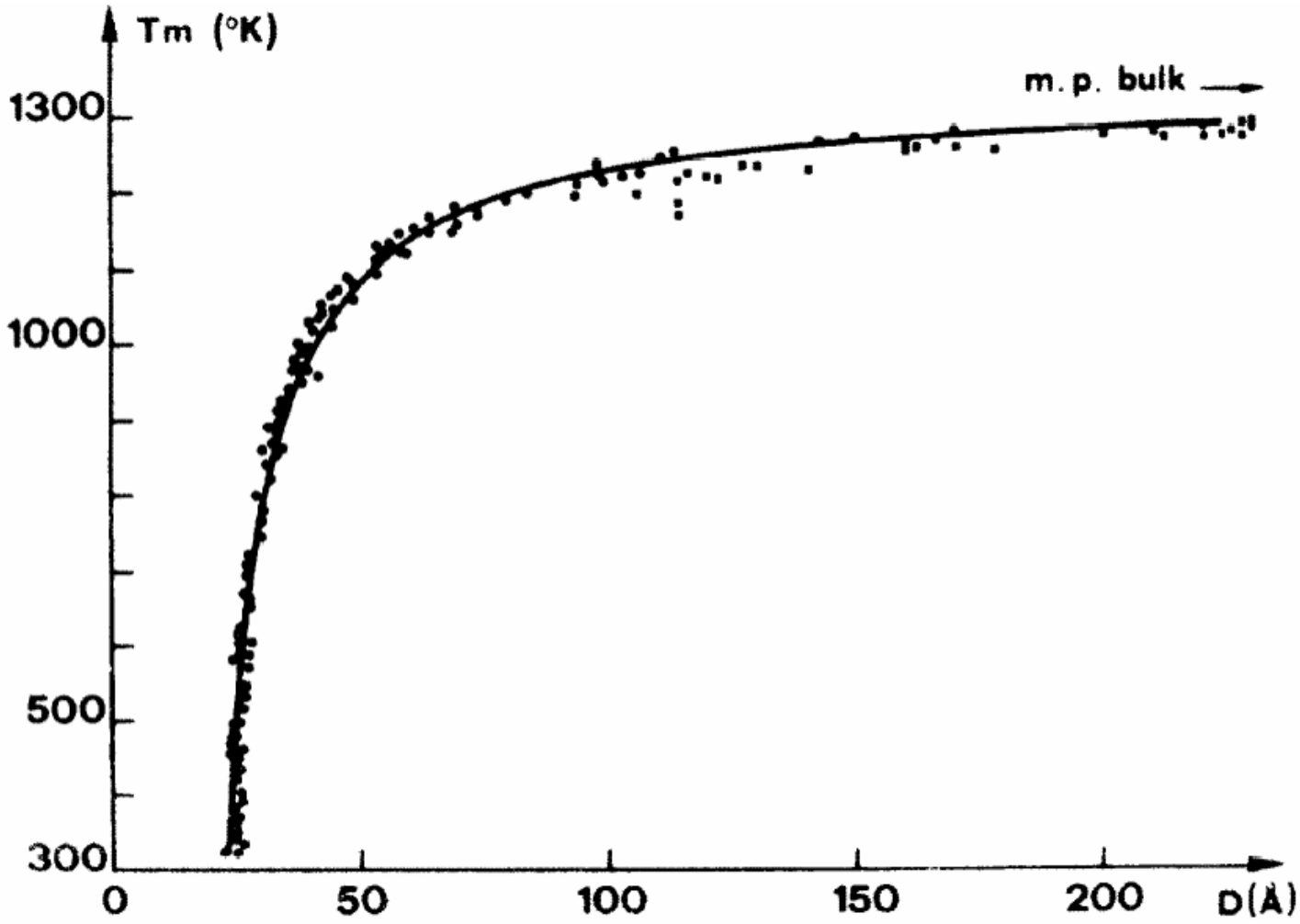
Als-Nielsen and McMorrow (2001)

Diffuse Scattering acquires Structure using CXD

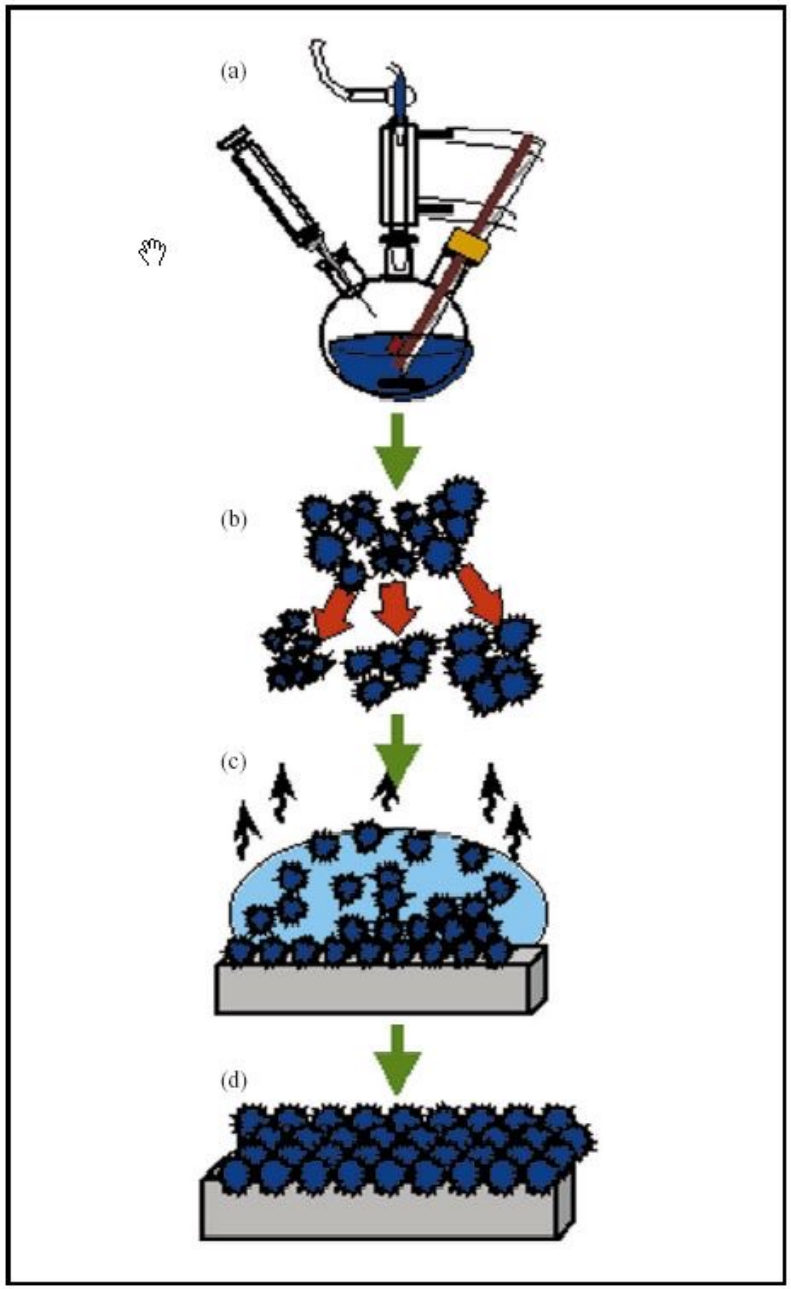


Size-dependent Melting of Au Particles

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

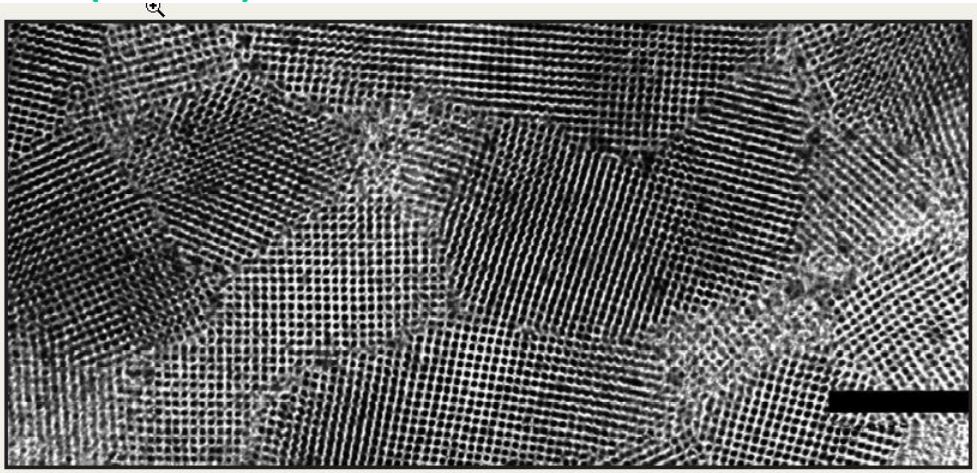


Chemical Synthesis of Nanocrystals

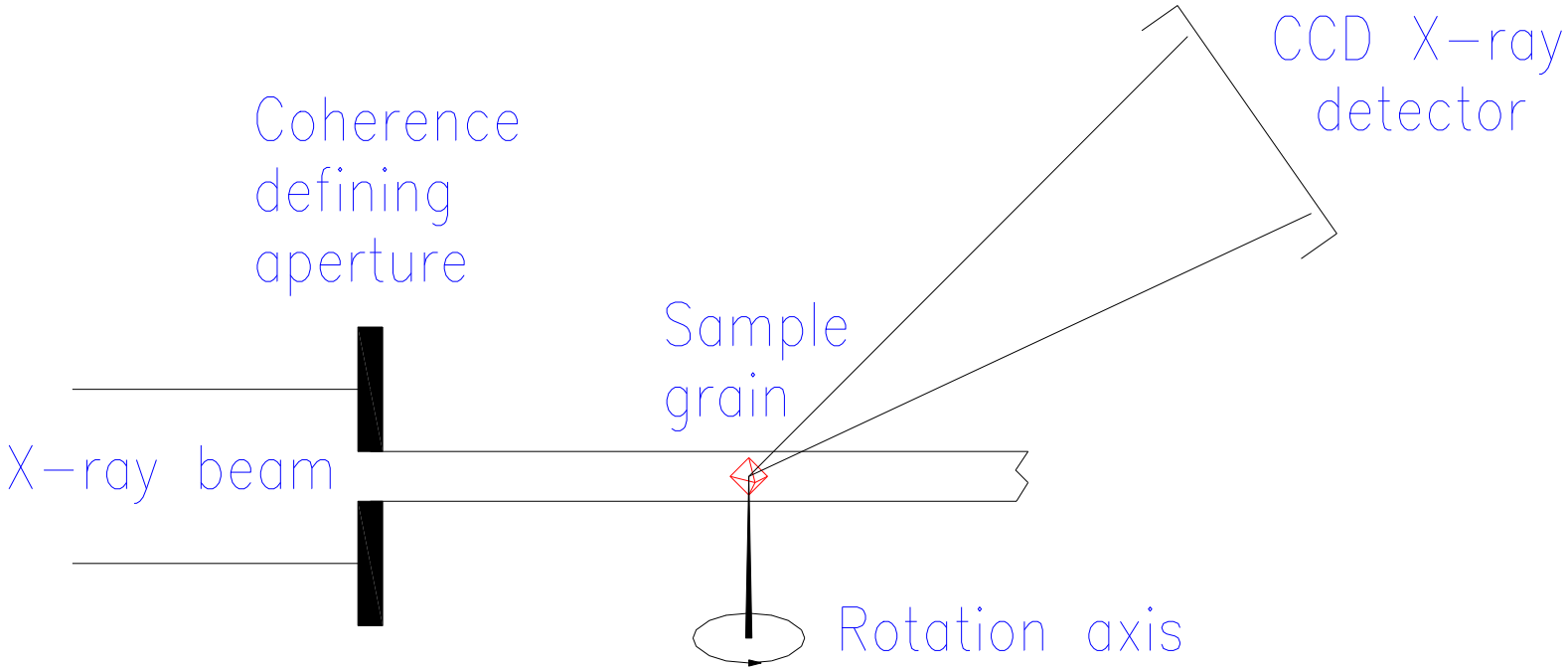


- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

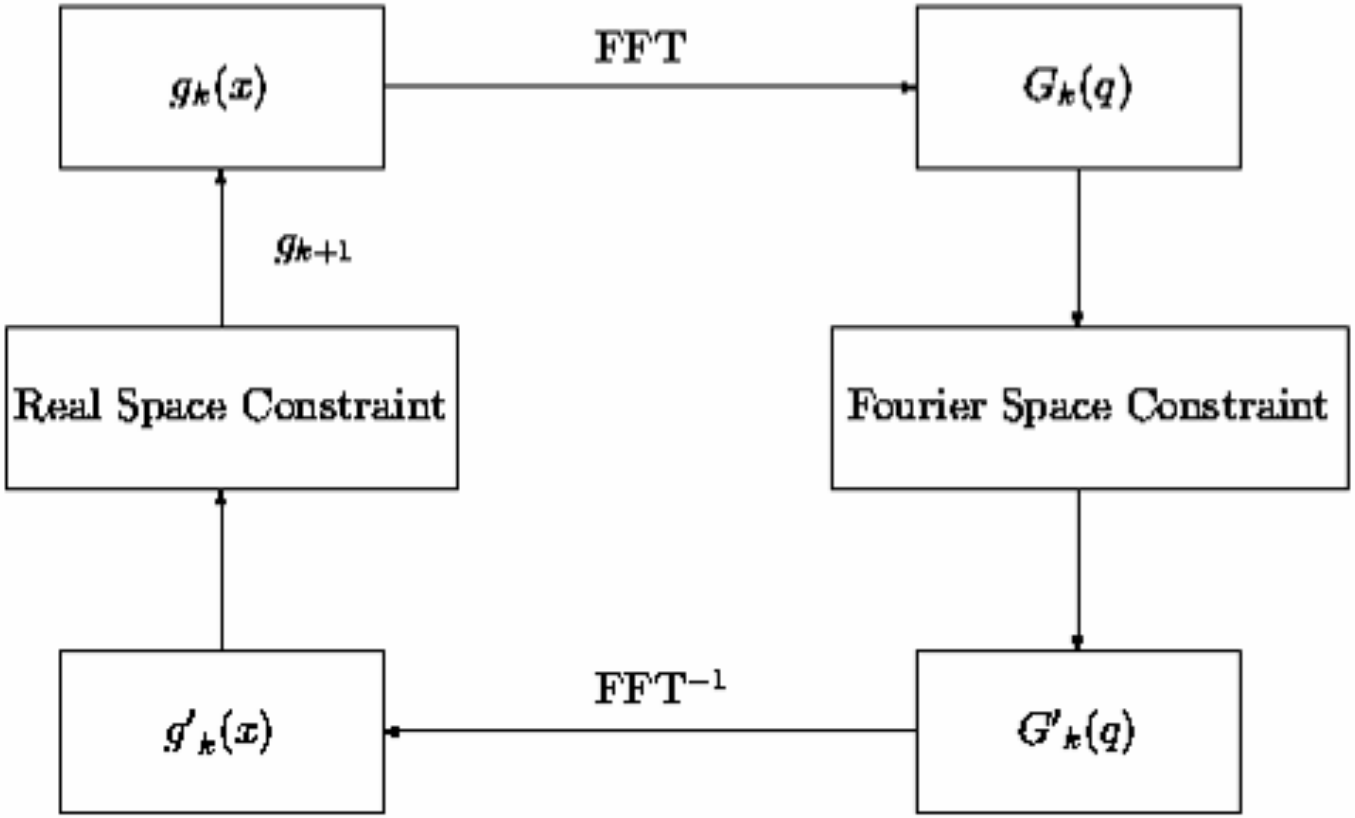
C. B. Murray, IBM J. Res. & Dev. **45** 47 (2001)



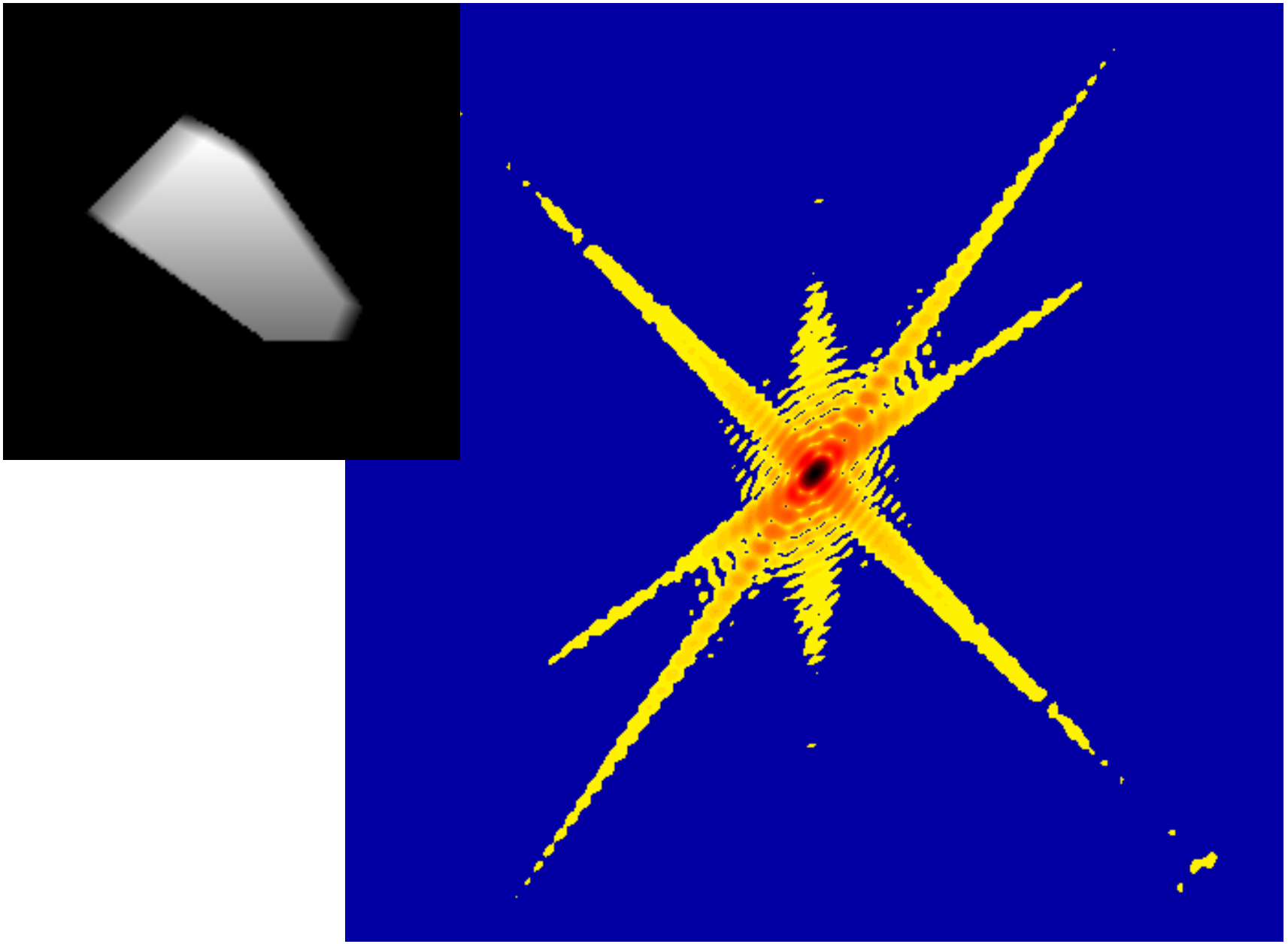
Lensless X-ray Microscope



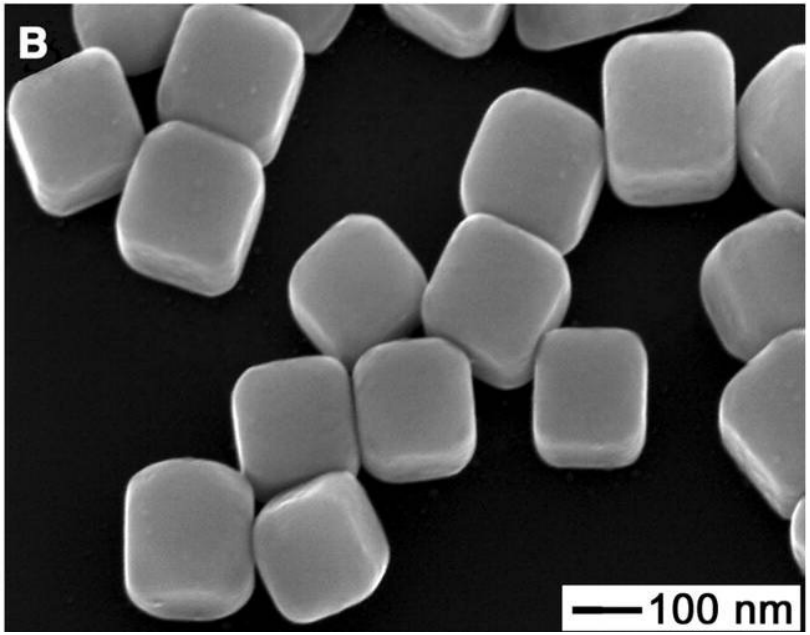
Generic "Error Reduction" method

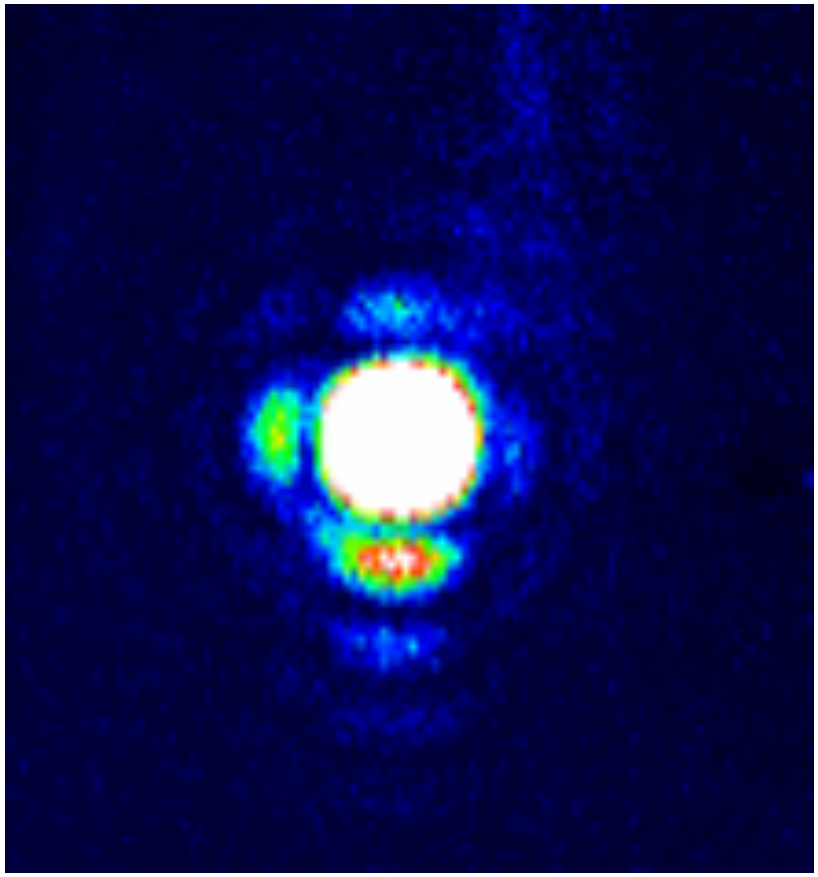


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)



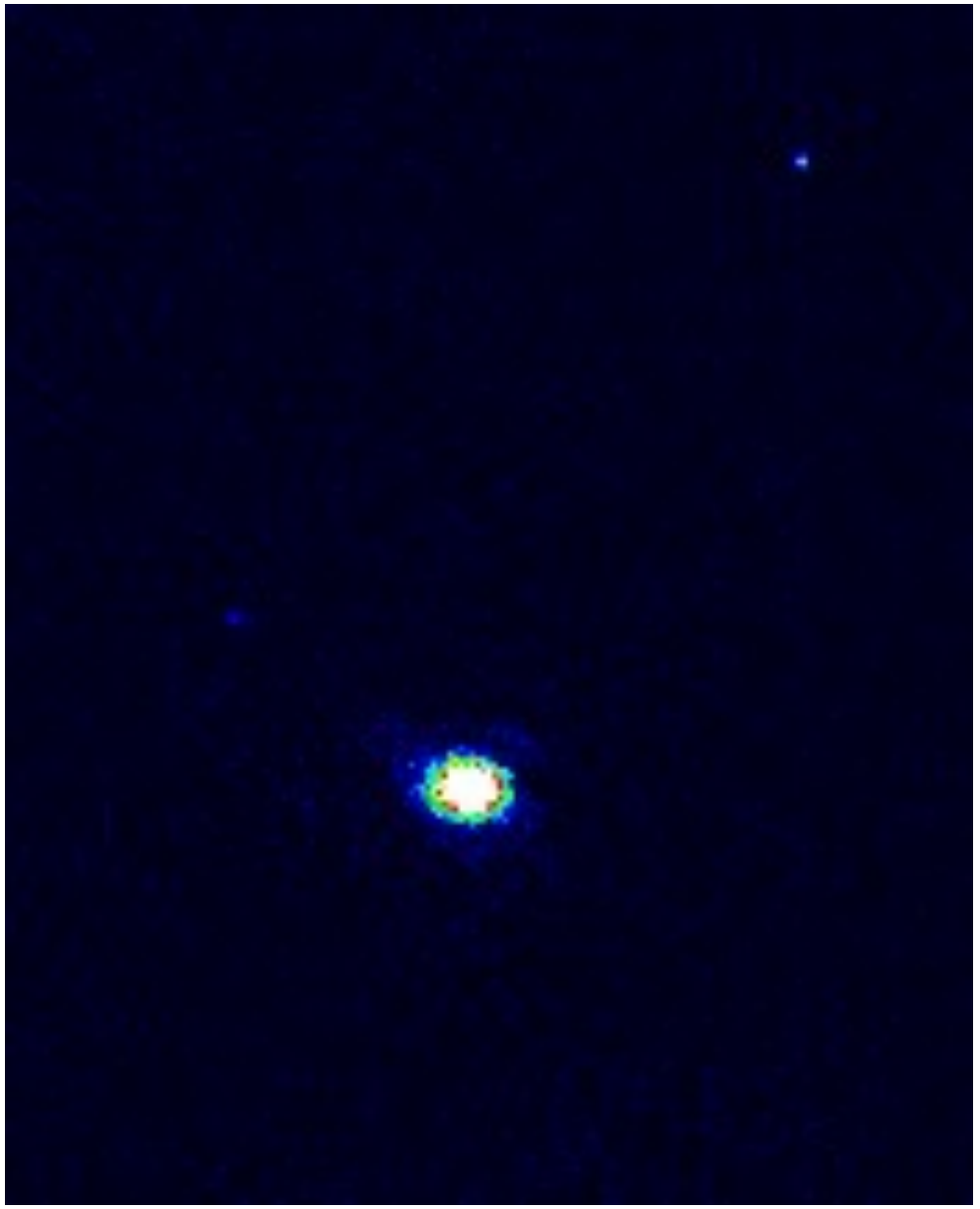
Chemically Synthesized Silver Nanocubes

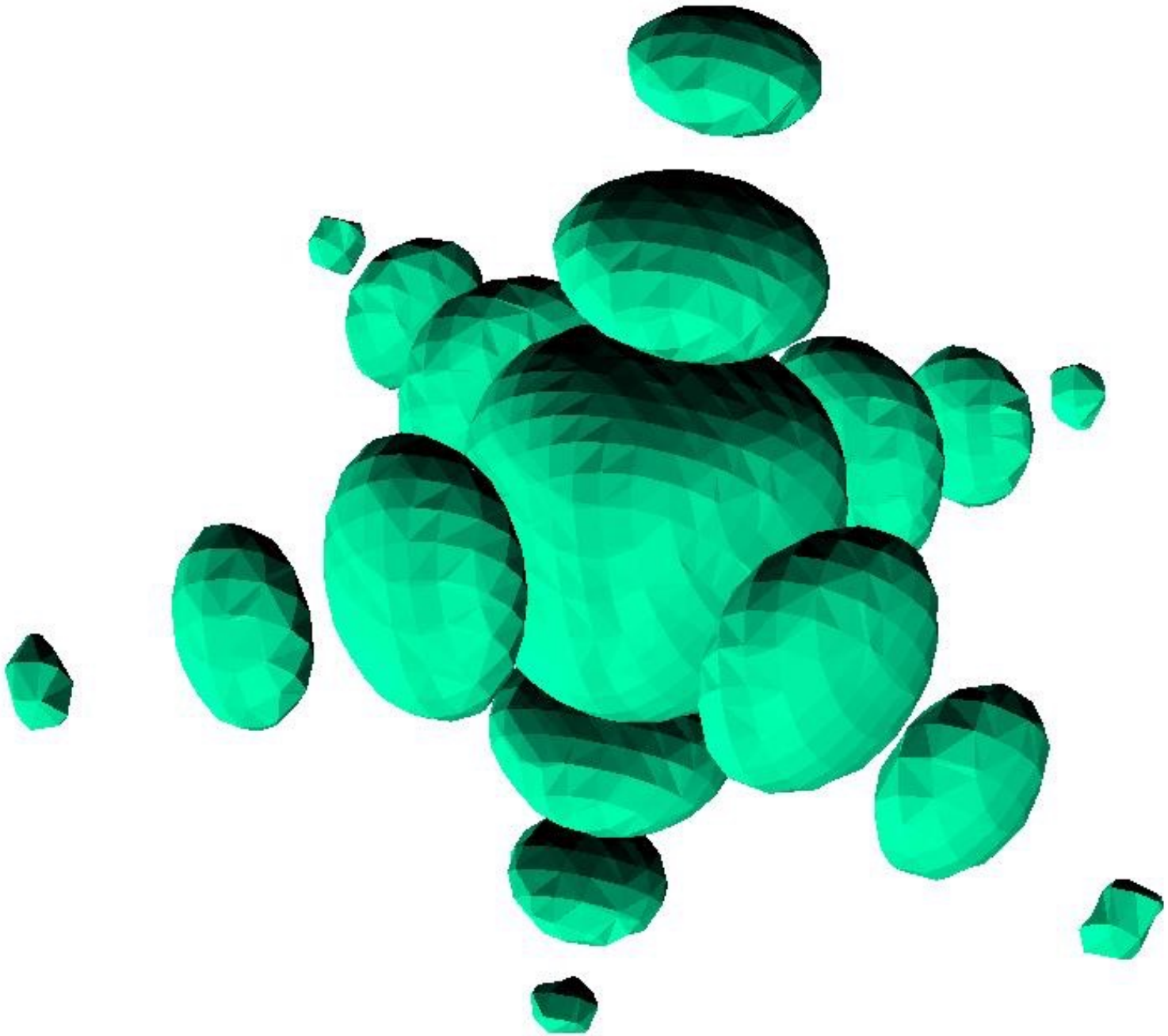


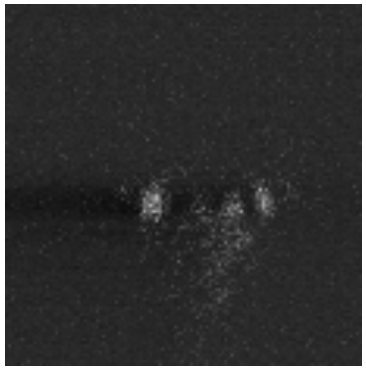


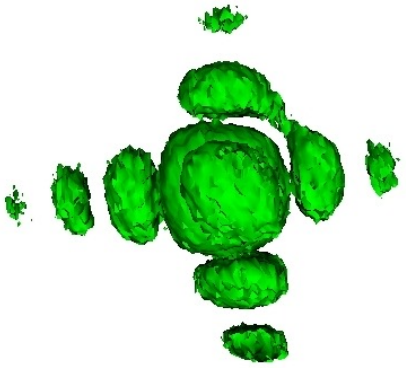
Yugang Sun and Younan Xia,
Science 298 2177 (2003)

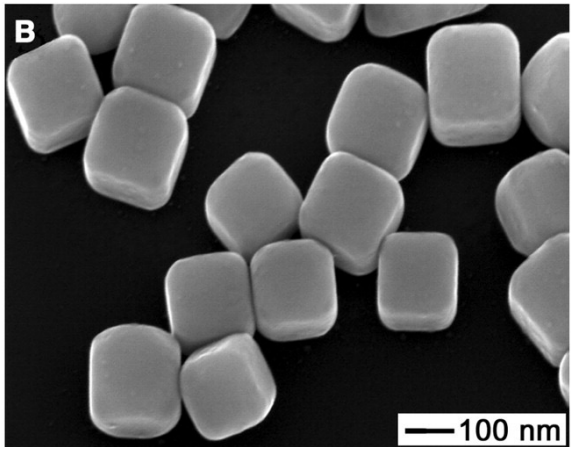
Rocking scan of Ag cubes with 0.01° steps

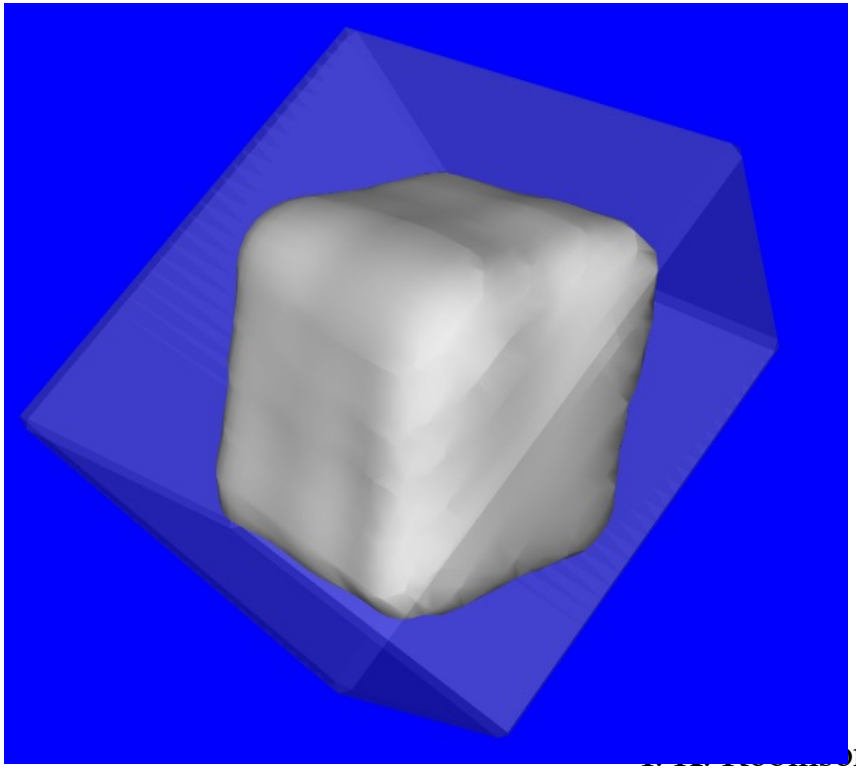


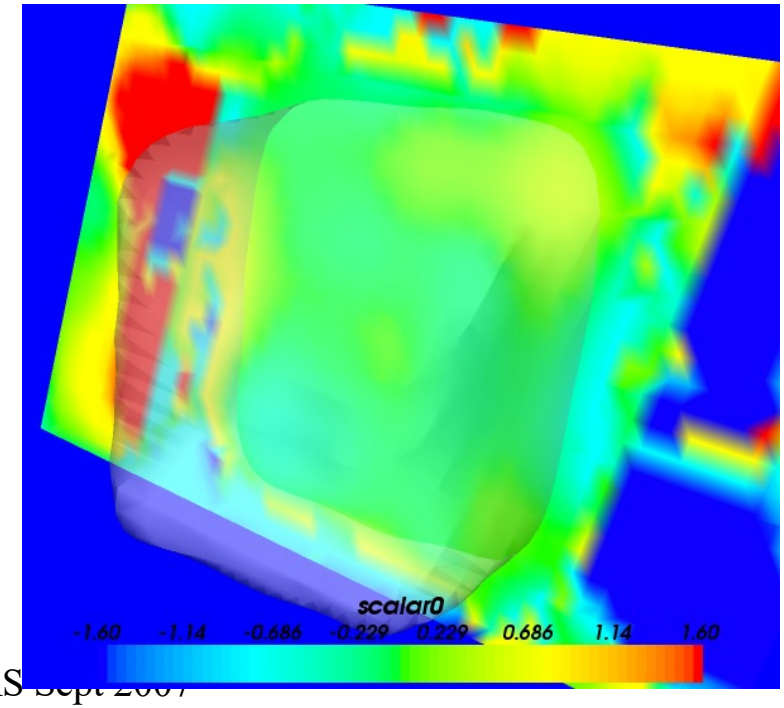




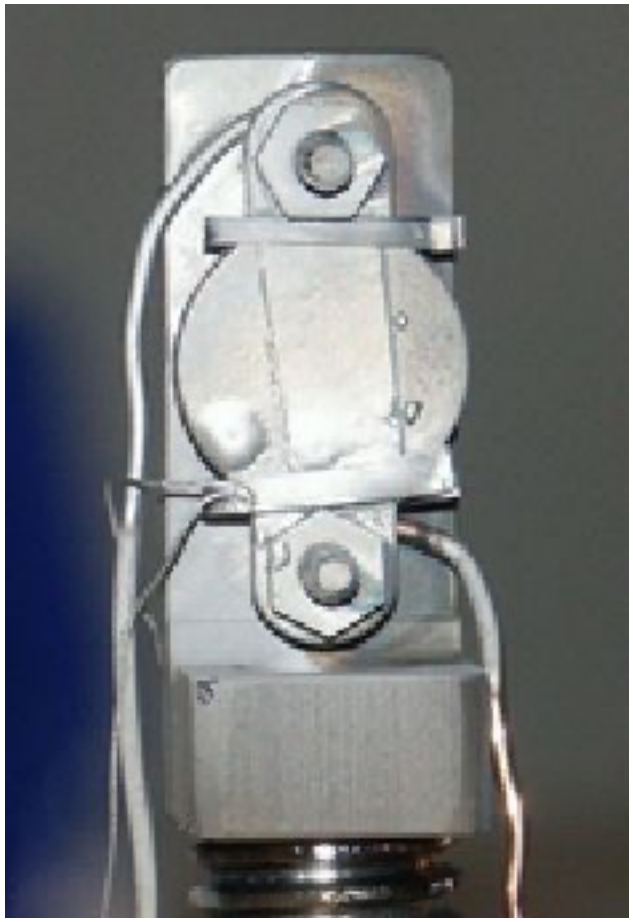


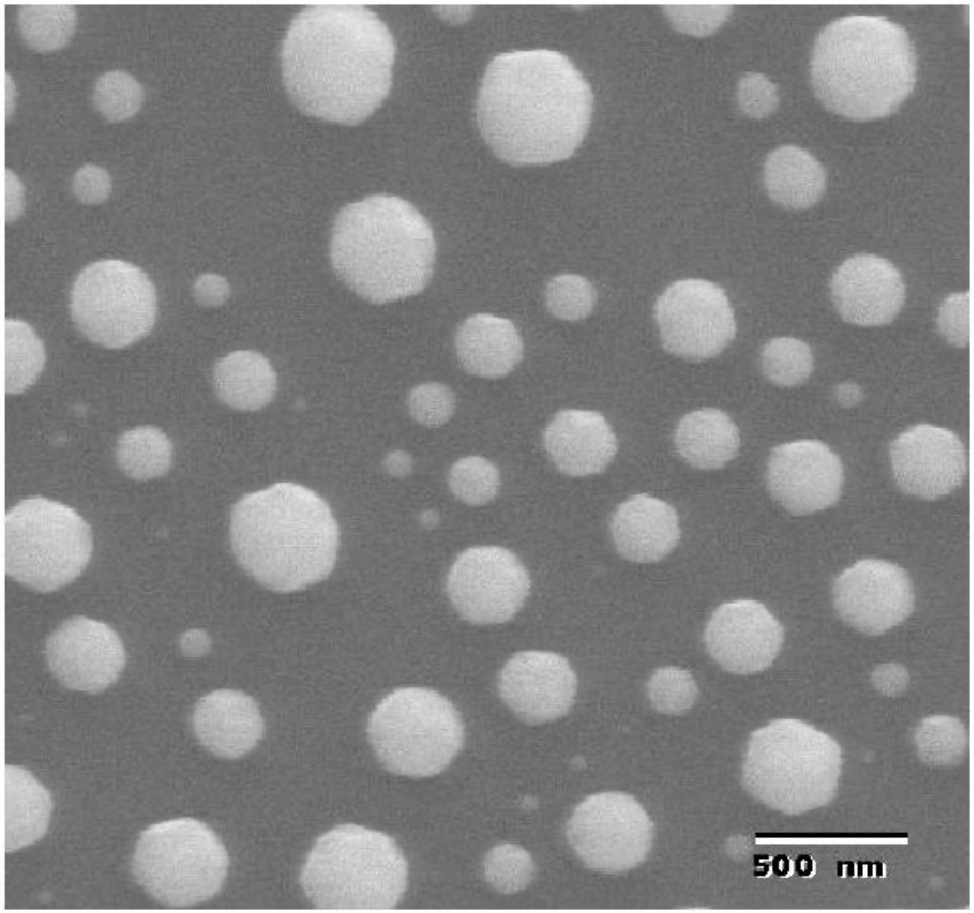

B
100 nm



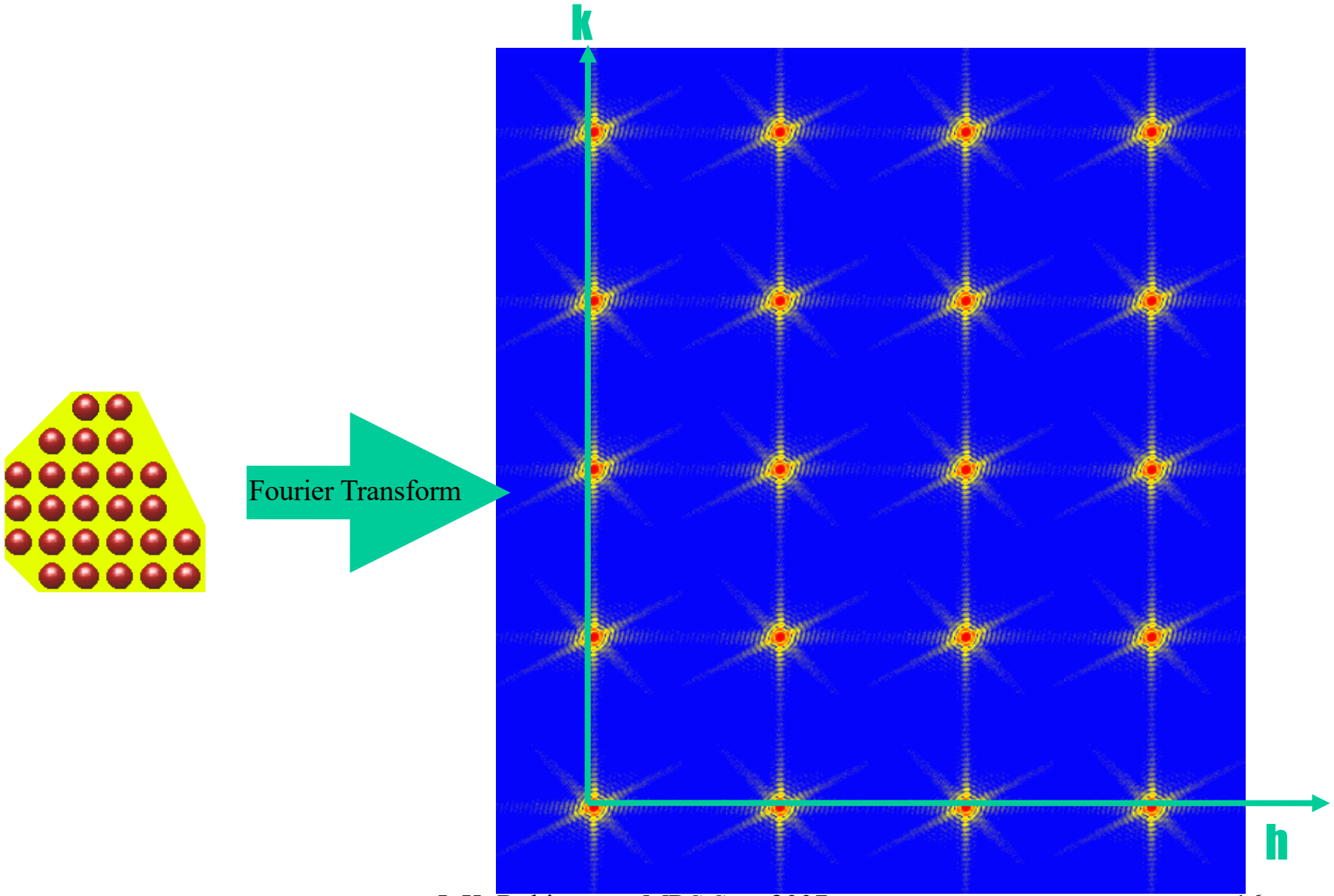

scalar0
-1.60 -1.14 -0.686 -0.229 0.229 0.686 1.14 1.60

In situ growth of Pb crystals





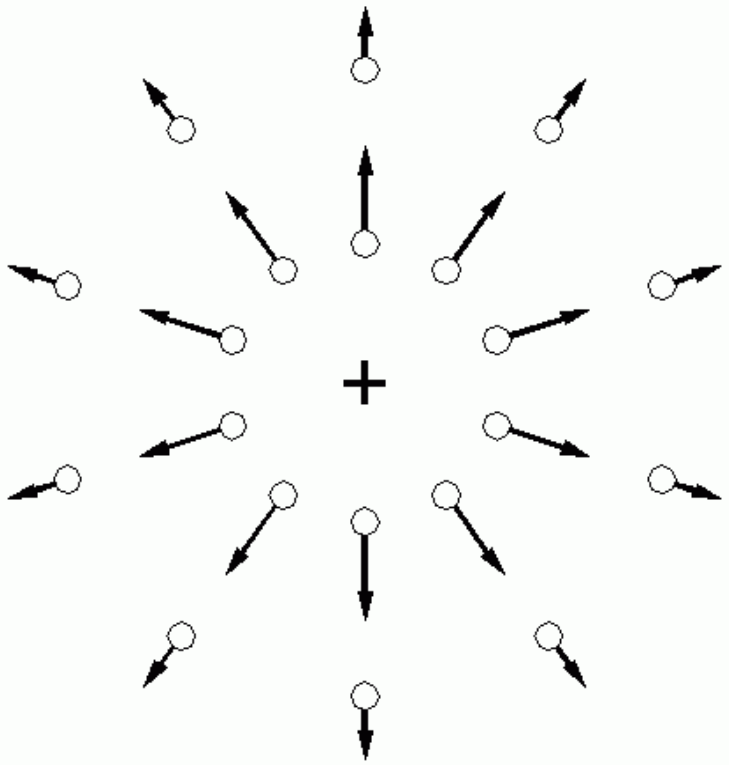
Coherent Diffraction from Crystals

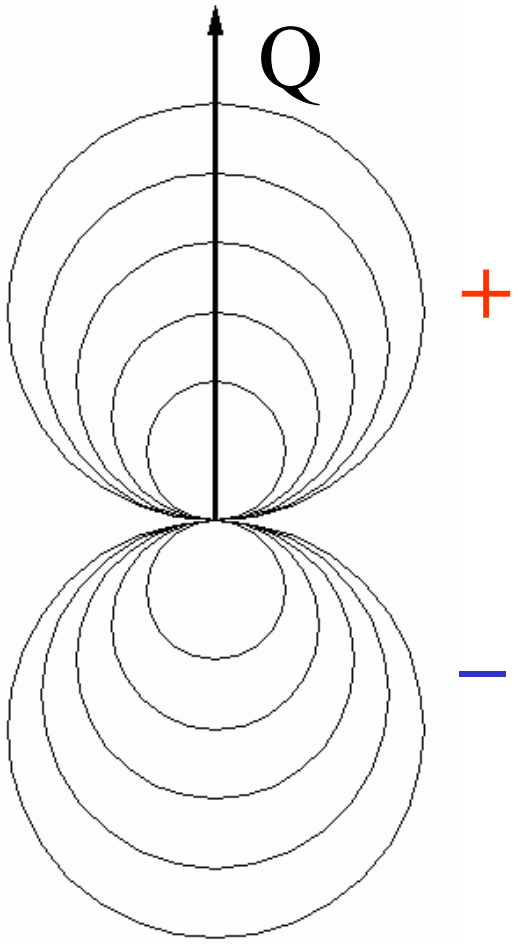


Diffraction by Strain of Point Defect

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

Imaginary density





Good statistics, 3D diffraction data

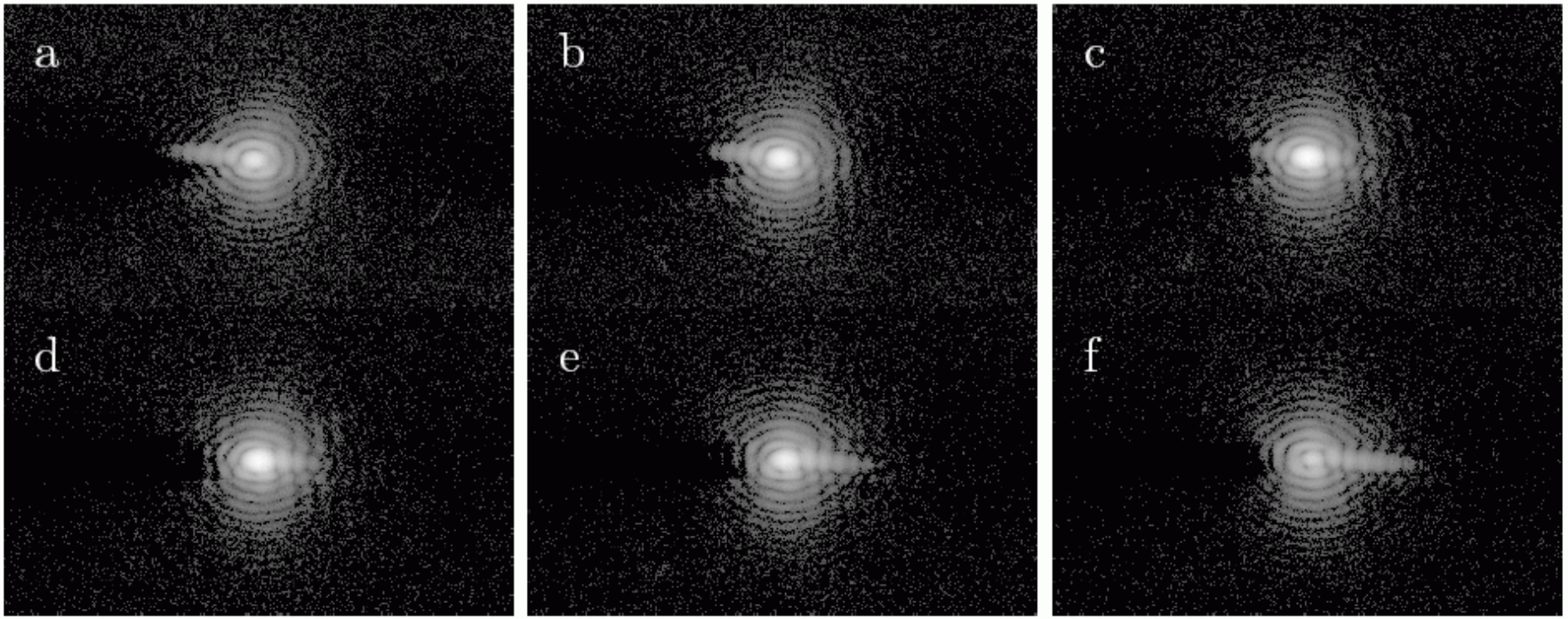
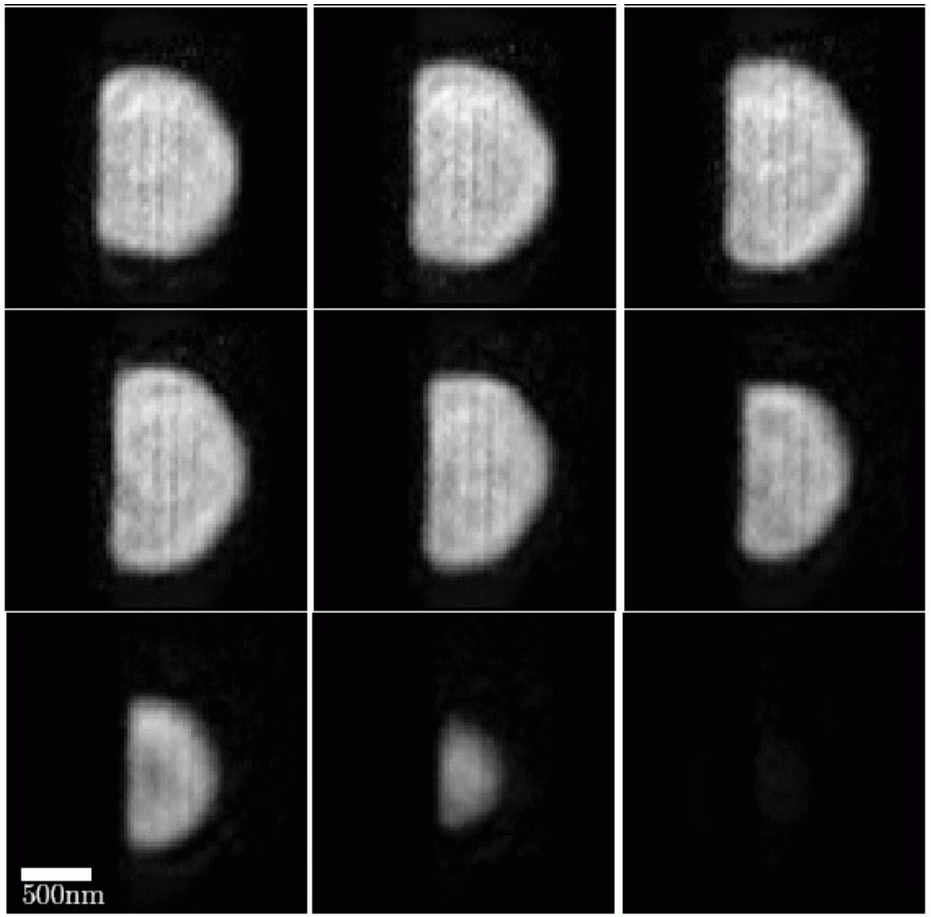
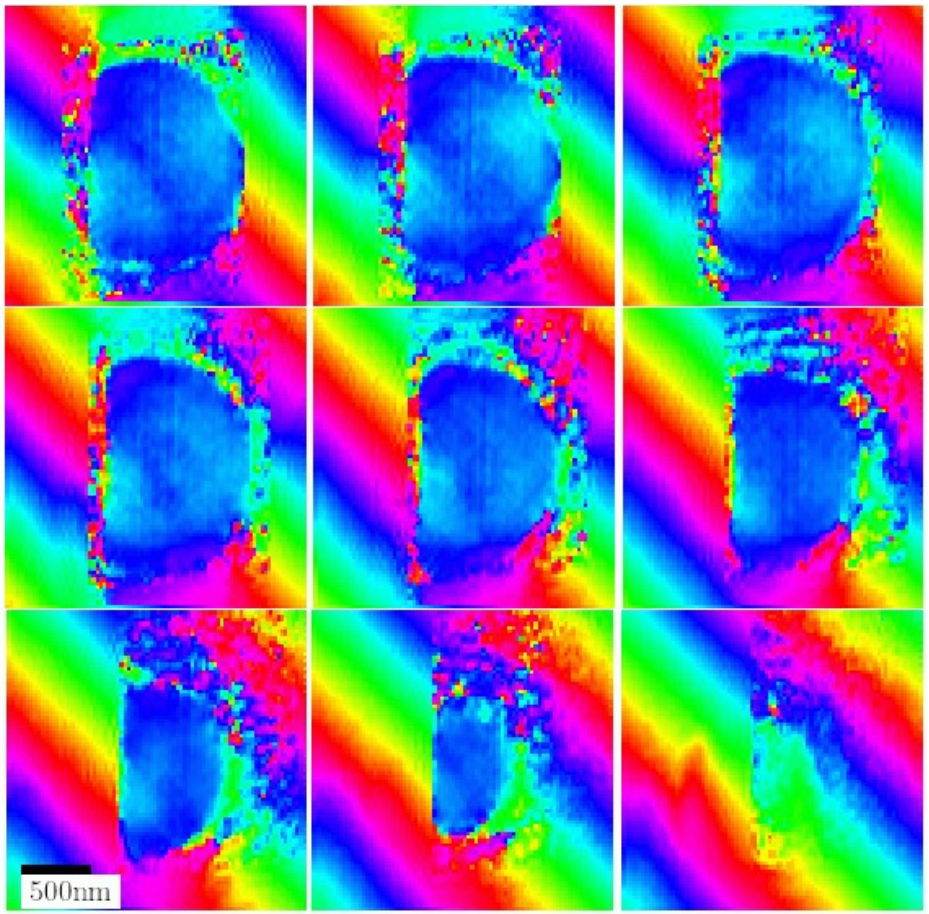


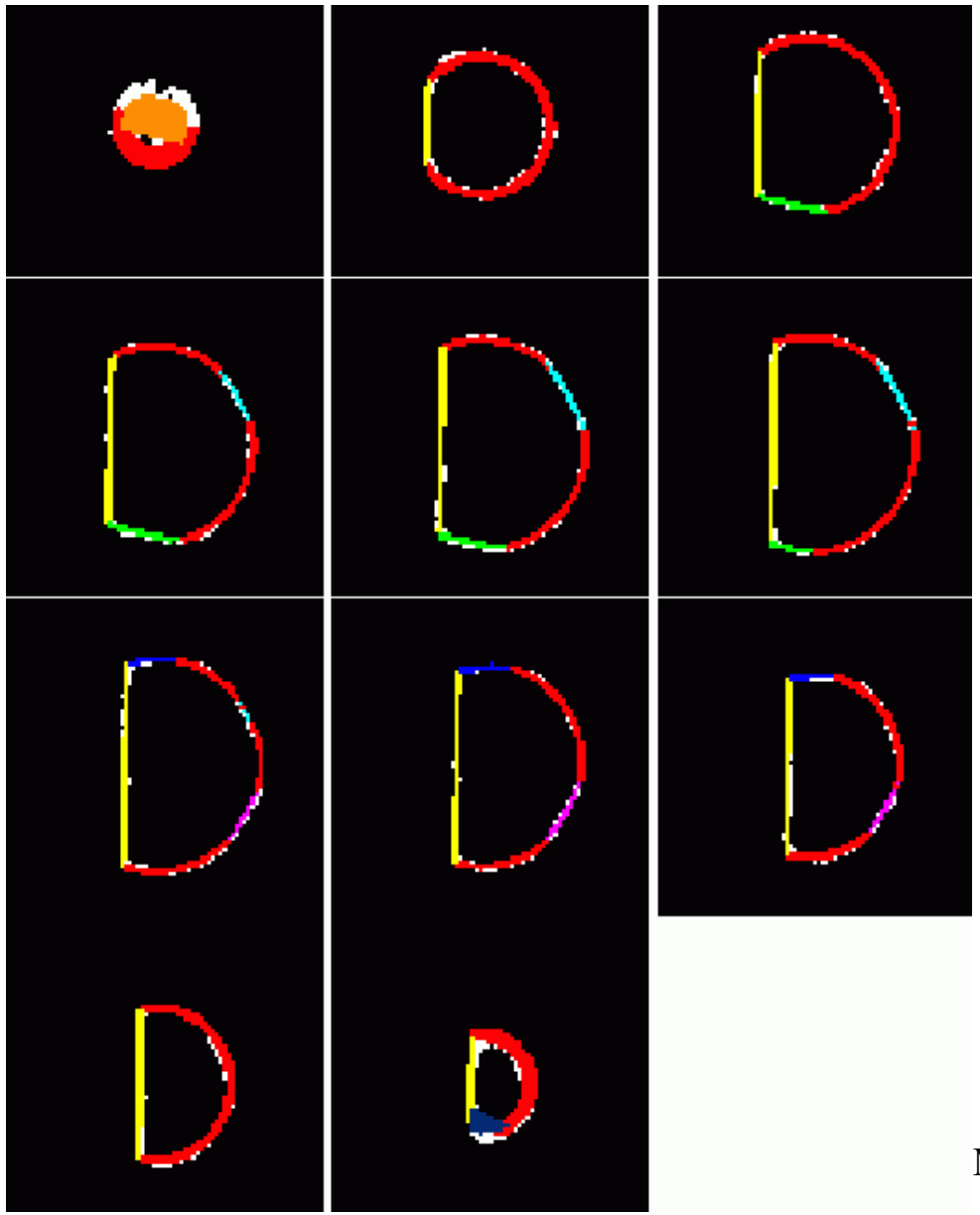
Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

Complex Density (amplitude *and* phase)



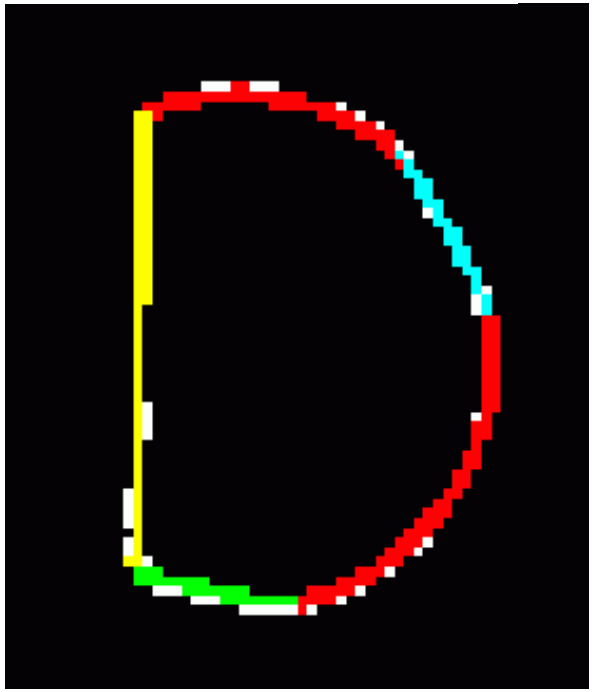


Fitting to facetted shape

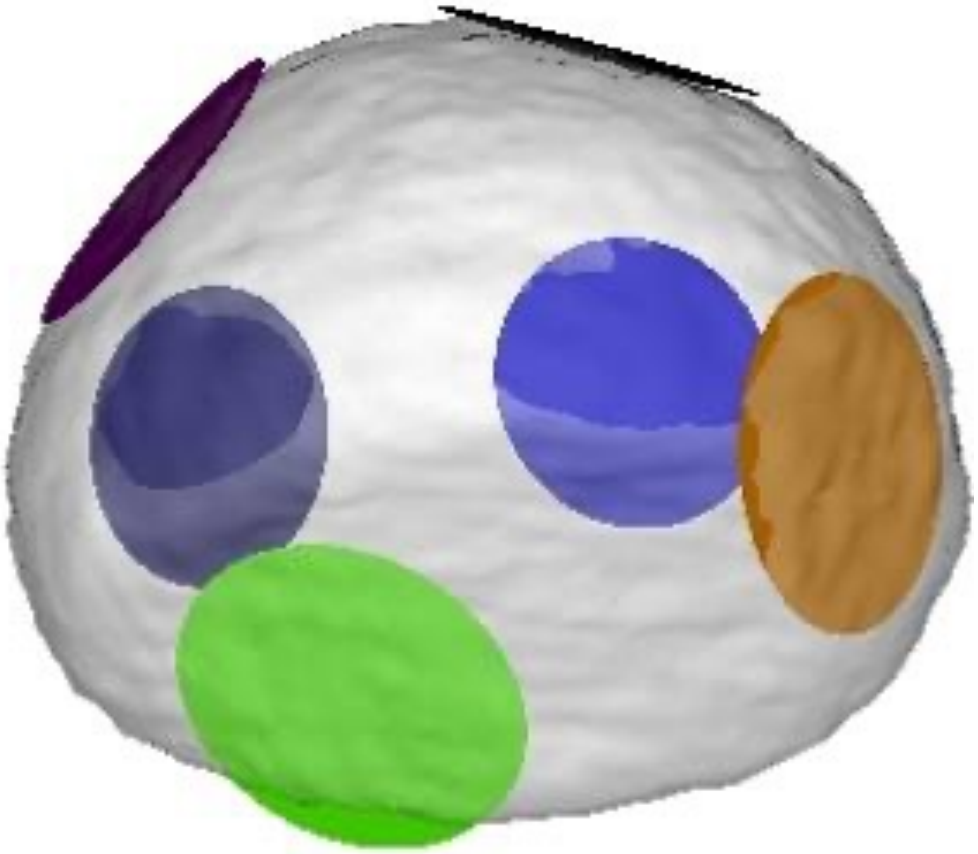


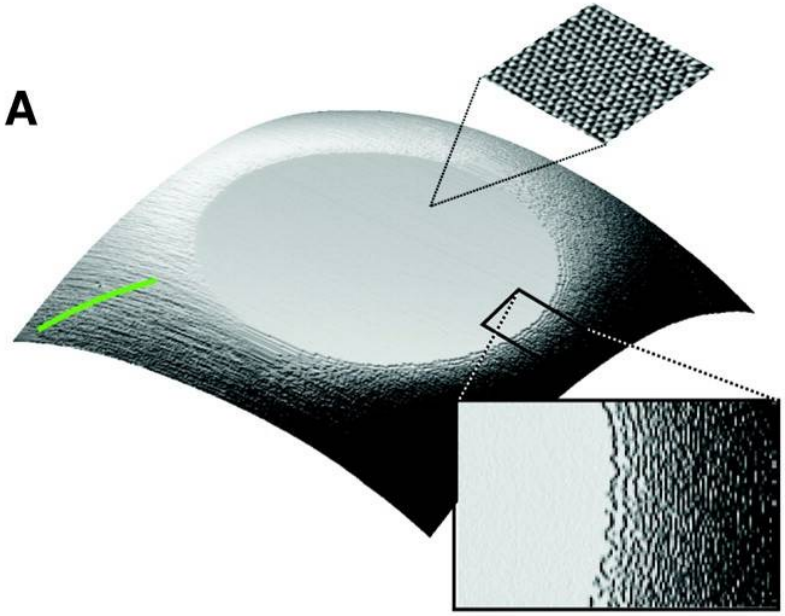
	$\|R\|$		P0	P1	P2	P3	P4	P5	P6
	9.4	P0	0	85	149	79	134	106	71
	25.7	P1		0	123	164	83	76	102
	25.1	P2			0	72	67	74	110
	25.9	P3				0	111	106	76
	25.4	P4					0	113	68
	25.4	P5						0	176
	26.0	P6							0 0

Angles between facets



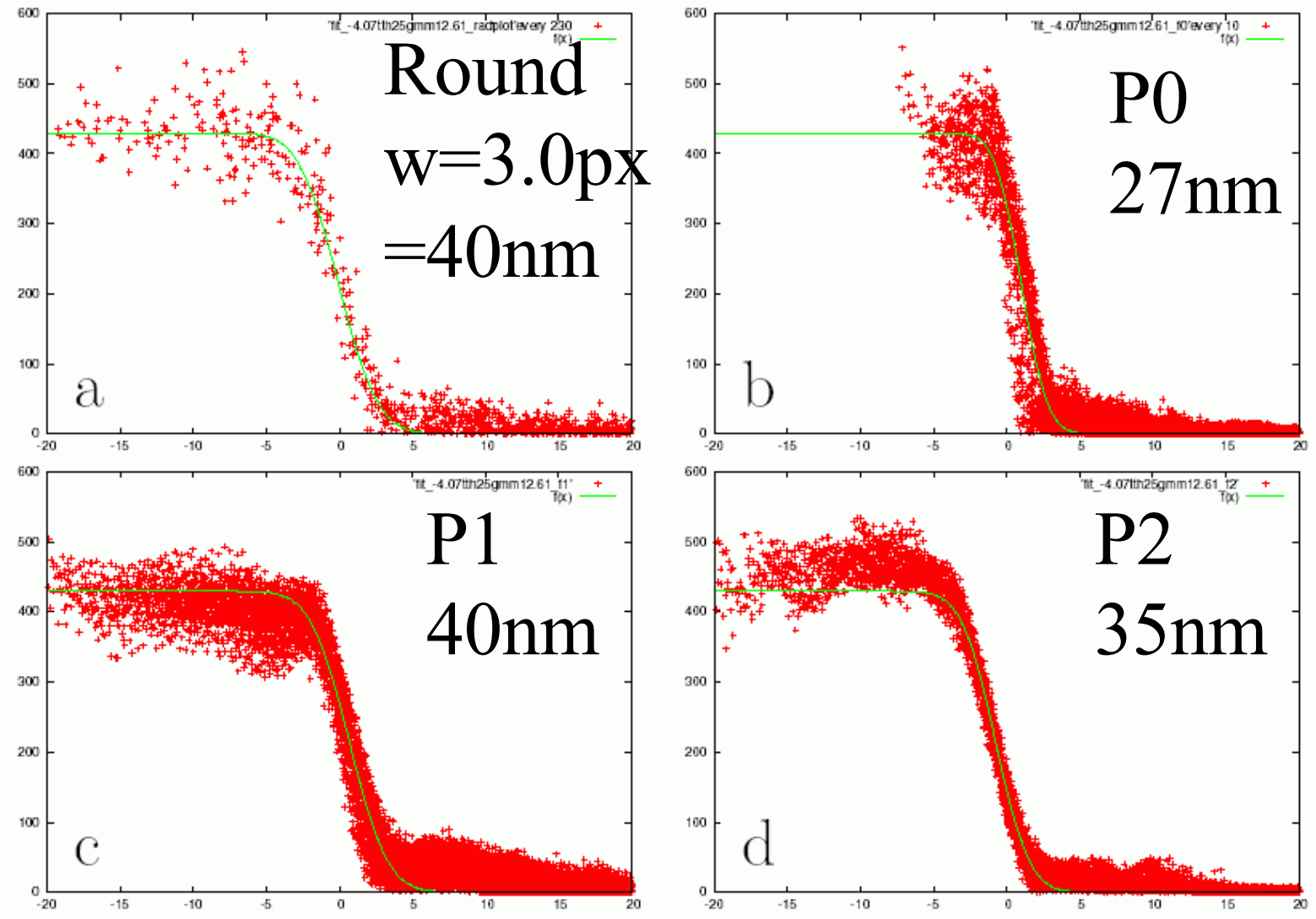
Facets of Equilibrium Crystal Shape



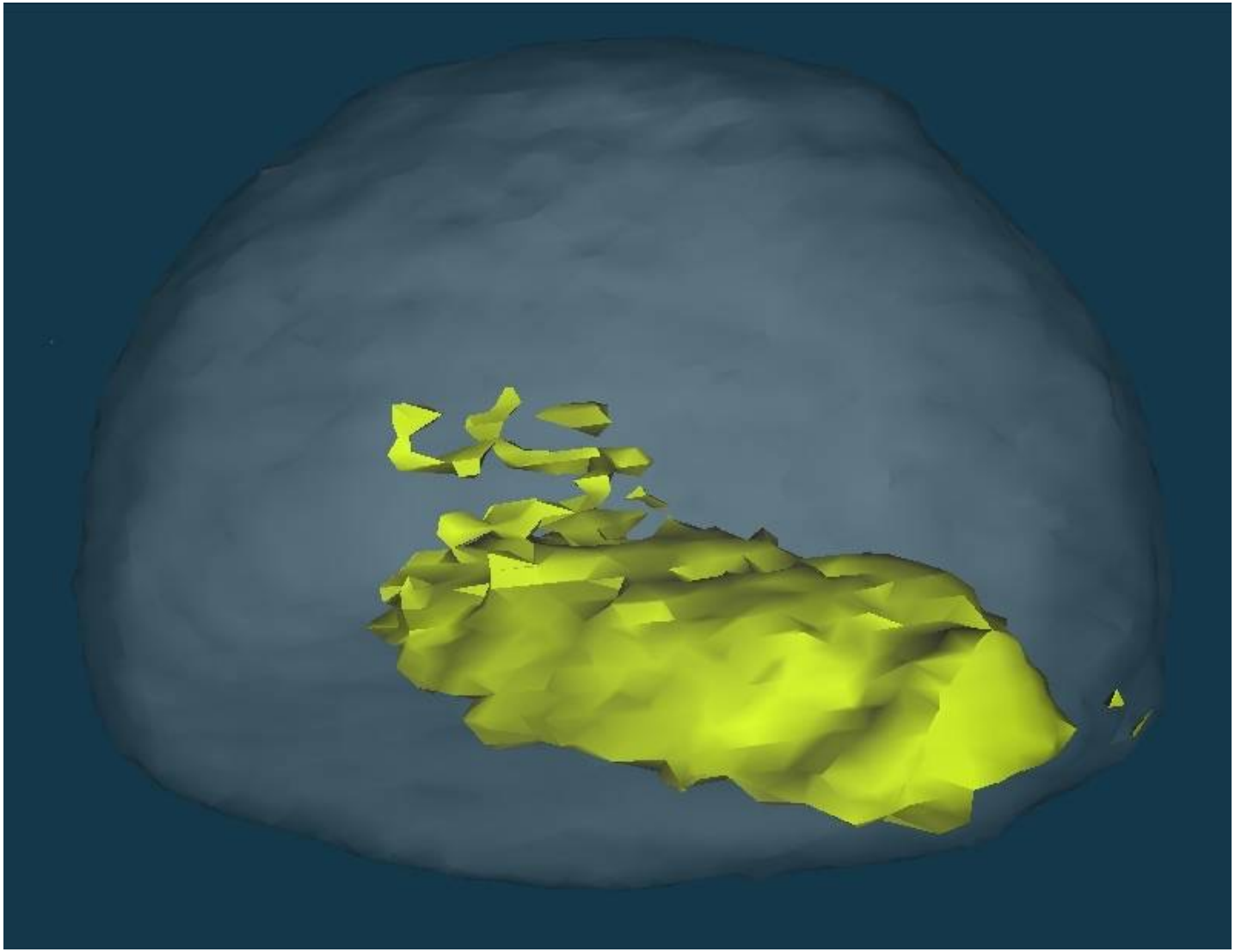


Thurmer K, Williams E, Reutt-Robey J
Science **297** 2033 (2002)

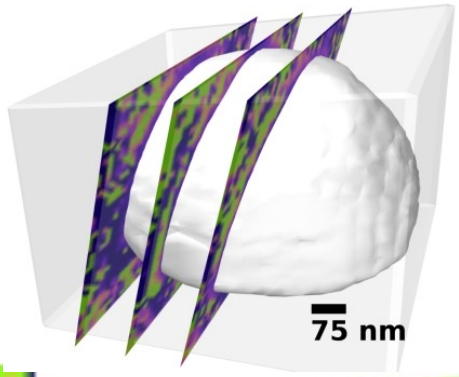
Density distribution across surface

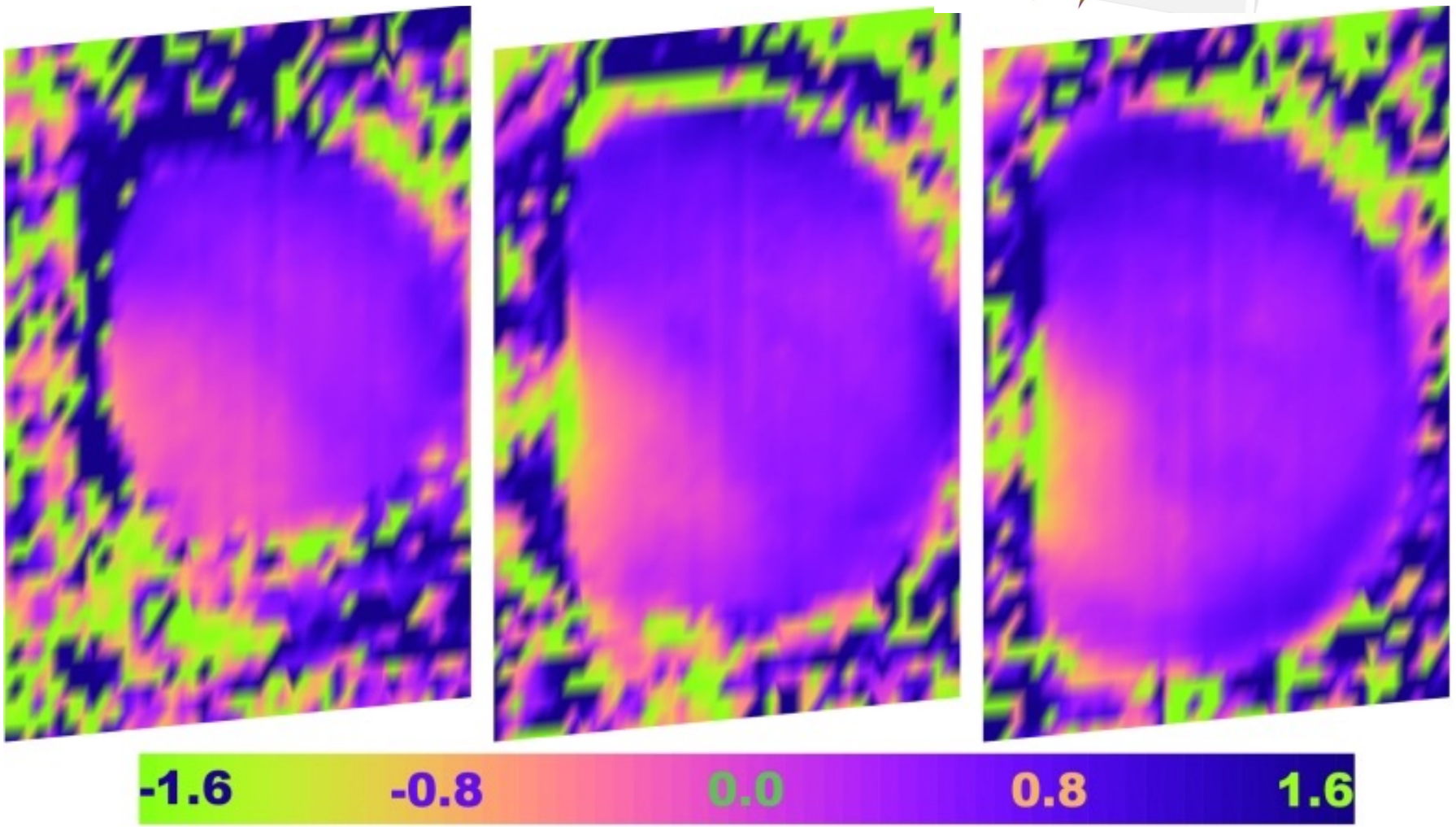


Modeling of 3D Phase Bump

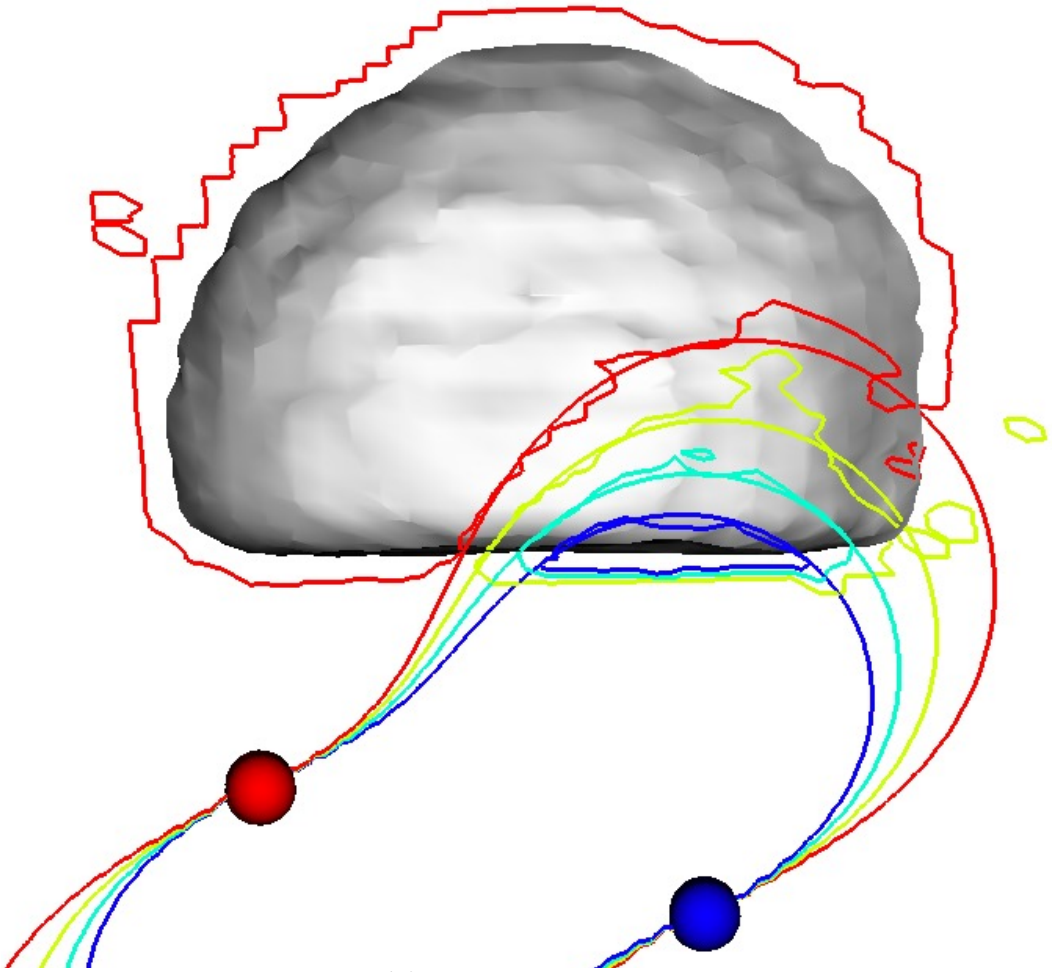


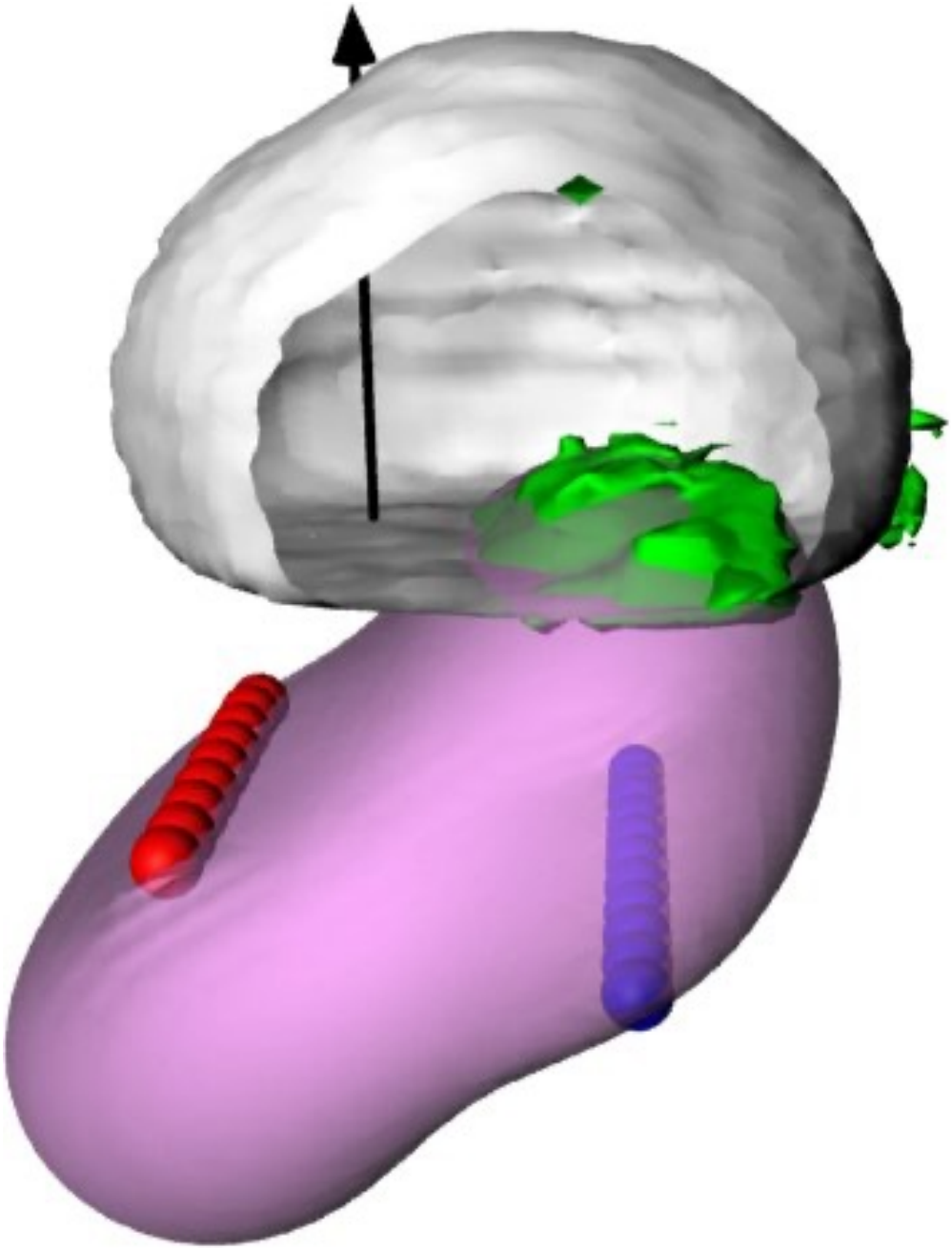
3D phase map sections





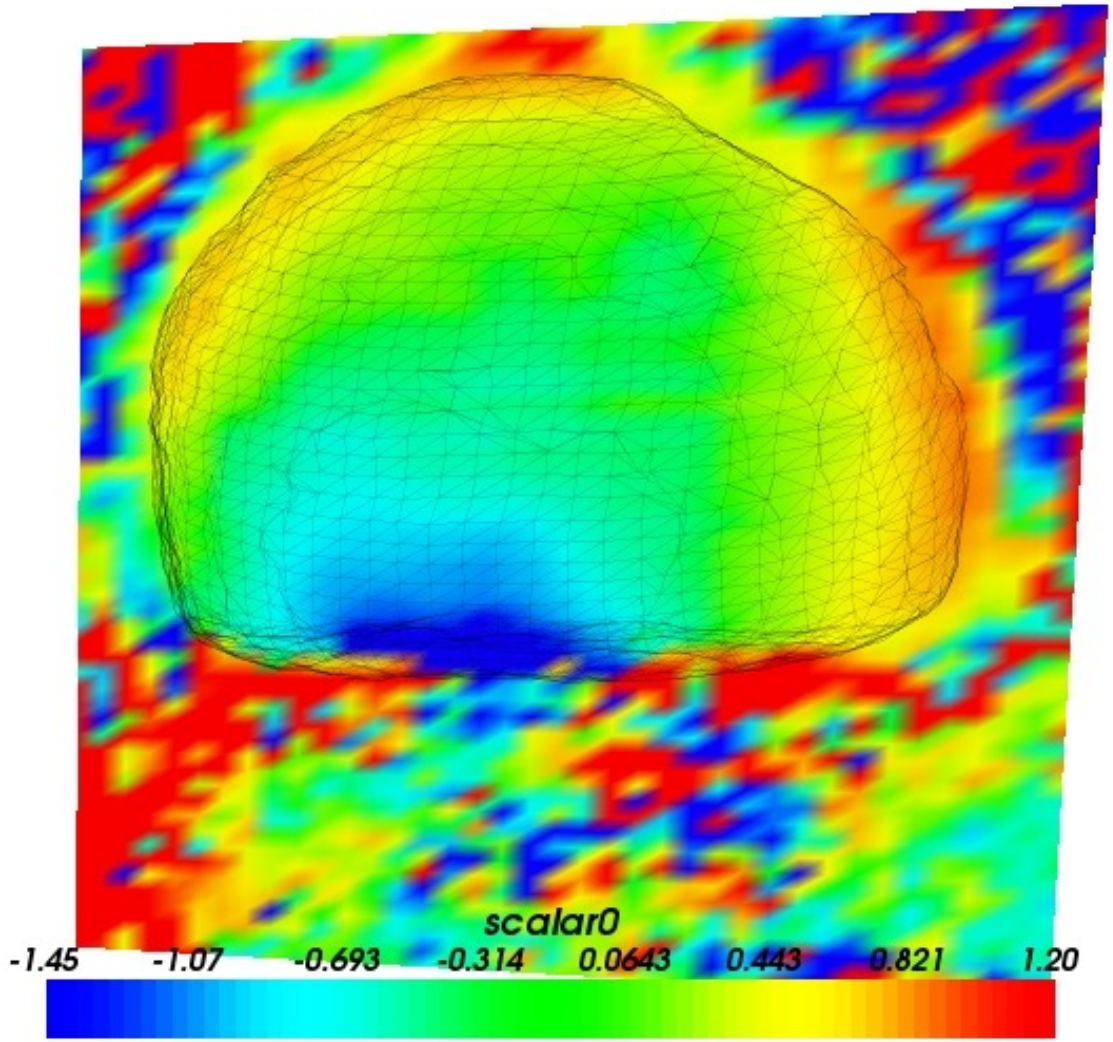
Field lines of Point Charges





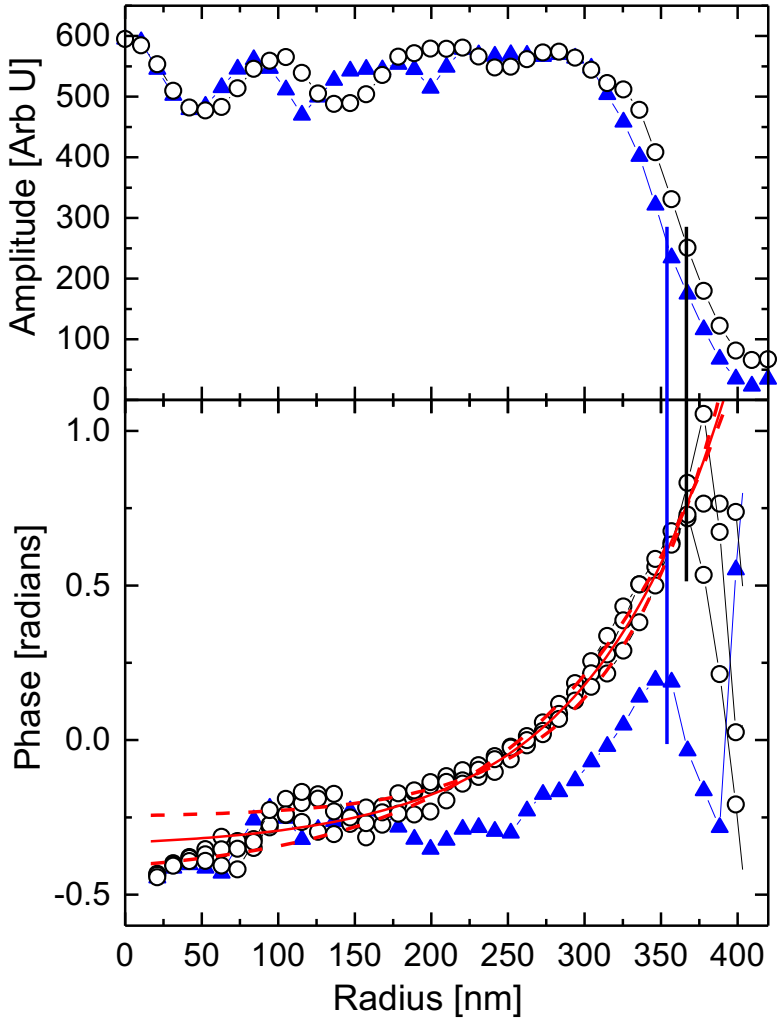
Contours showing Positive Phase

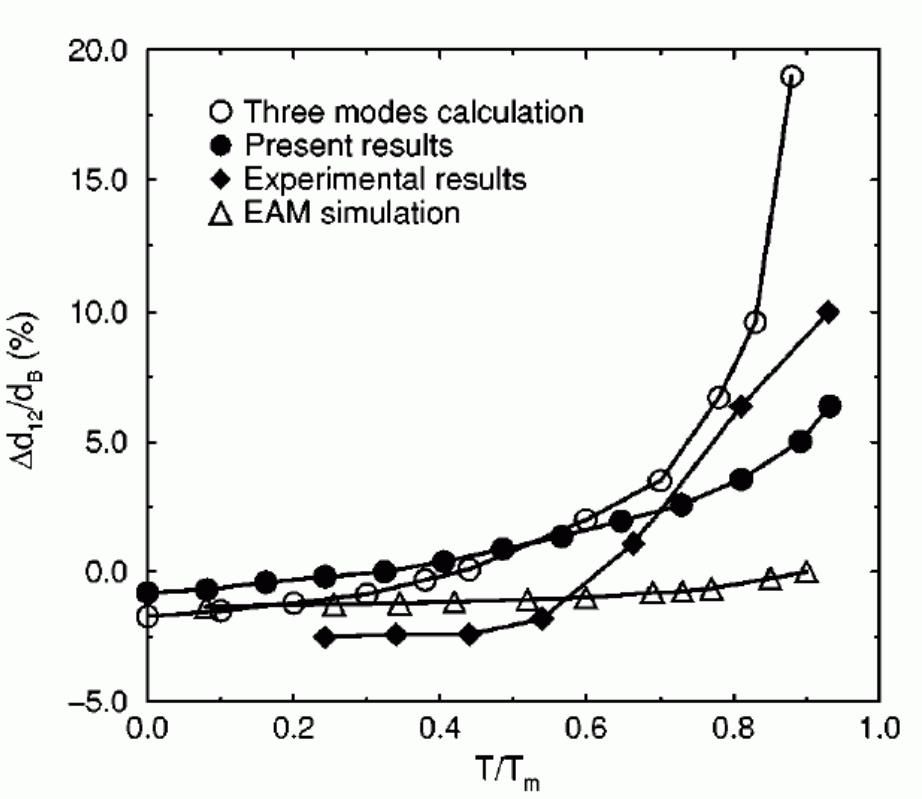
including correction for refraction by crystal



Surface Thermal Expansion

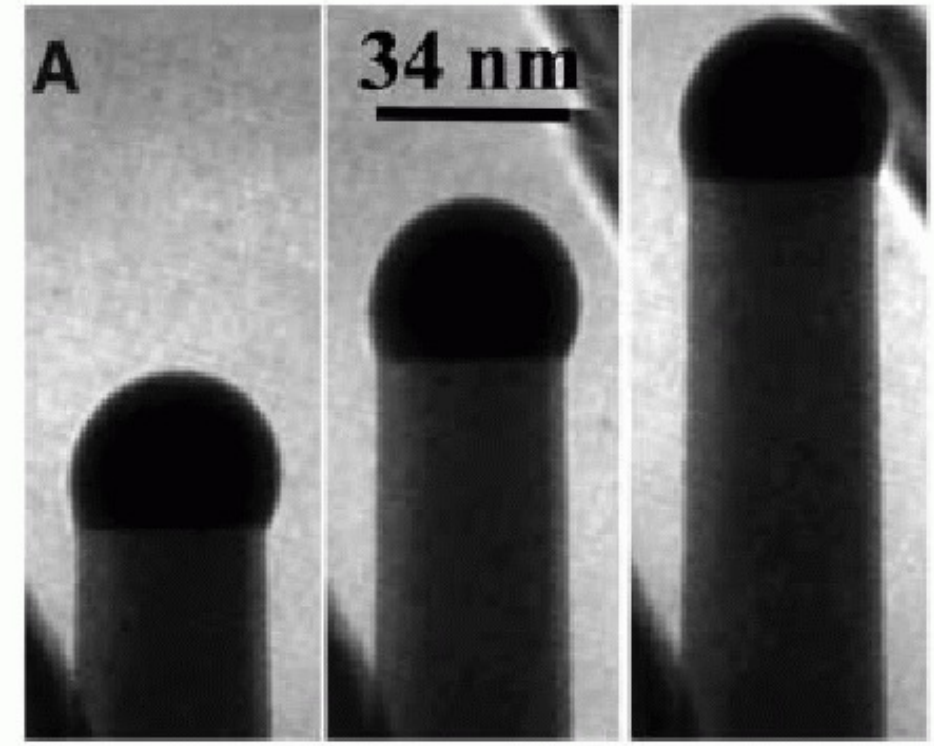
Ag(111): Scheffler et al PRB 59 970 (1999)

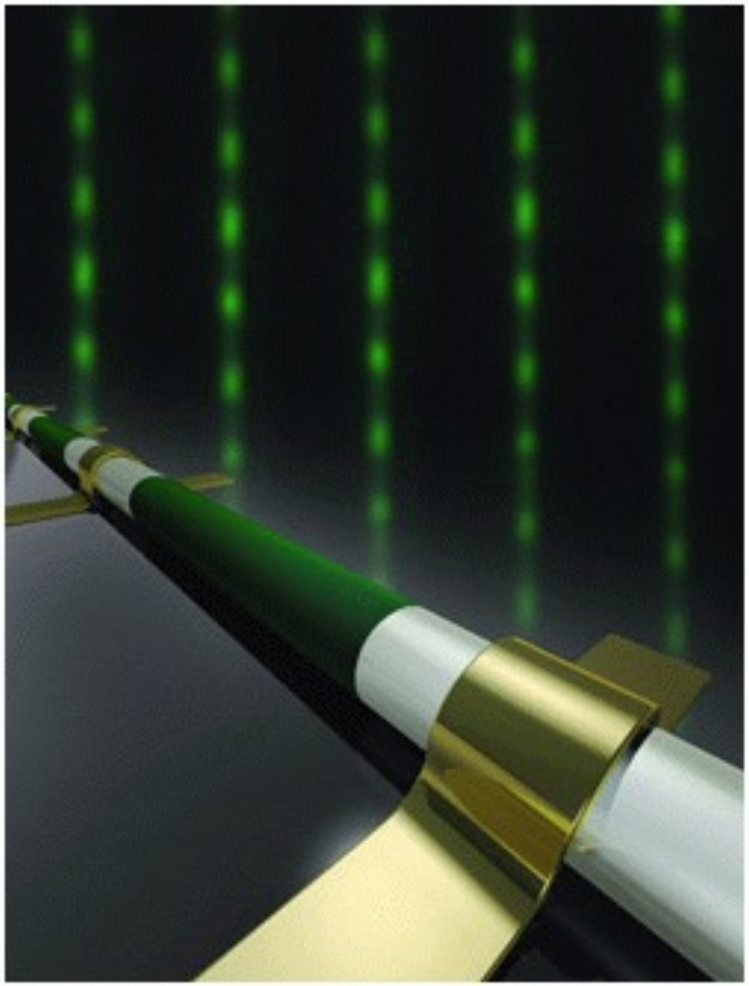




VLS growth of nanowires

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



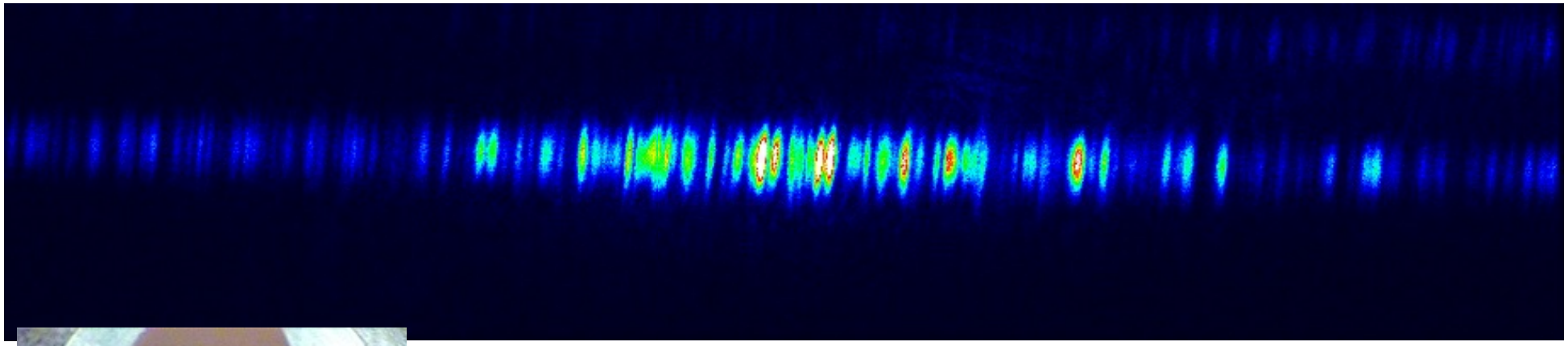


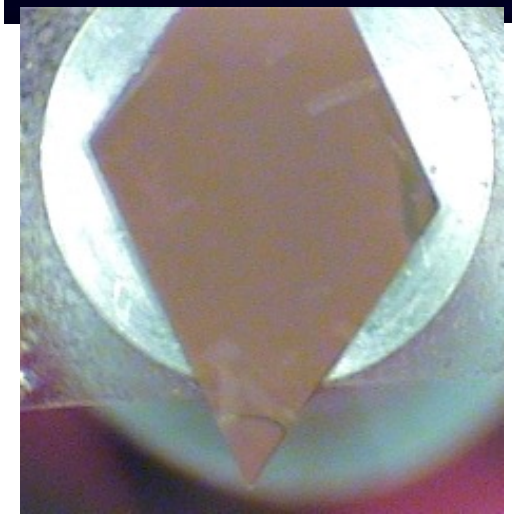
NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

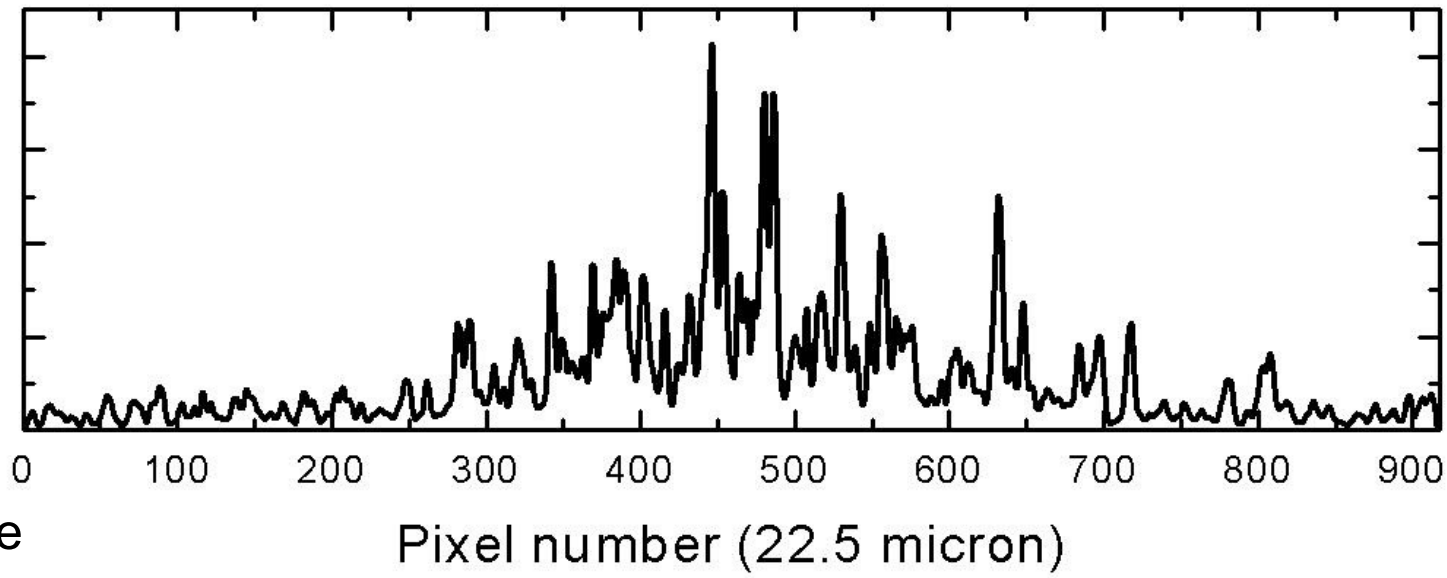
I. K. Robinson, eMRS S

GaAs Nanowire "Barcode"

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



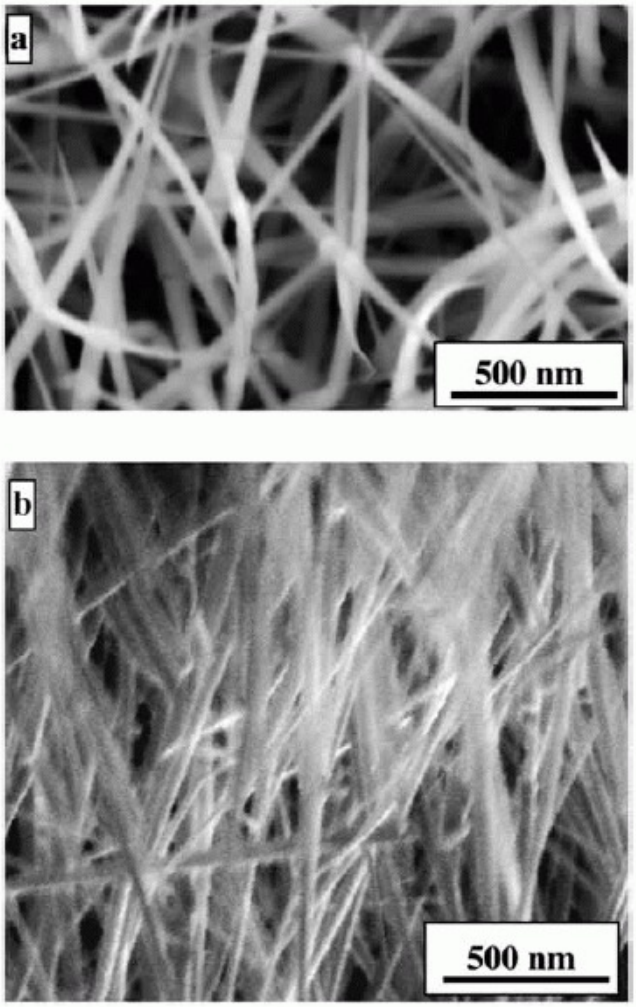


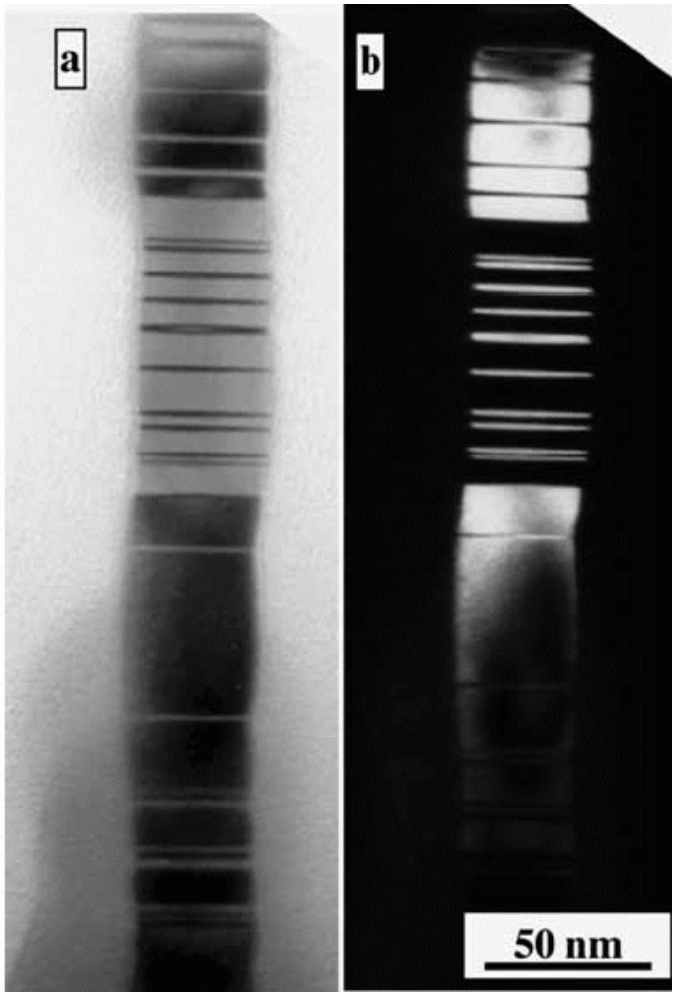


GaAsNW1106-22.spe
B9348 from Philips

Dark Field TEM of GaAs Nanowires

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

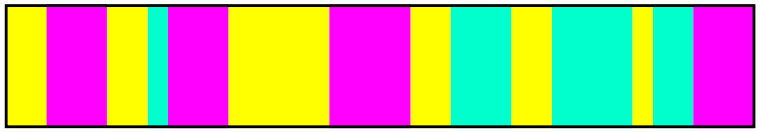




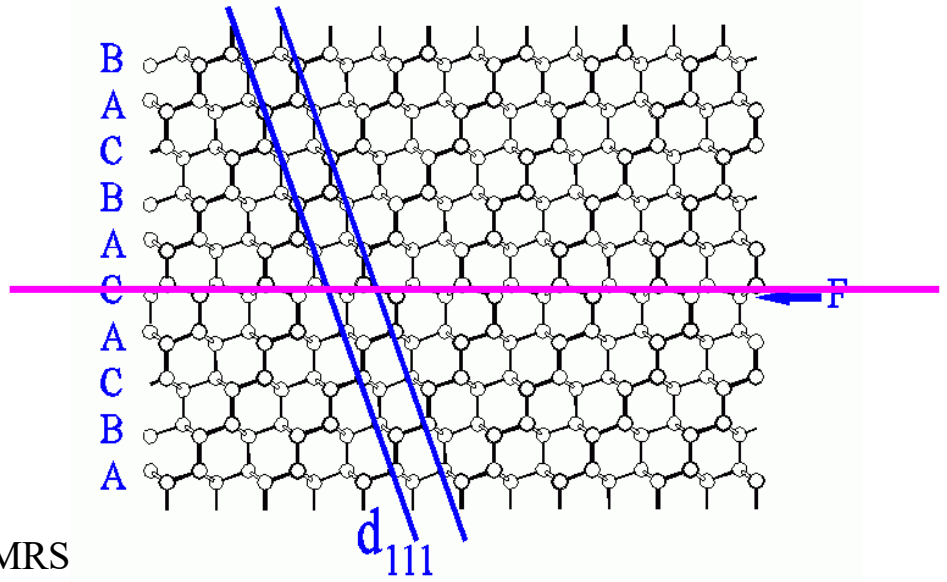
Models of Barcode Diffraction

(111) wires at (11-1) reflection

- Twinned stacking sequence

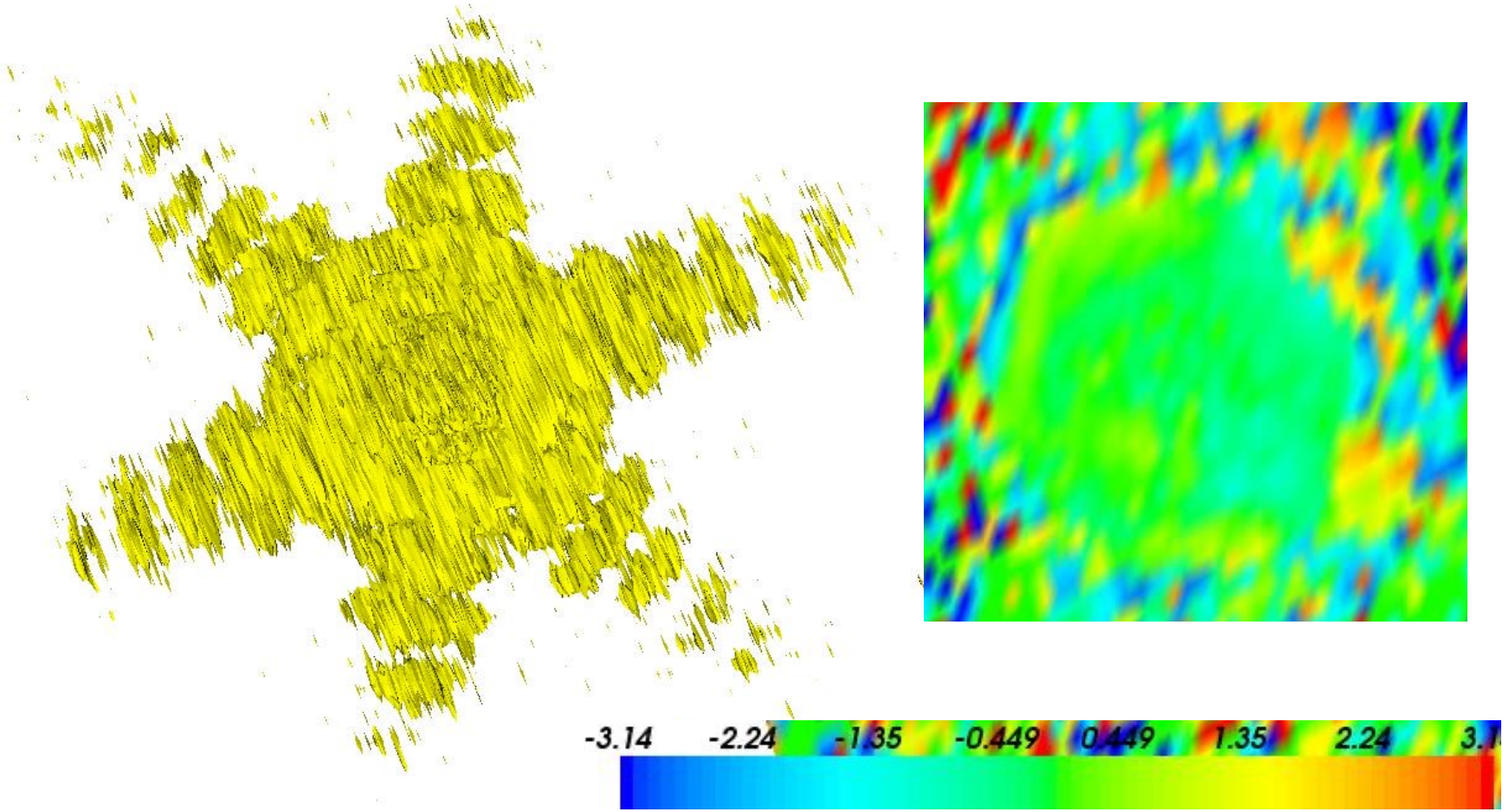


- Deformation faults



ZnO Nanowire Reconstruction

Ross Harder, Steven Leake, PhD project at UCL



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