3D Strain Mapping inside Individual Nanocrystals

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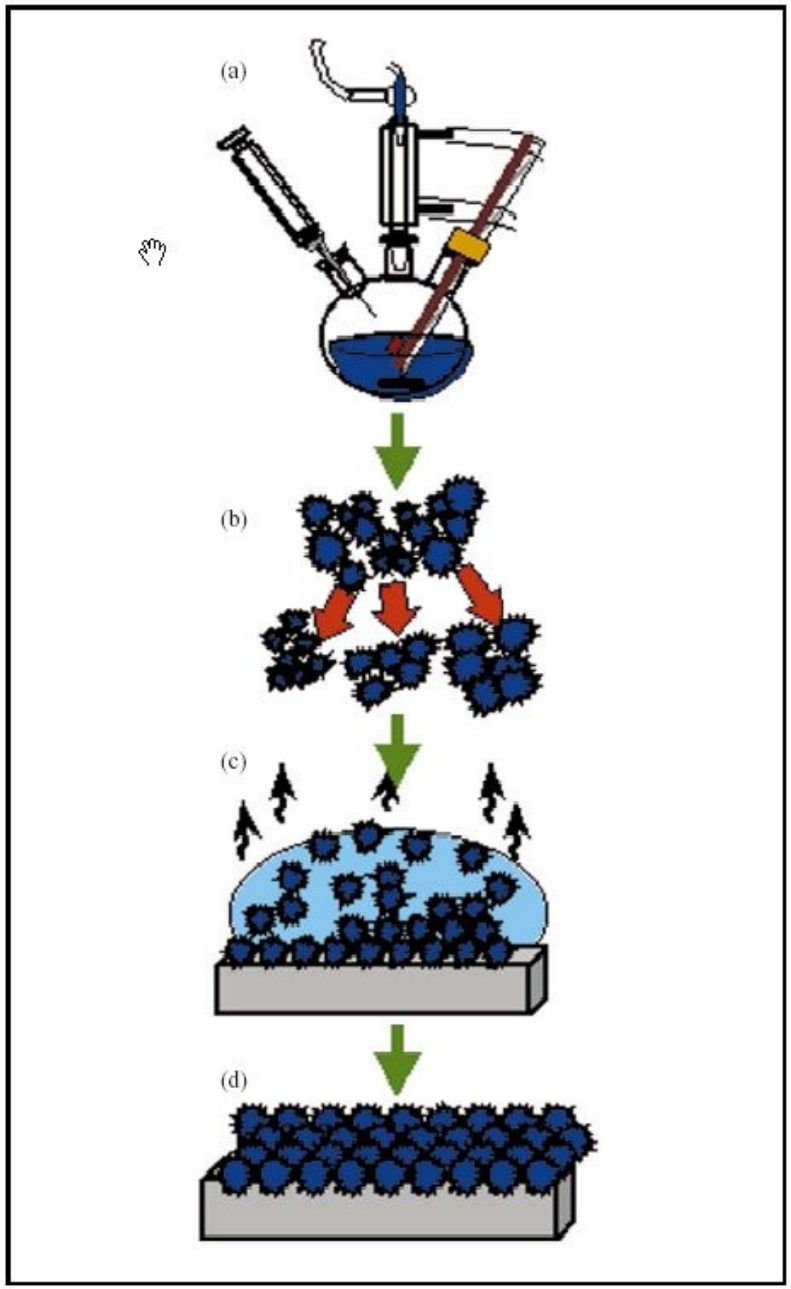
Outline

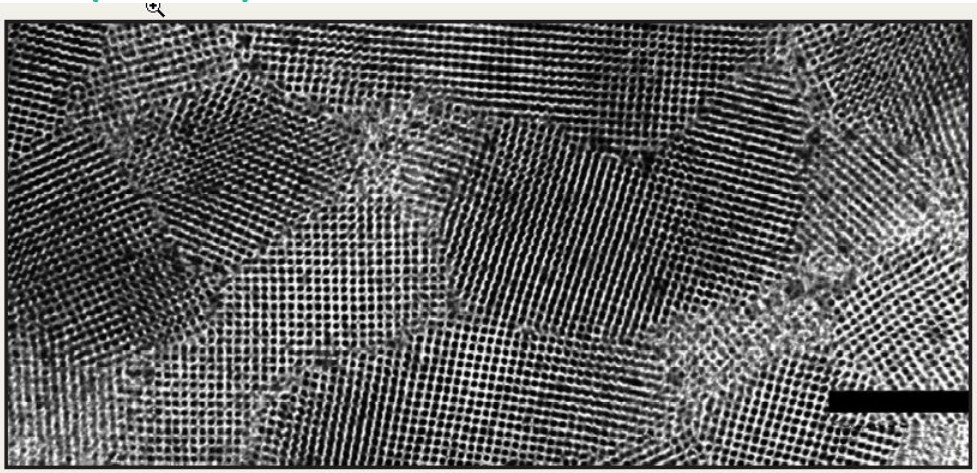
- Coherent x-ray diffraction
- CXD can solve the phase problem
- Extension to phase objects
- Nanocrystal structures
- Nanowire structures

Chemical Synthesis of Nanocrystals

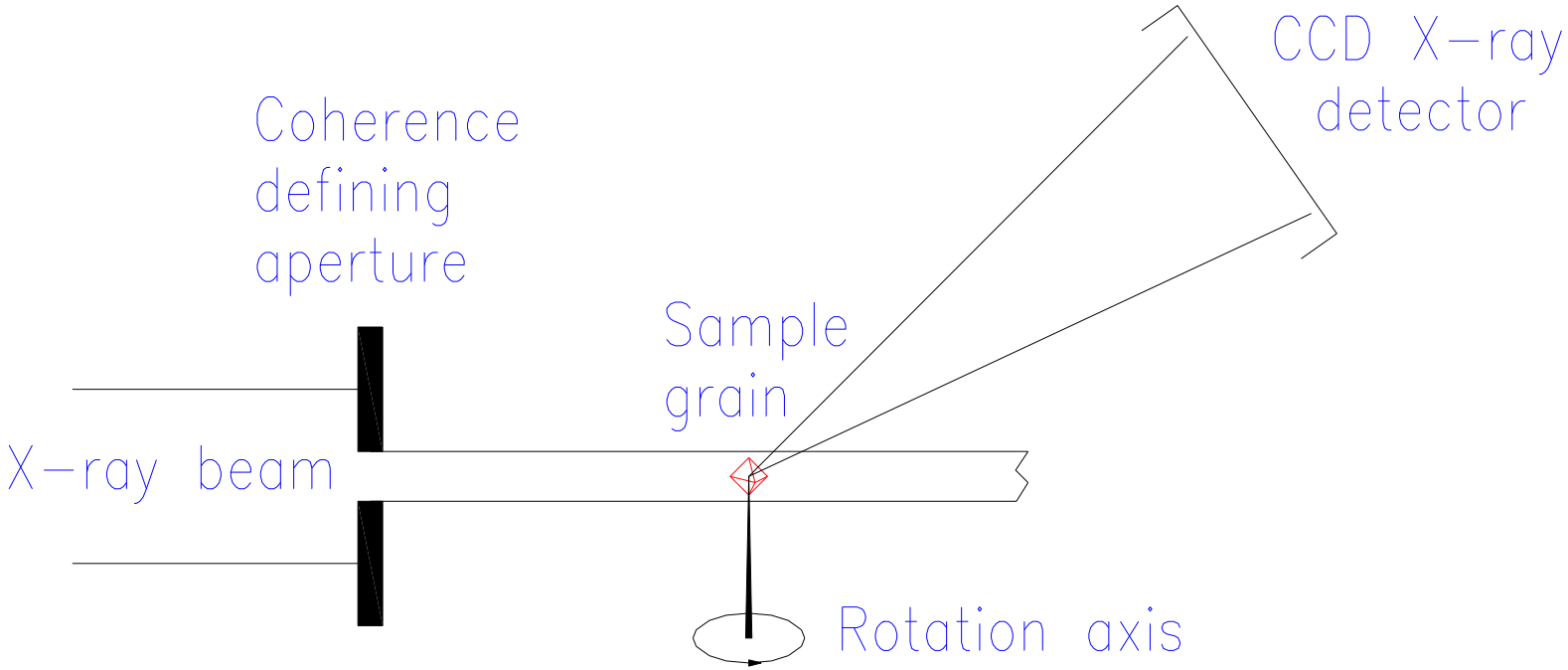


- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

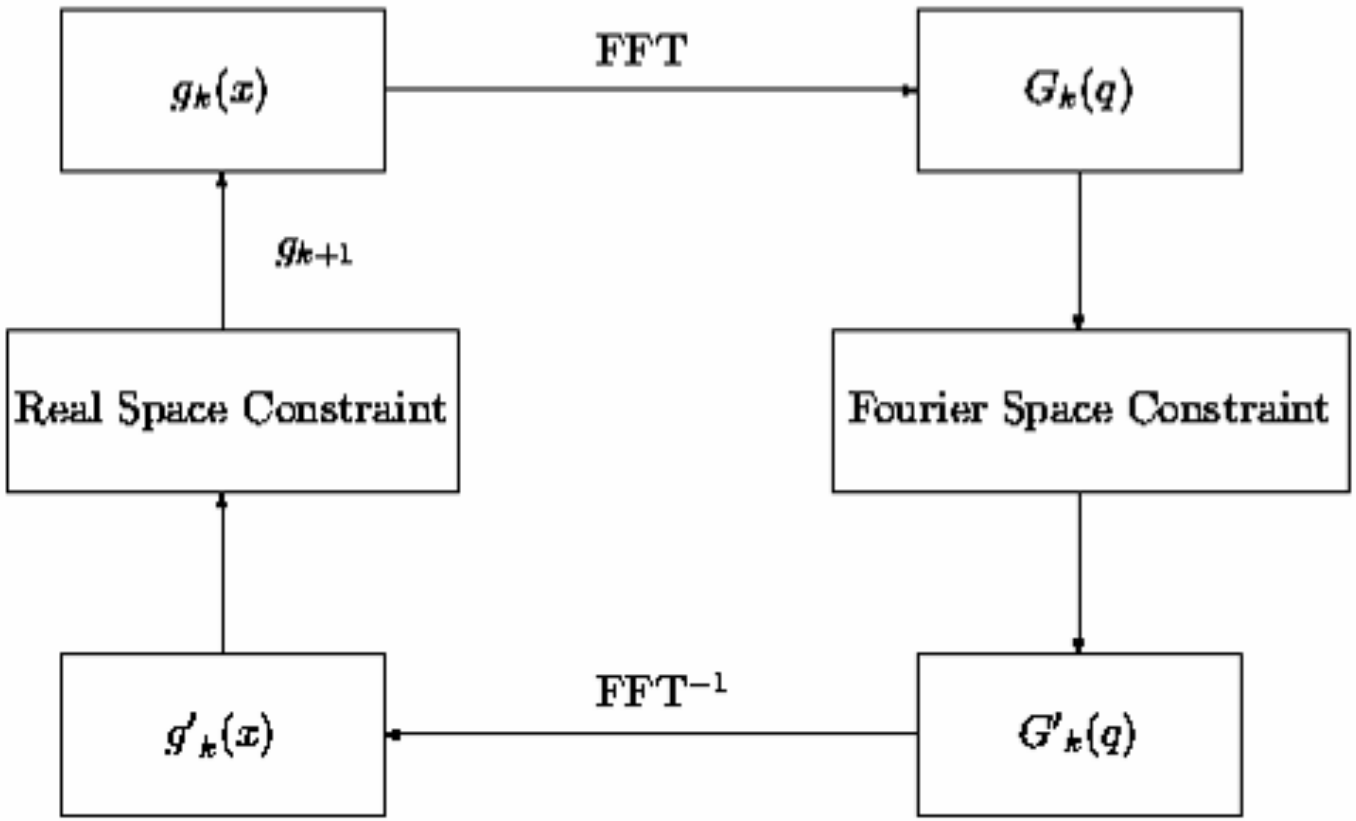
C. B. Murray, IBM J. Res. & Dev. **45** 47 (2001)



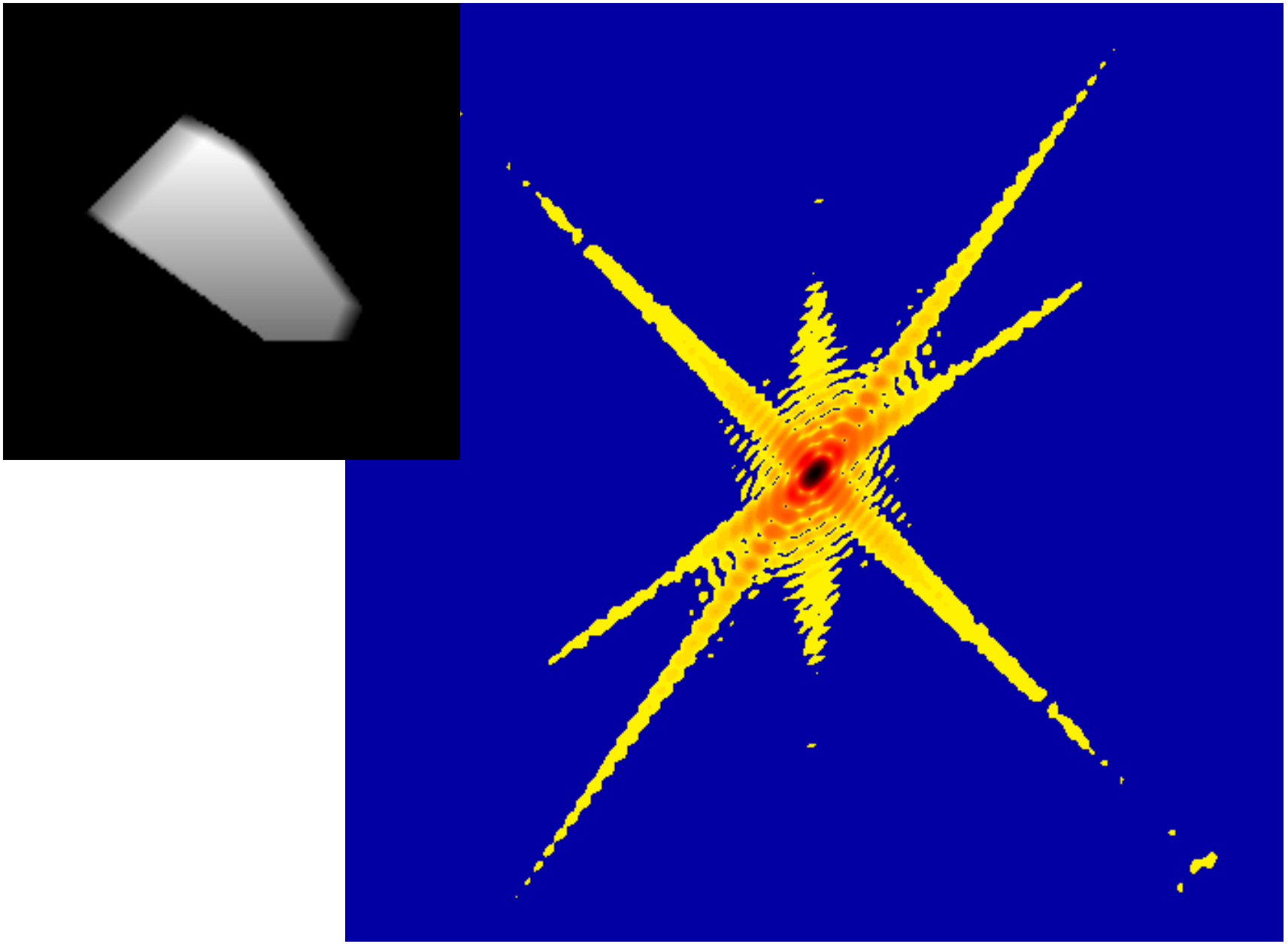
Lensless X-ray Microscope

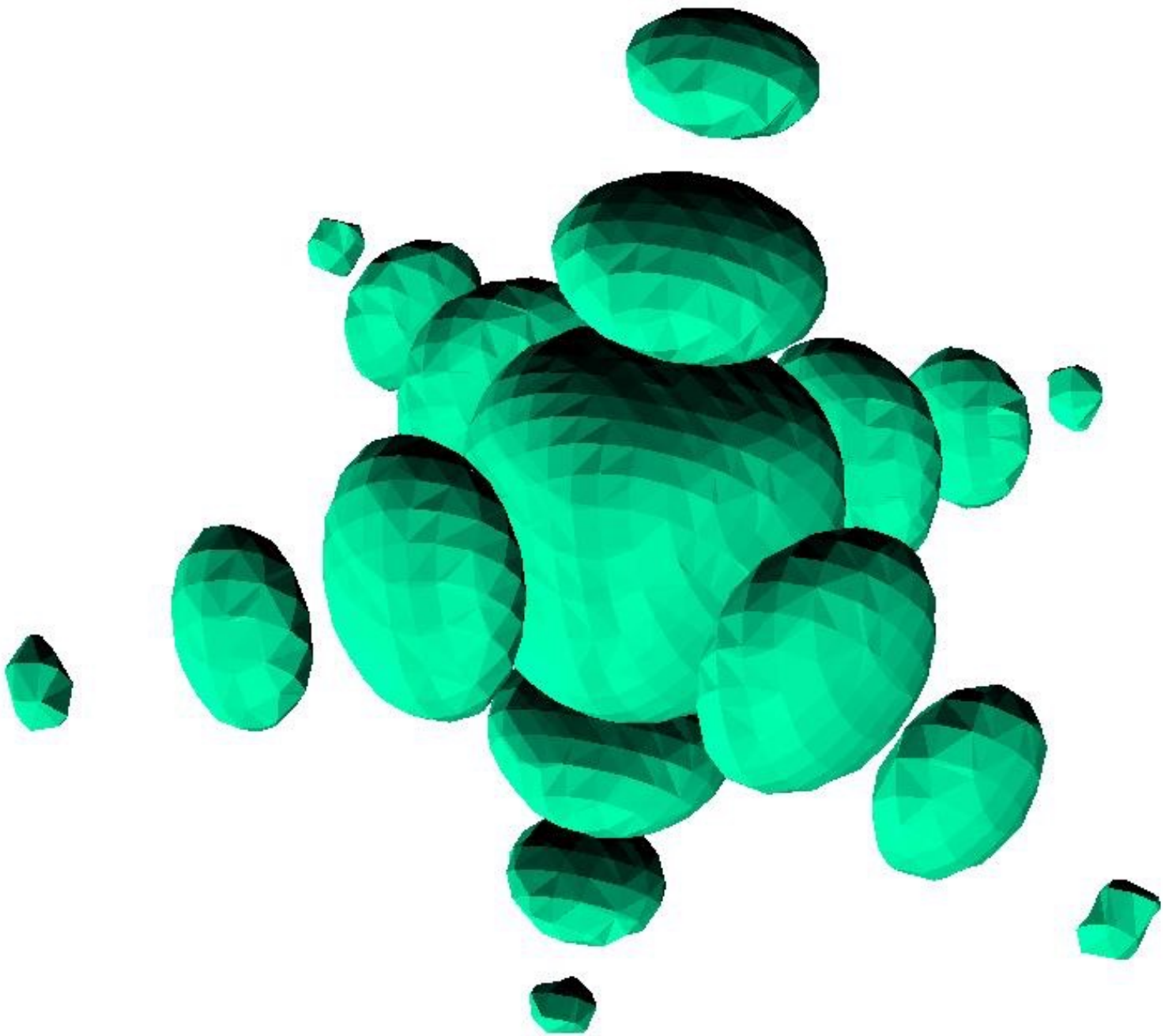


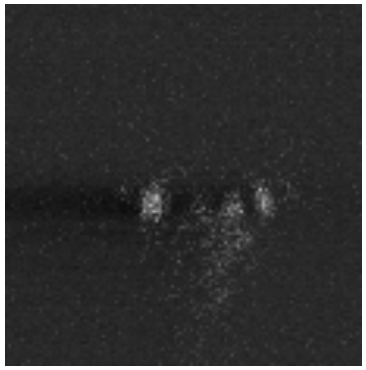
Generic "Error Reduction" method

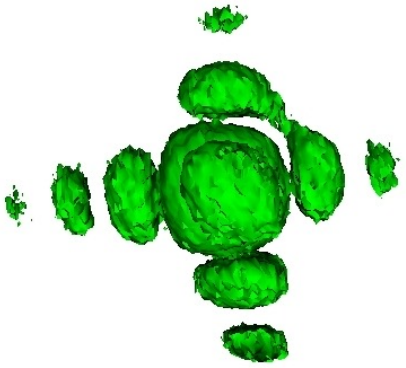


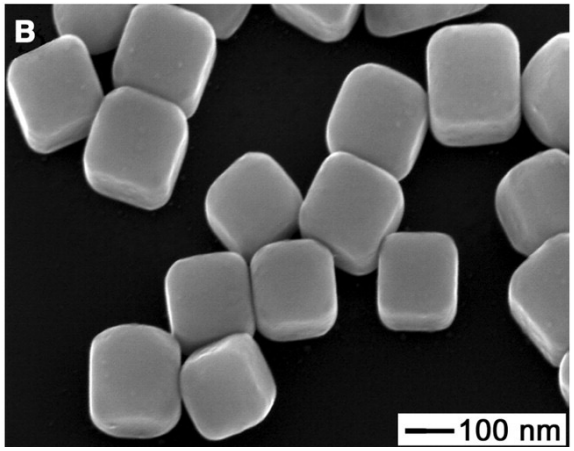
J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

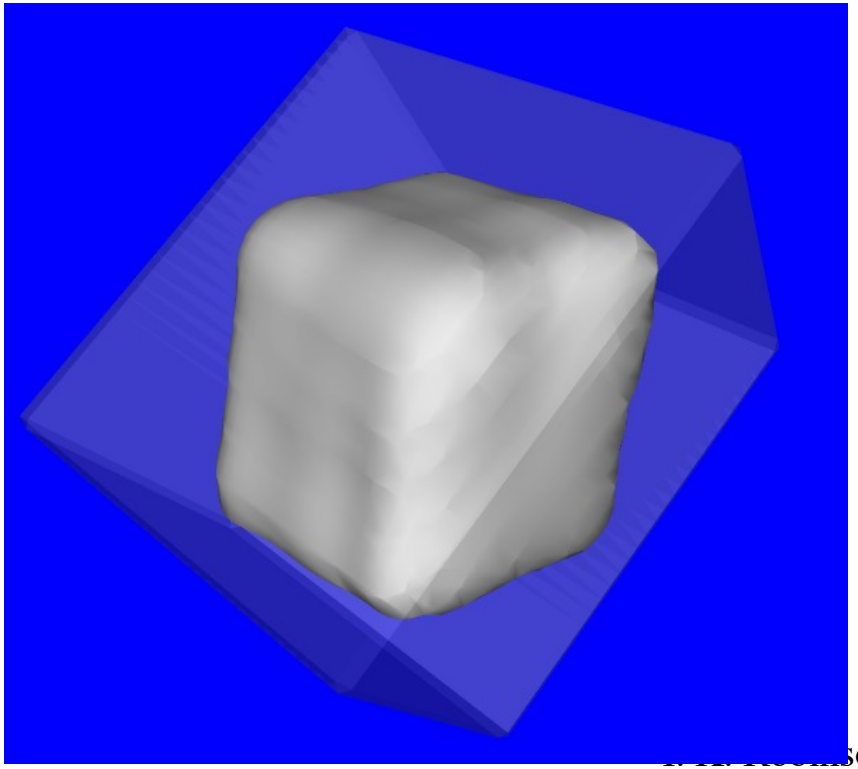


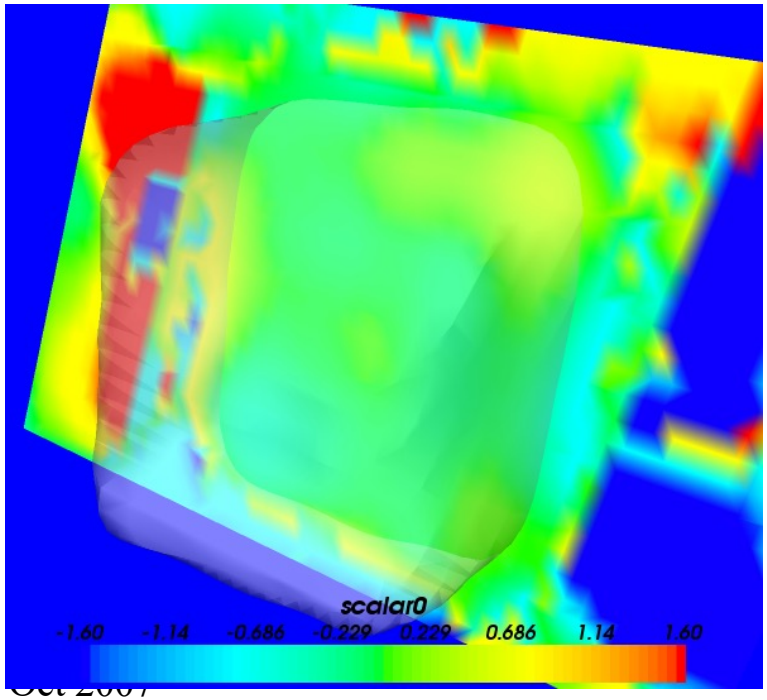




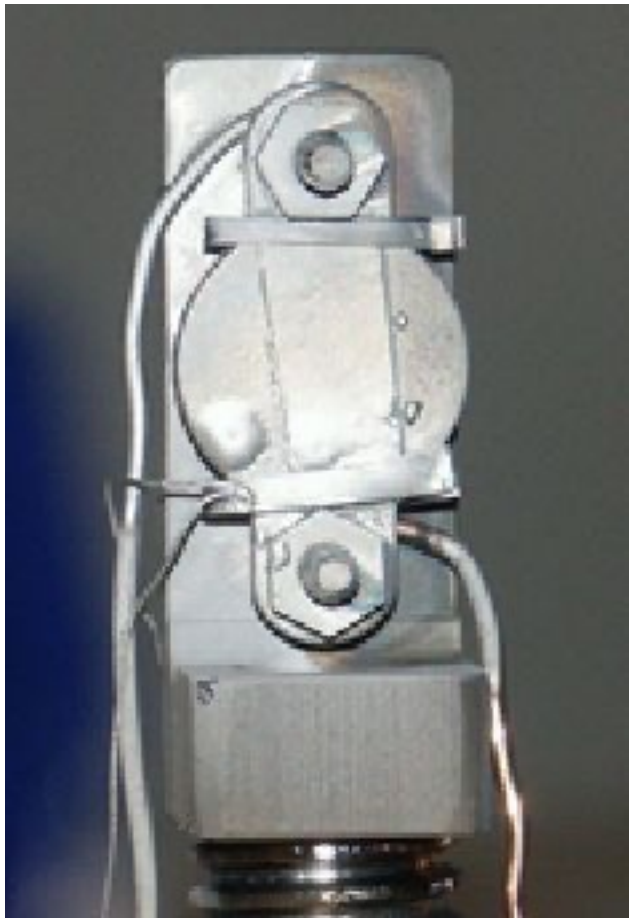


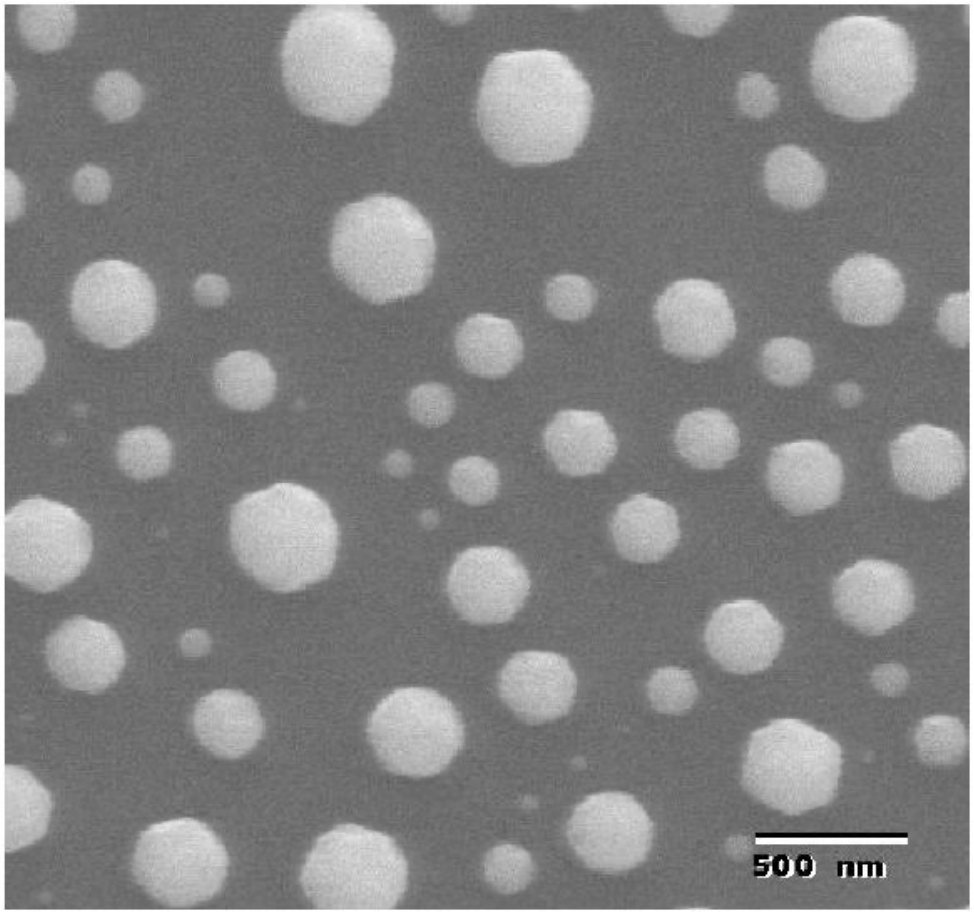

B
100 nm



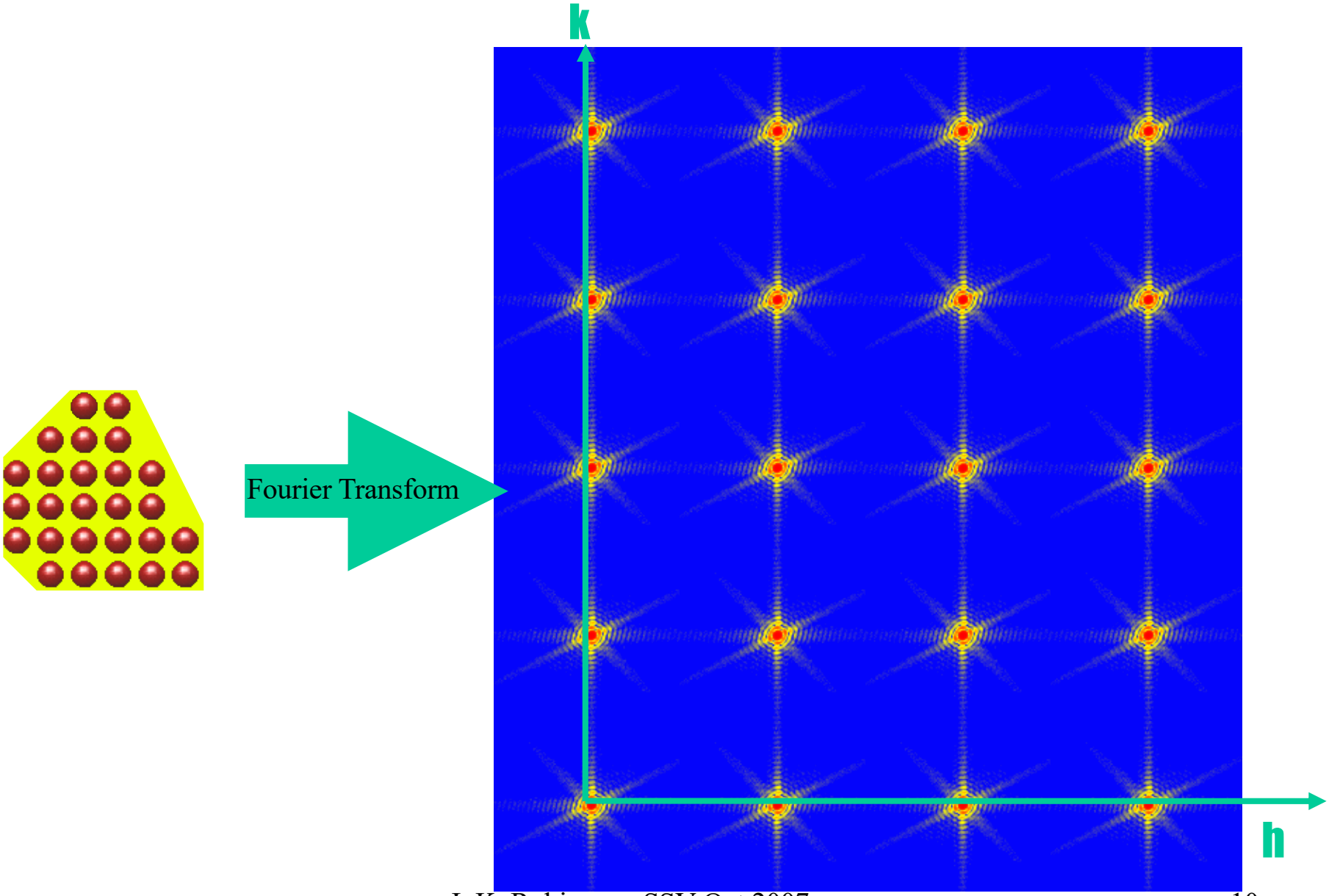

scalar0
-1.60 -1.14 -0.686 -0.229 0.229 0.686 1.14 1.60

In situ growth of Pb crystals





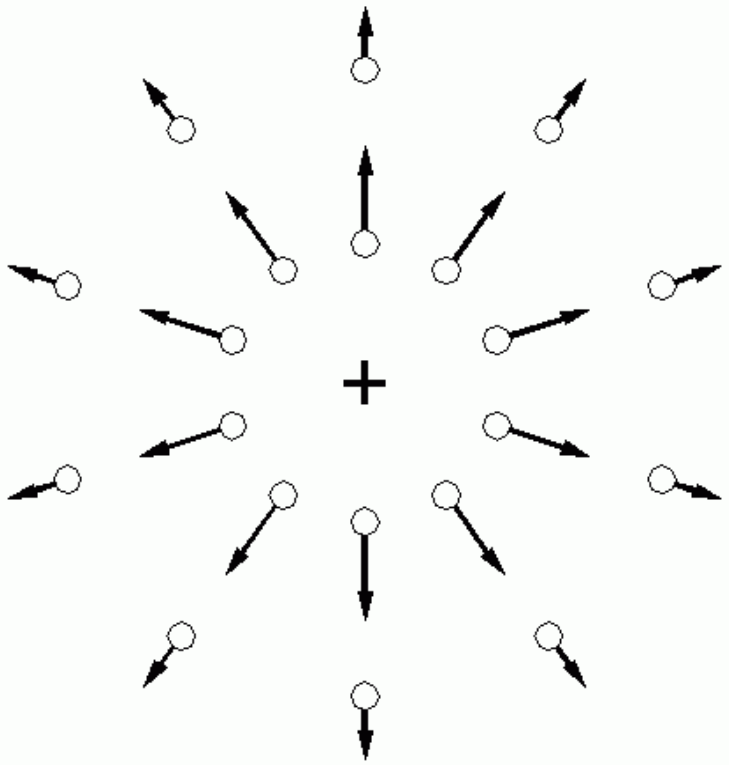
Coherent Diffraction from Crystals

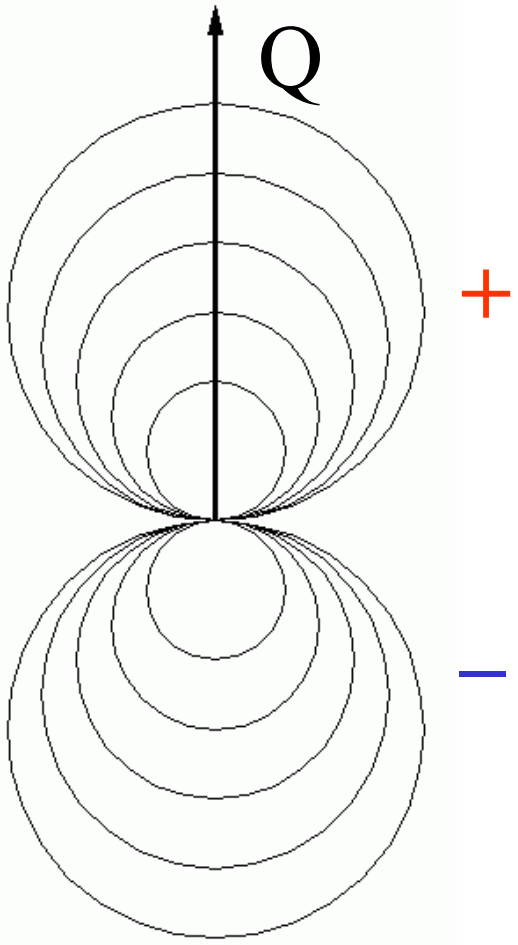


Diffraction by Strain of Point Defect

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

Imaginary density





Good statistics, 3D diffraction data

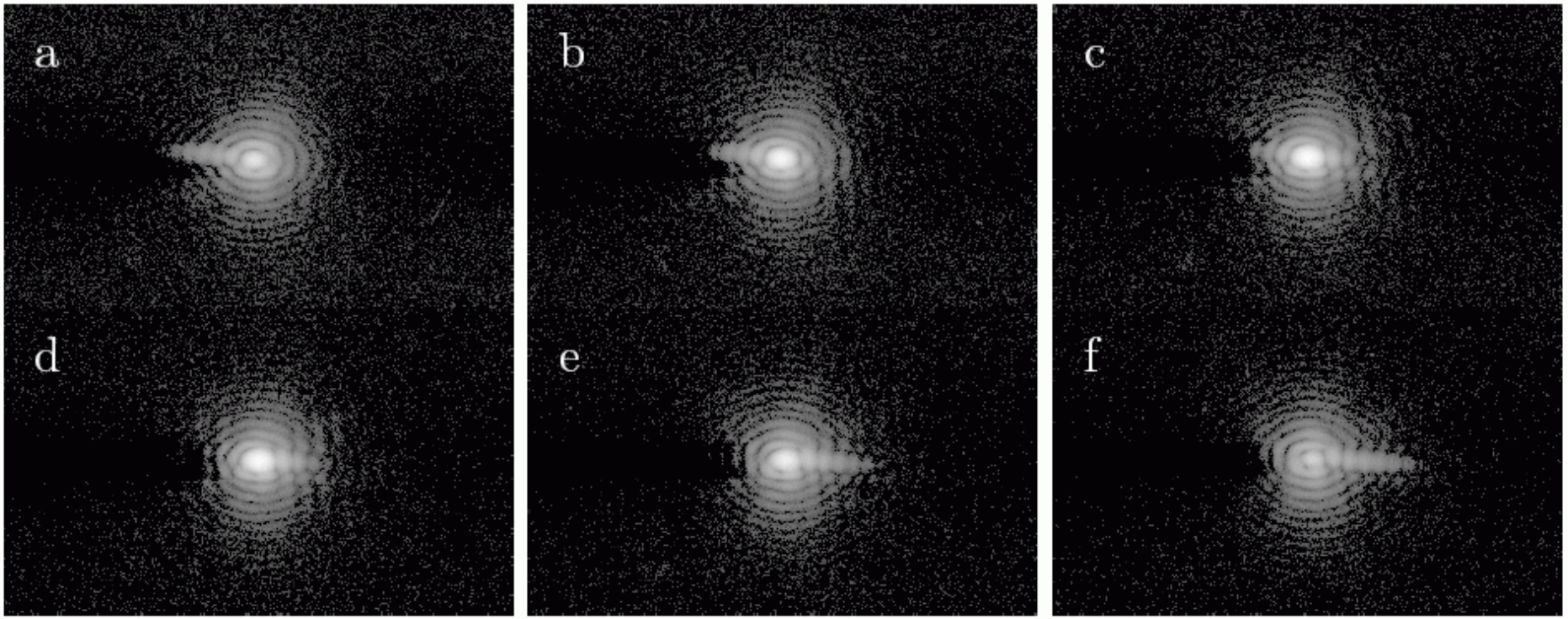
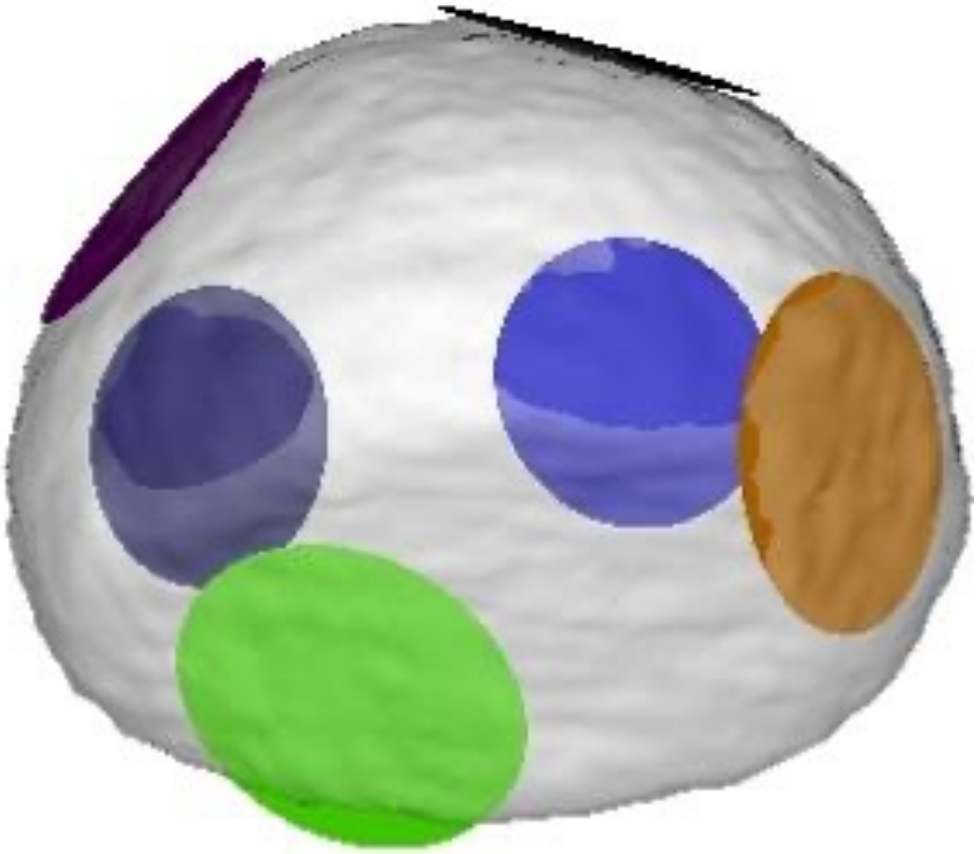
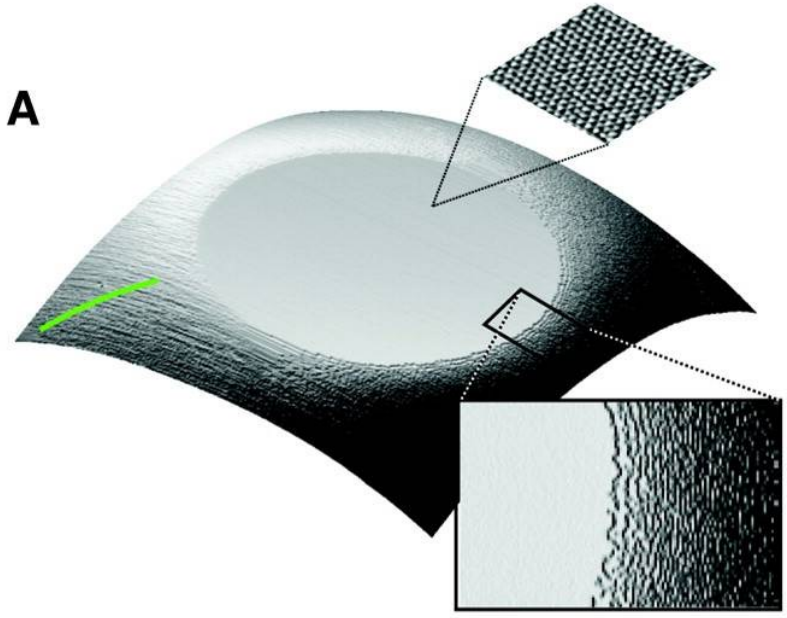


Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

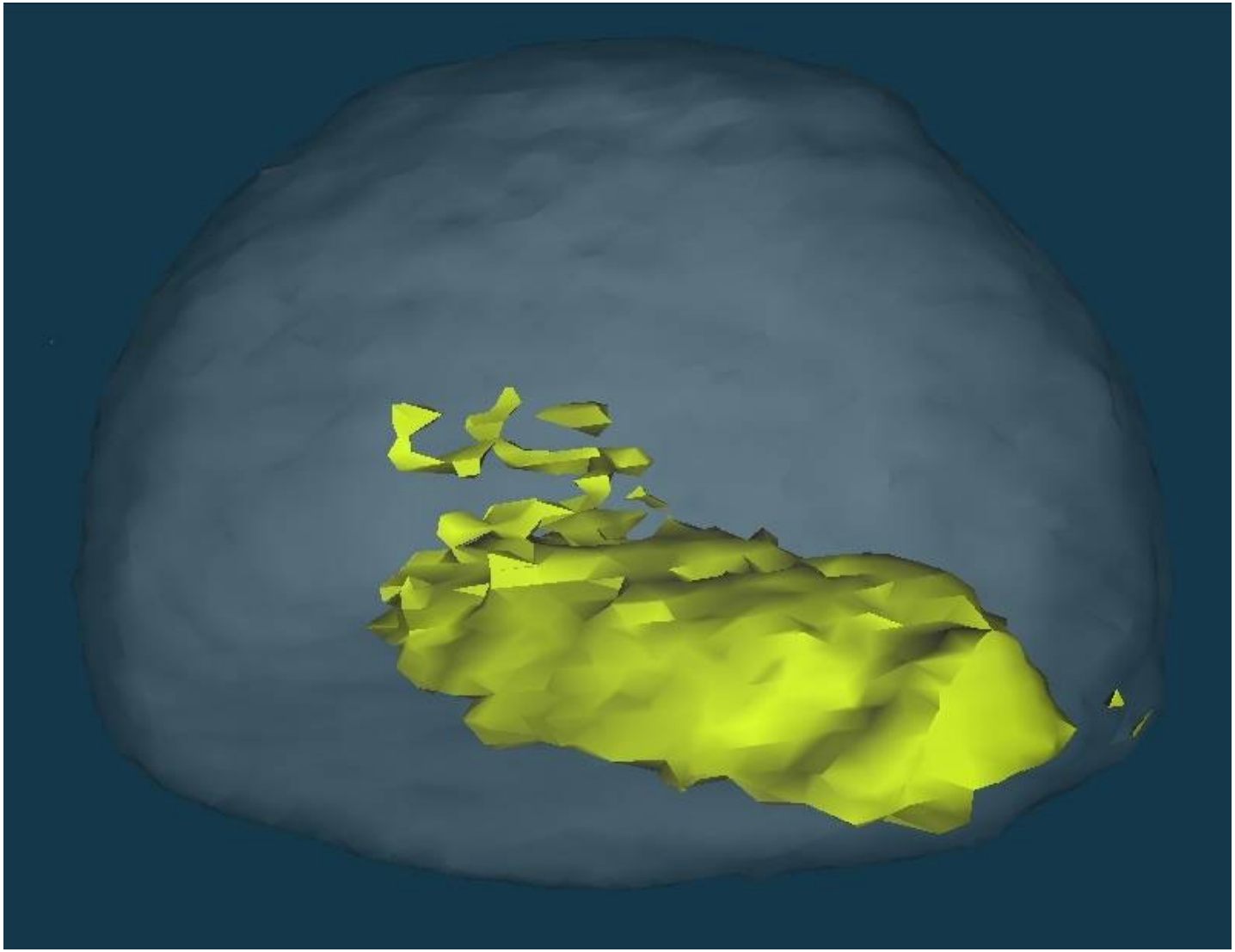
Facets of Equilibrium Crystal Shape



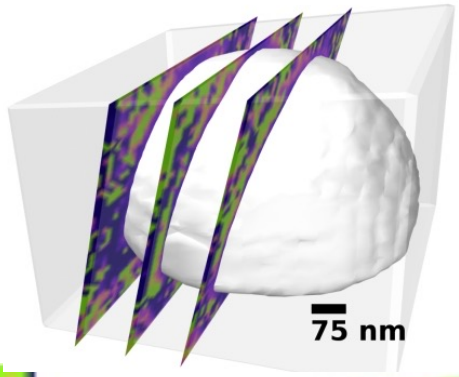


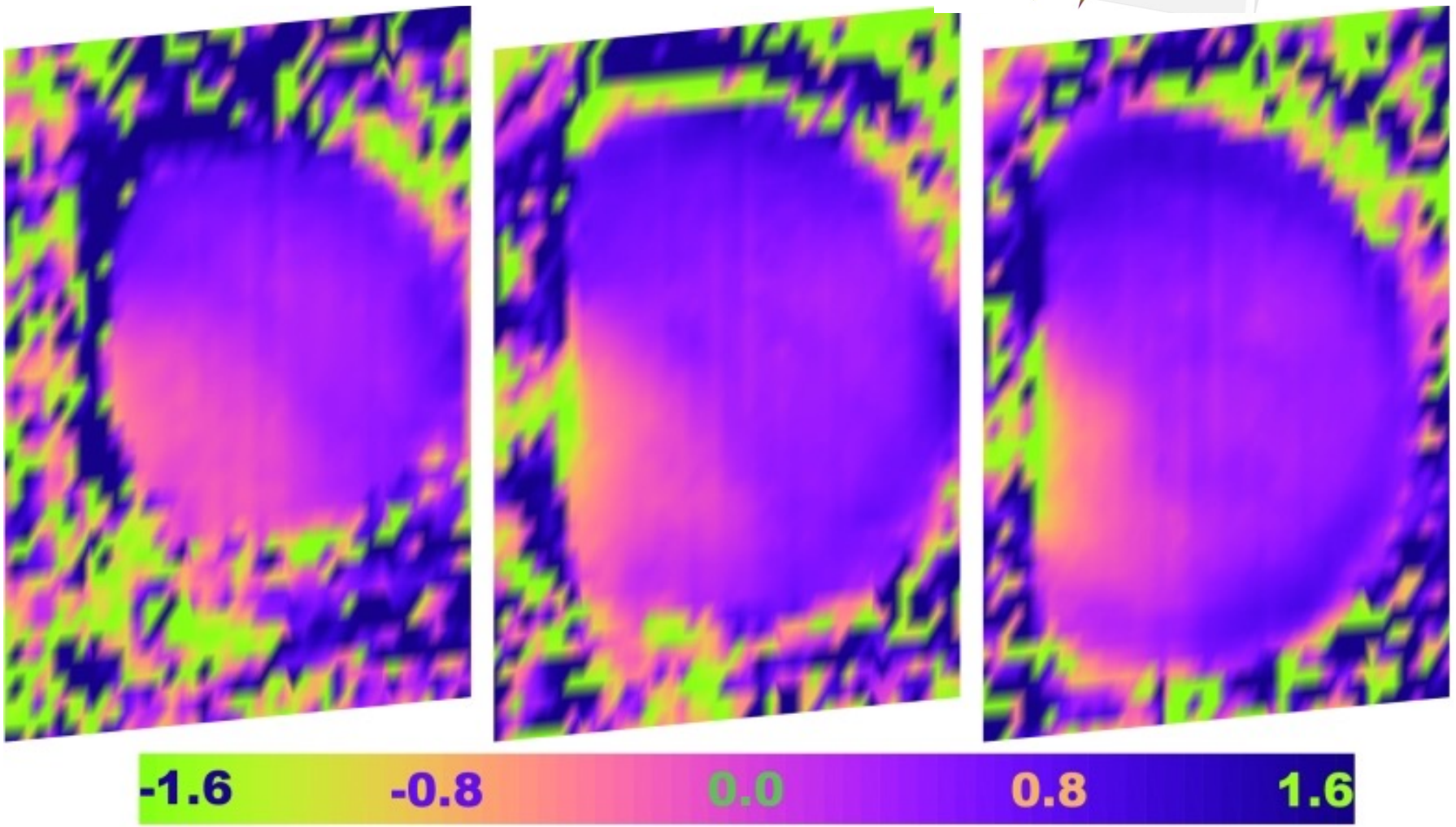
Thurmer K, Williams E, Reutt-Robey J
Science **297** 2033 (2002)

Modeling of 3D Phase Bump

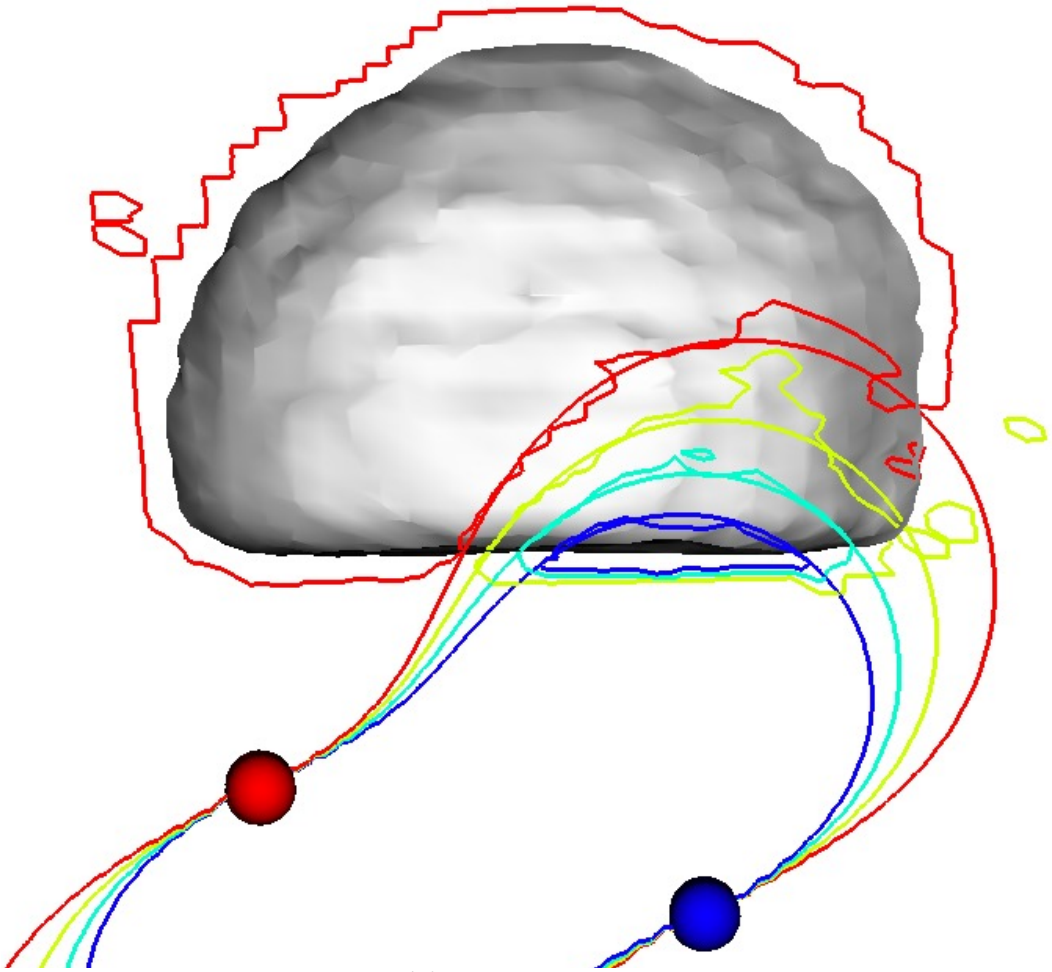


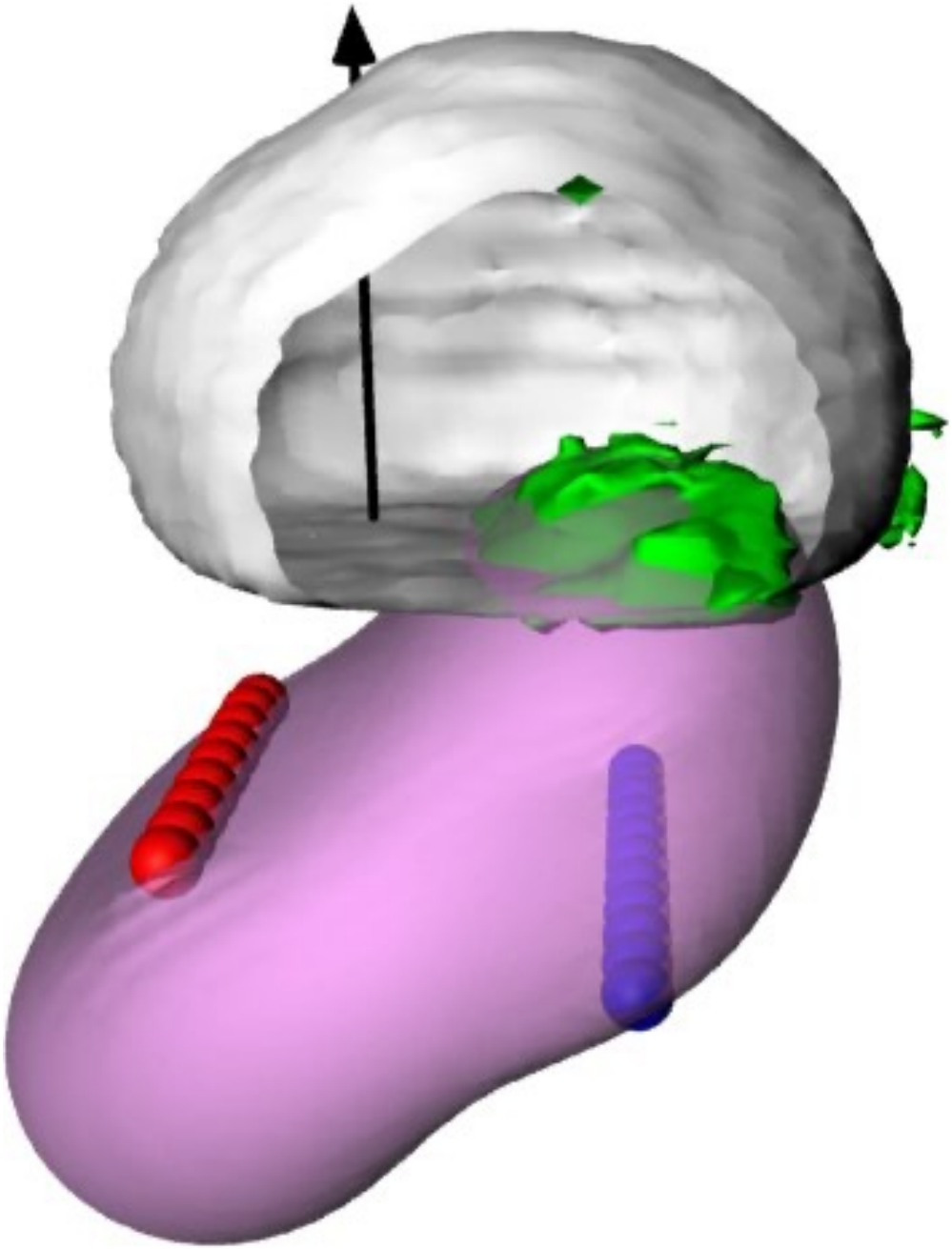
3D phase map sections





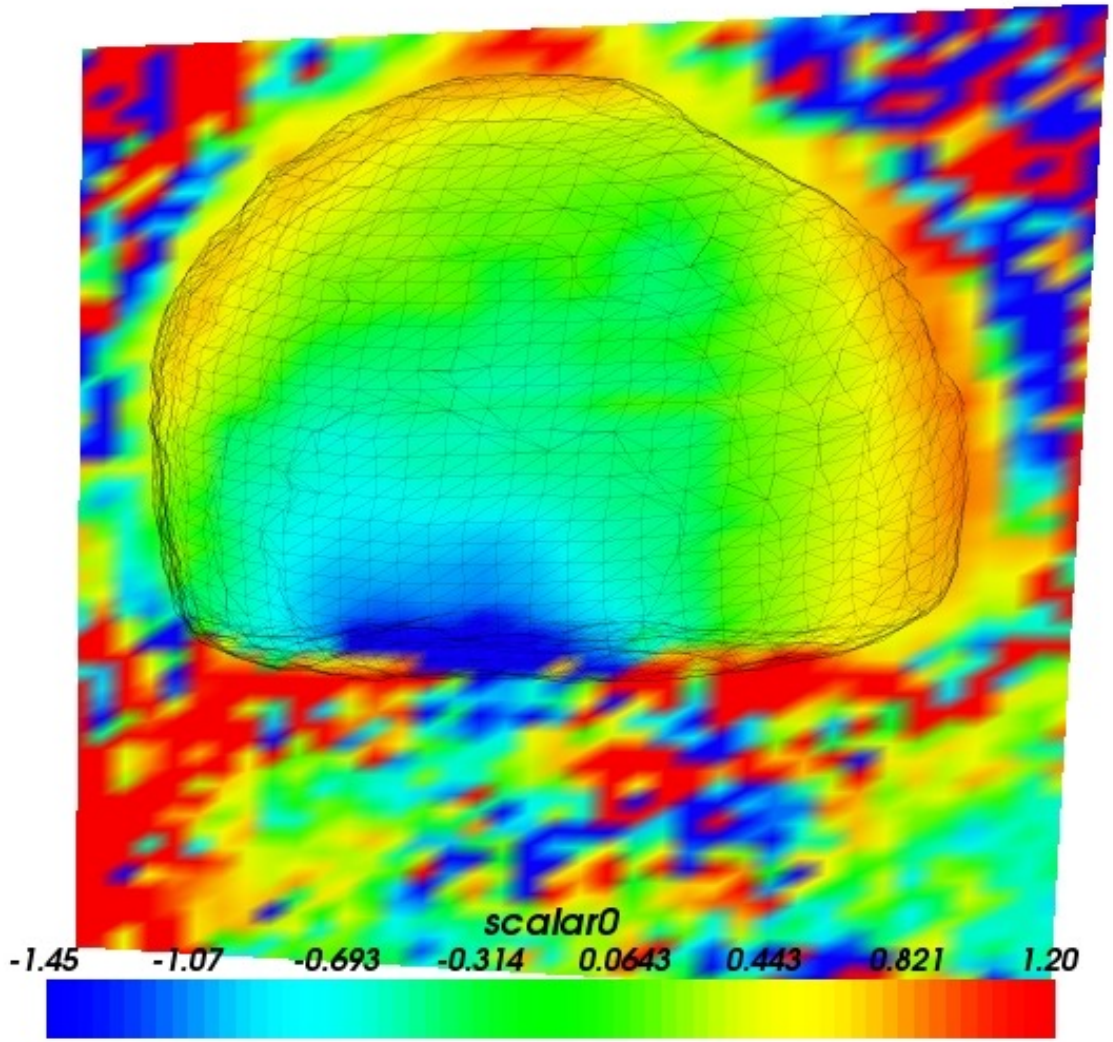
Field lines of Point Charges





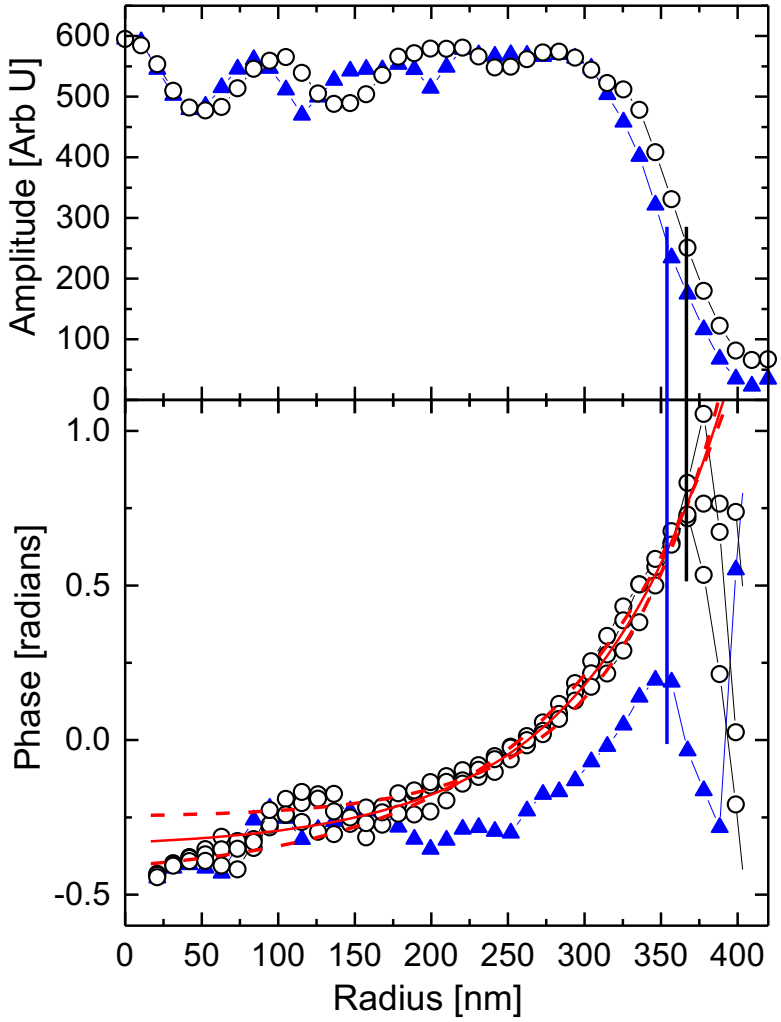
Contours showing Positive Phase

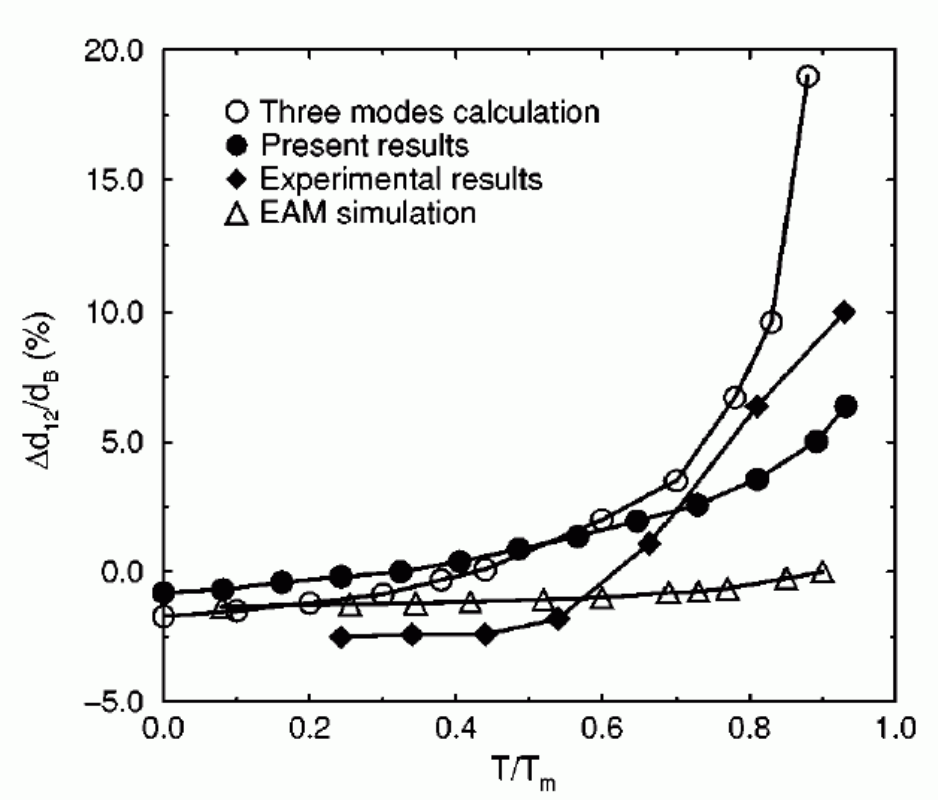
including correction for refraction by crystal



Surface Thermal Expansion

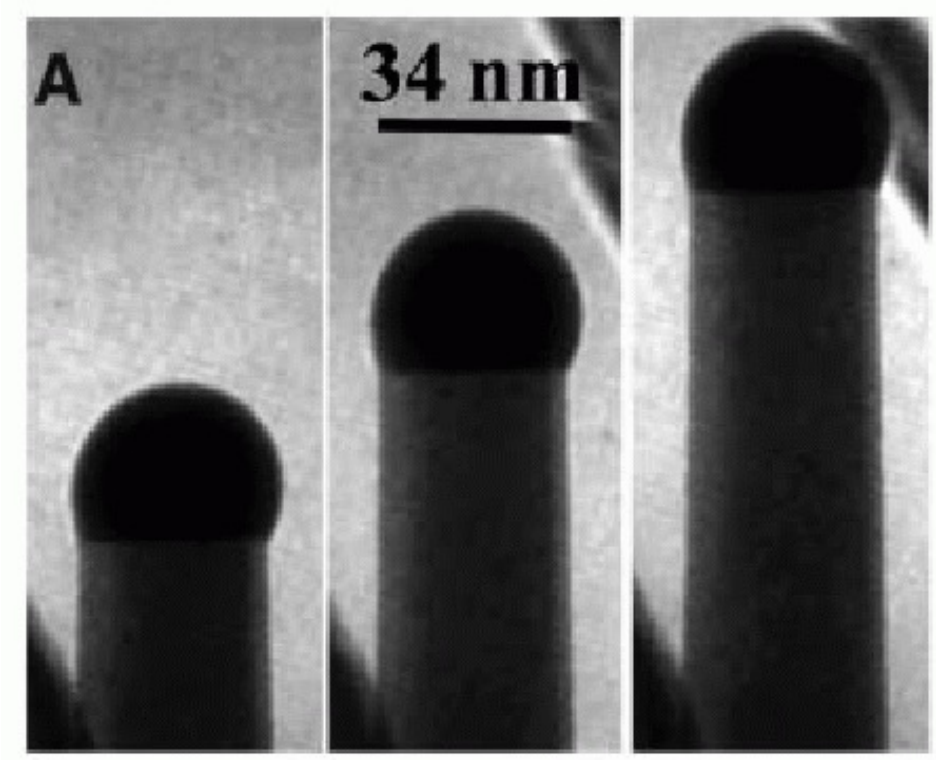
Ag(111): Scheffler et al PRB 59 970 (1999)

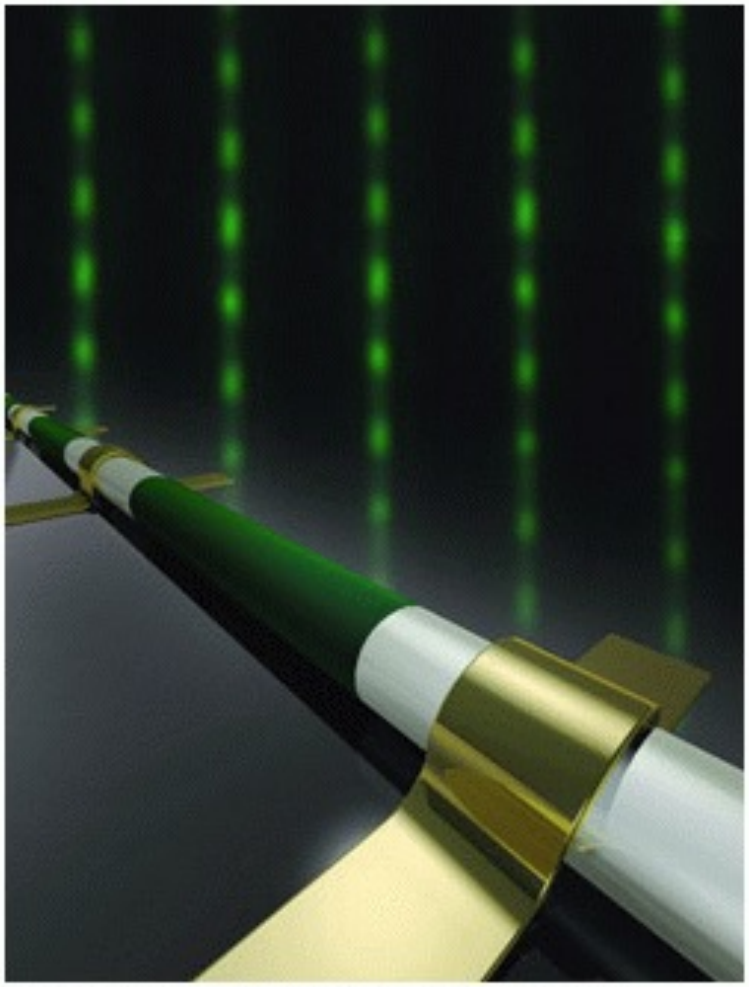




VLS growth of nanowires

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

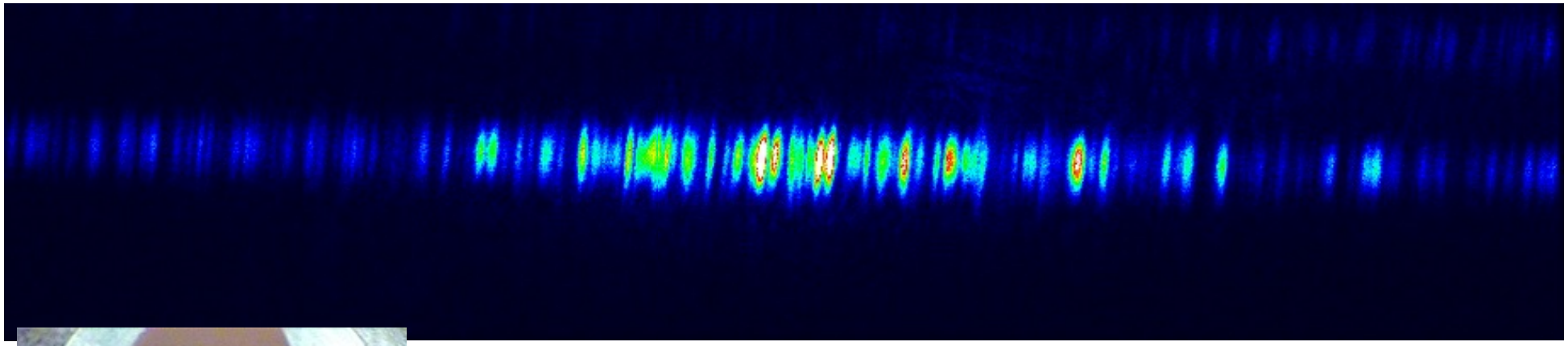


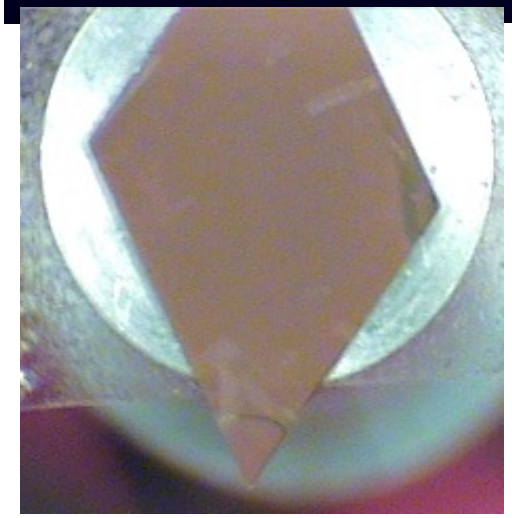


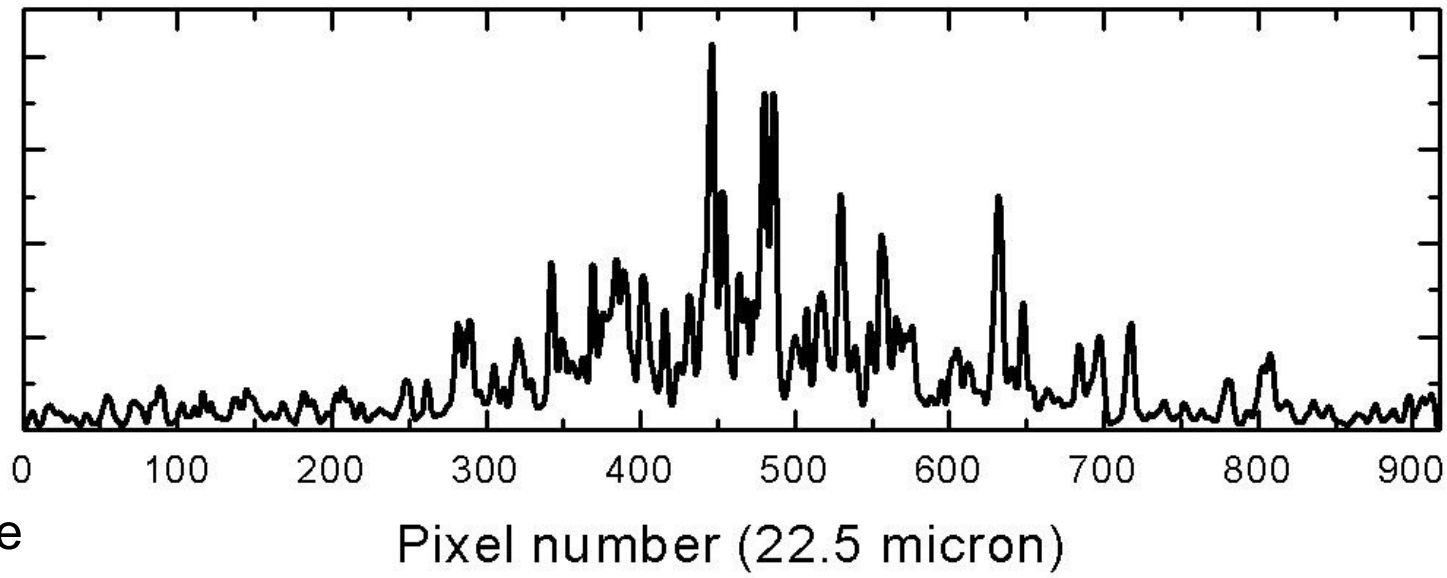
NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

GaAs Nanowire "Barcode"

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



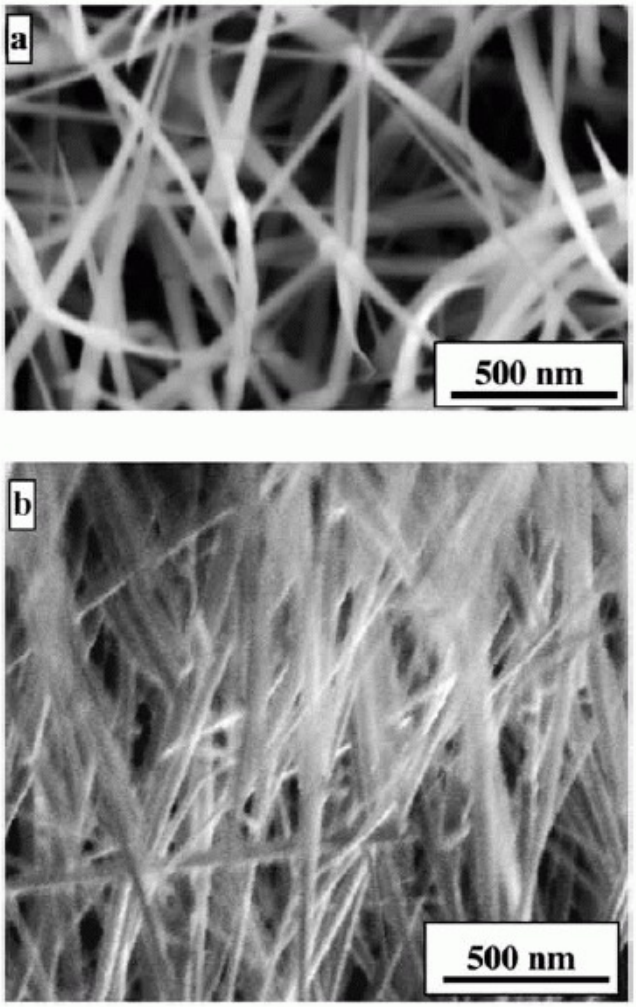


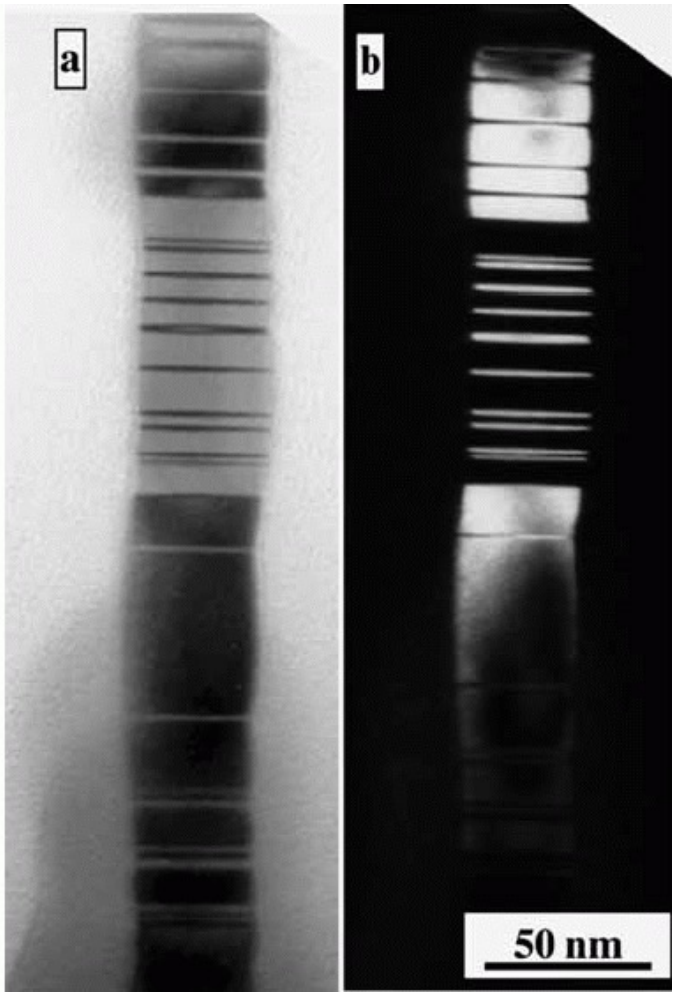


GaAsNW1106-22.spe
B9348 from Philips

Dark Field TEM of GaAs Nanowires

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

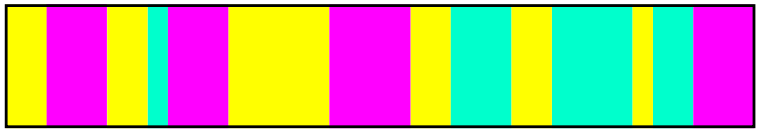




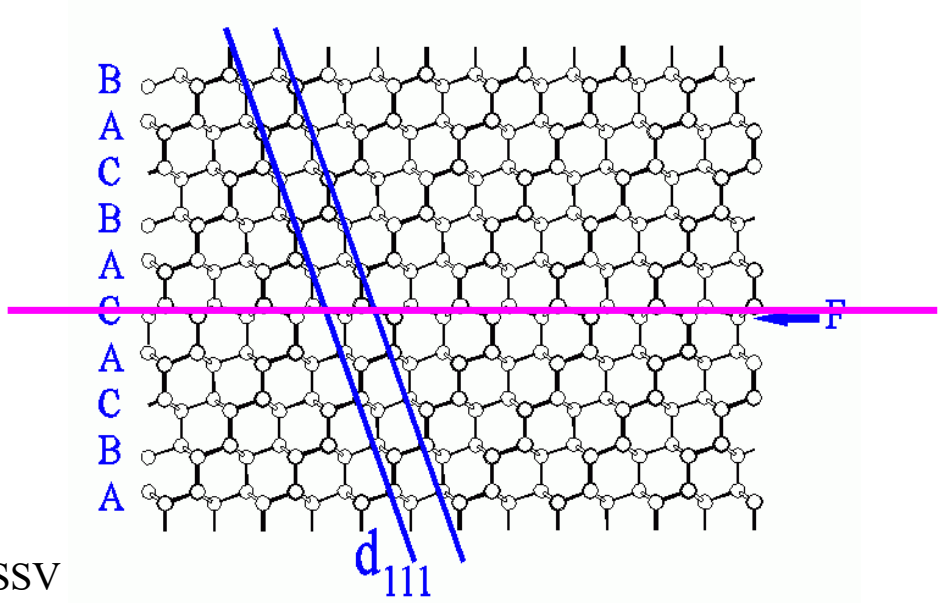
Models of Barcode Diffraction

(111) wires at (11-1) reflection

- Twinned stacking sequence

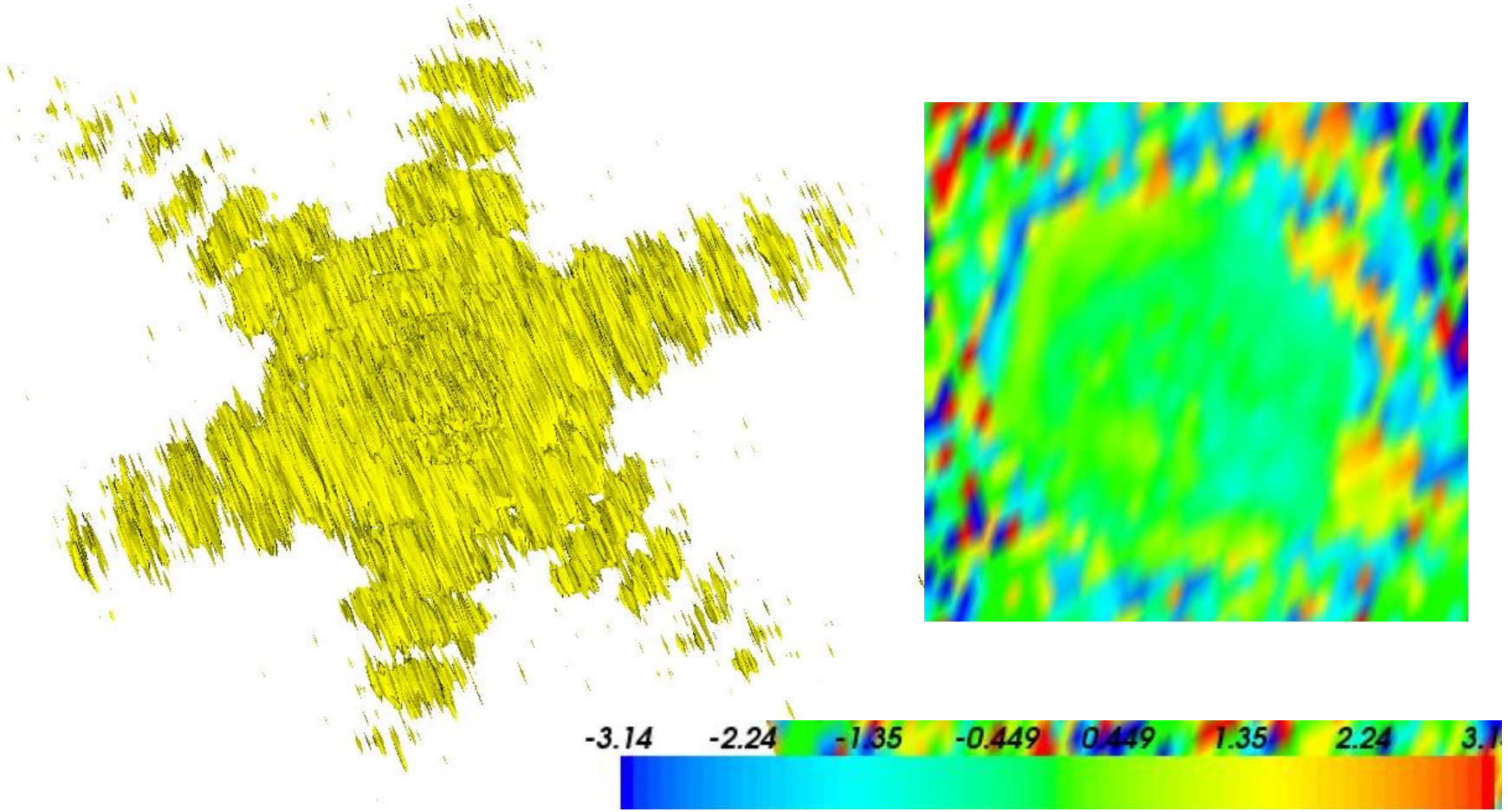


- Deformation faults



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