Coherent X-ray Diffraction

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Diamond Light Source

MISCA-II
Oviedo
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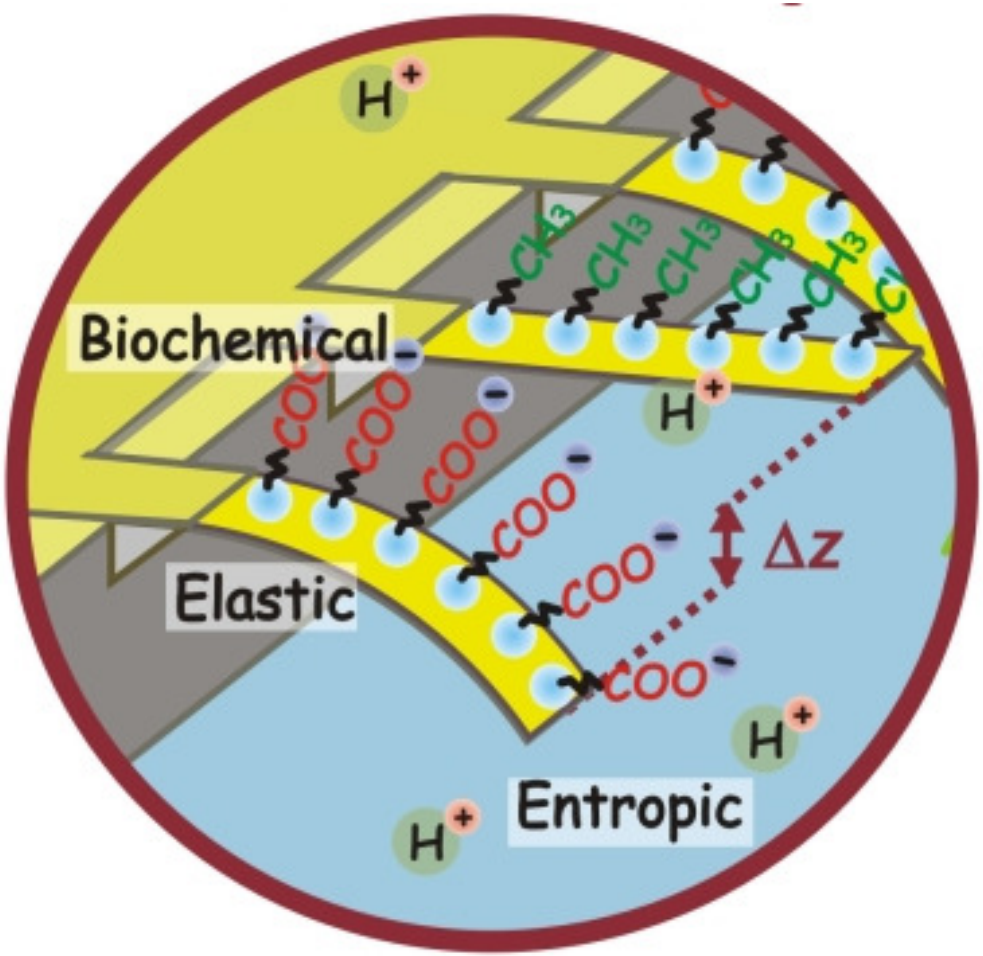
Outline

- Coherent x-ray diffraction
- Solving the phase problem
- Nanocrystal structures
- Exploration of crystal strain
- Nanowire structures

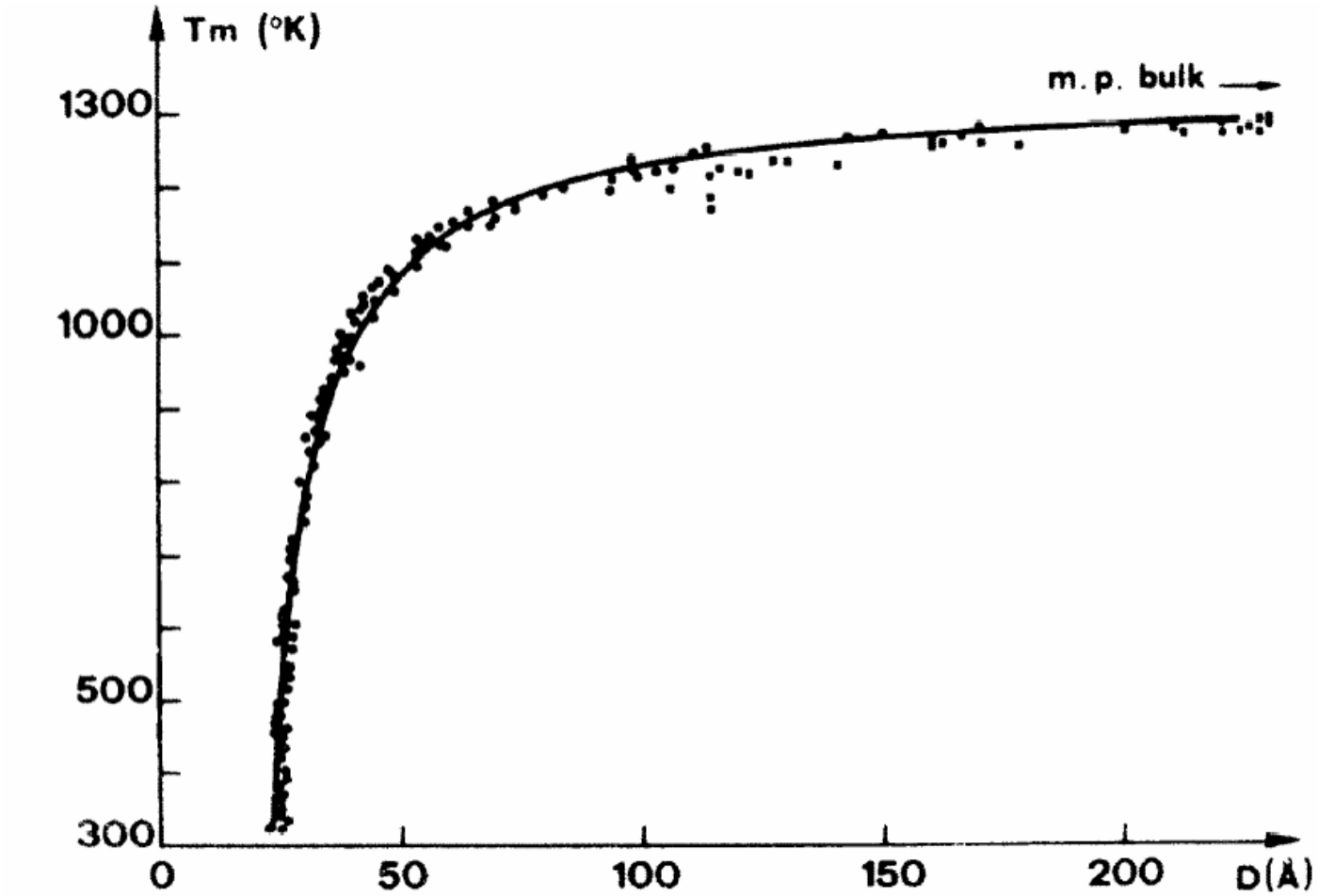
Nanocantilevers

Dr Rachel McKendrie

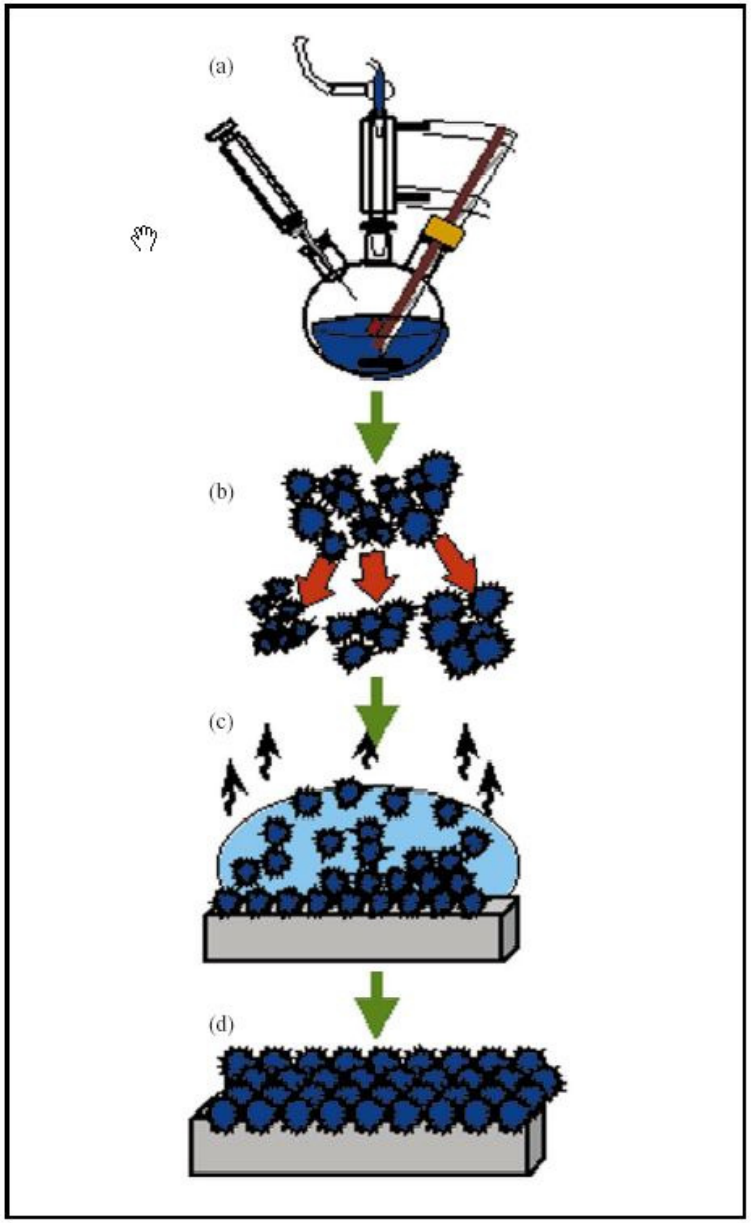


Size-dependent Melting of Au Particles

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

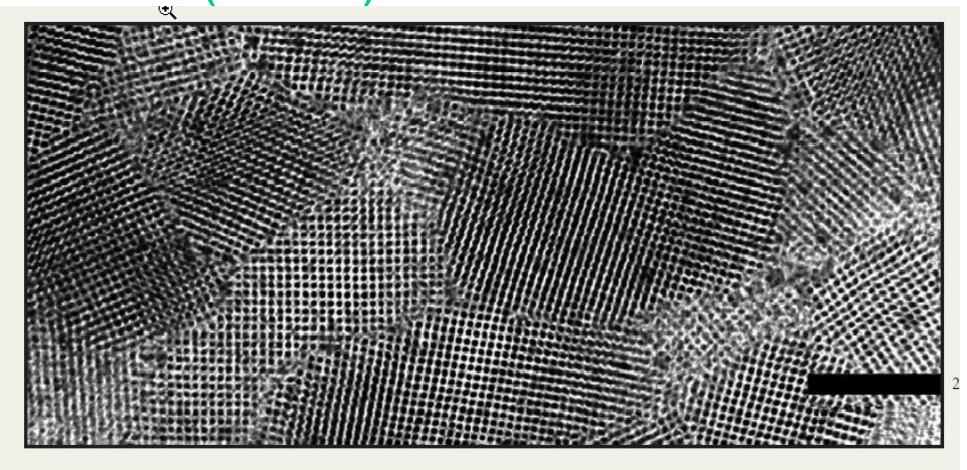


Chemical Synthesis of Nanocrystals



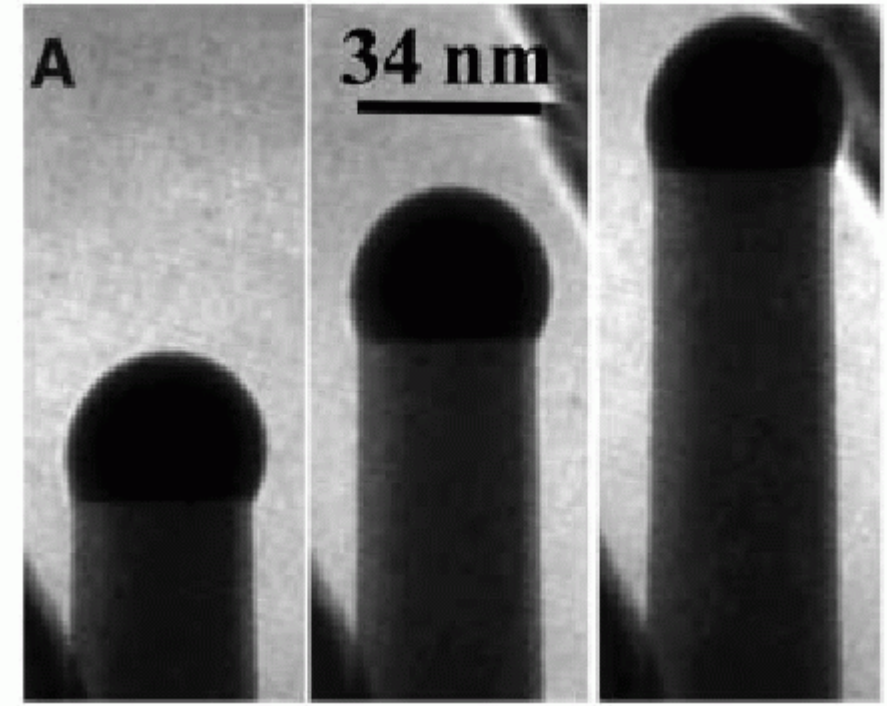
- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

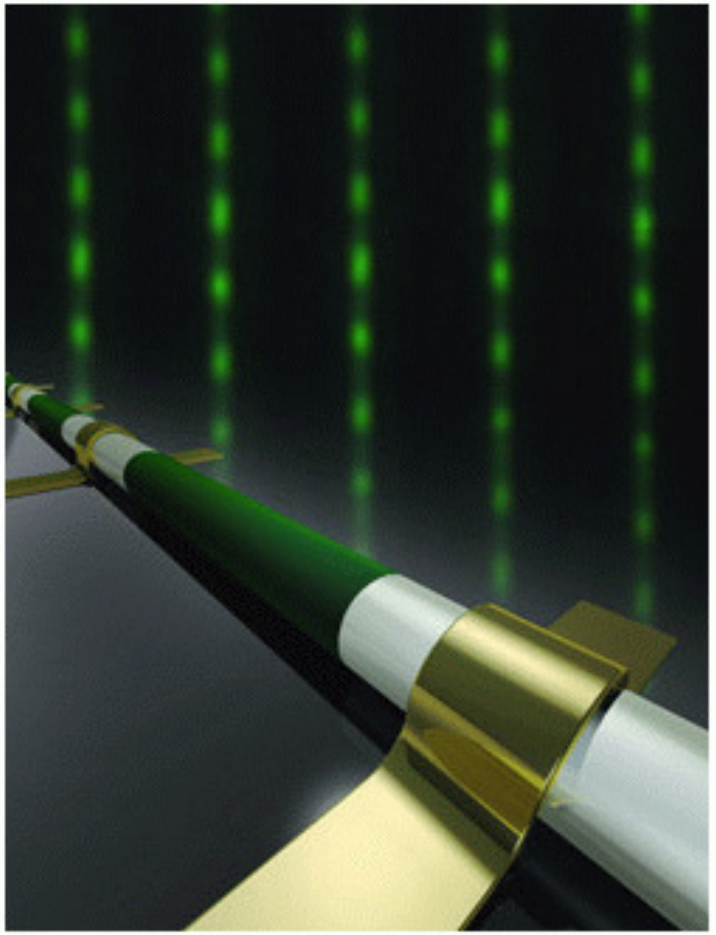
C. B. Murray, IBM J. Res. & Dev. **45** 47 (2001)



VLS growth of nanowires

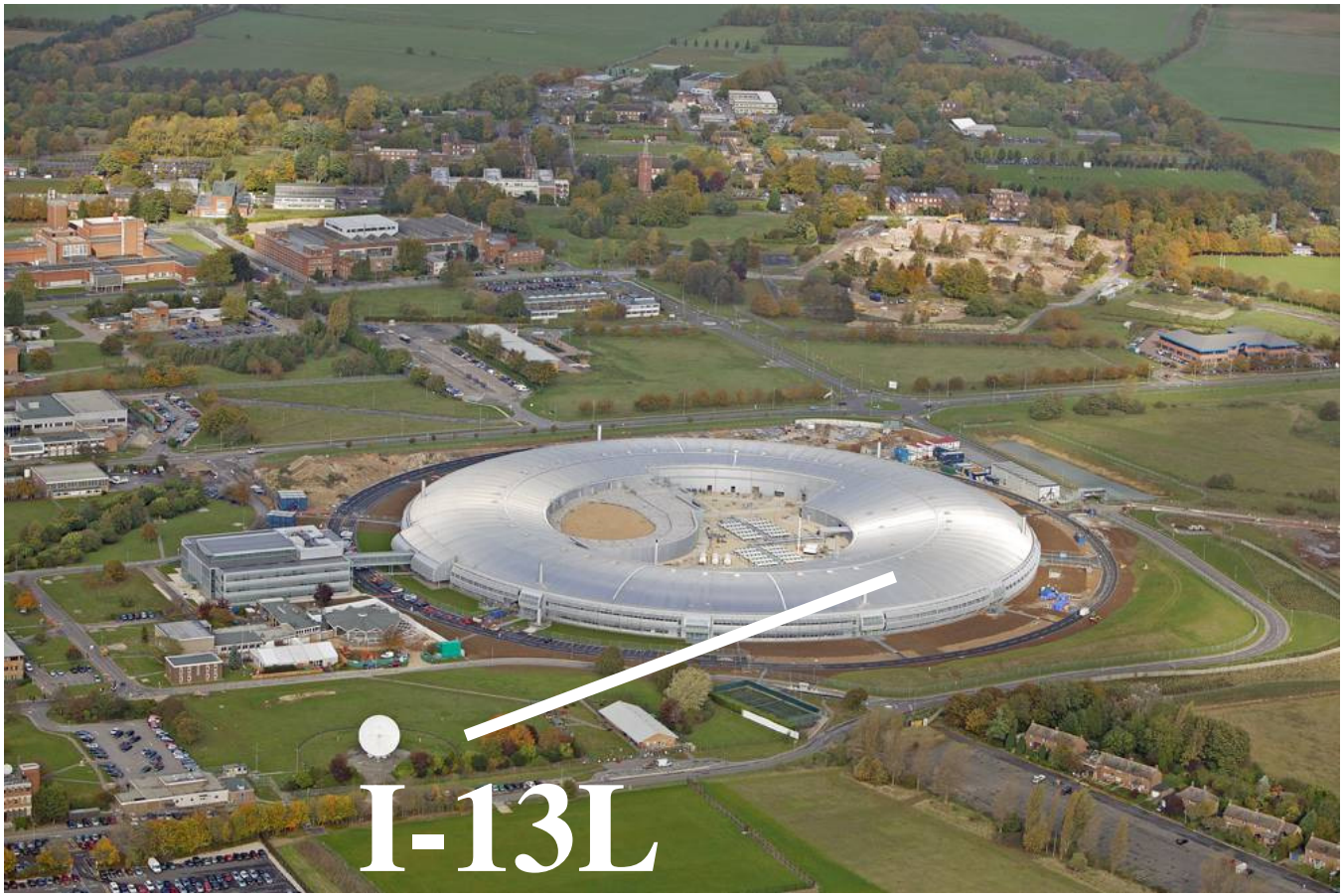
S. Kodambaka et al., Science 316 729 (2007)



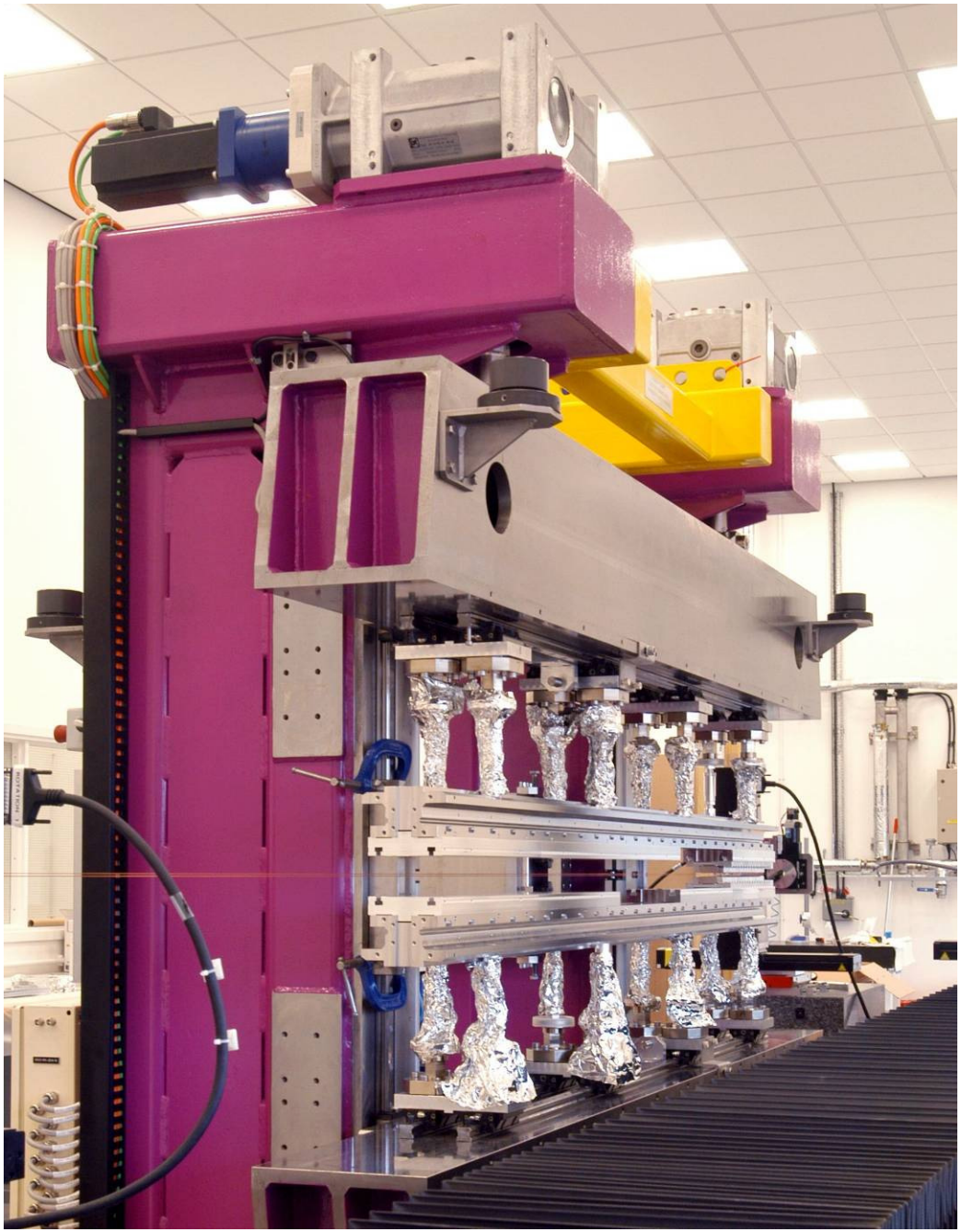


NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

Diamond Light Source (RAL)

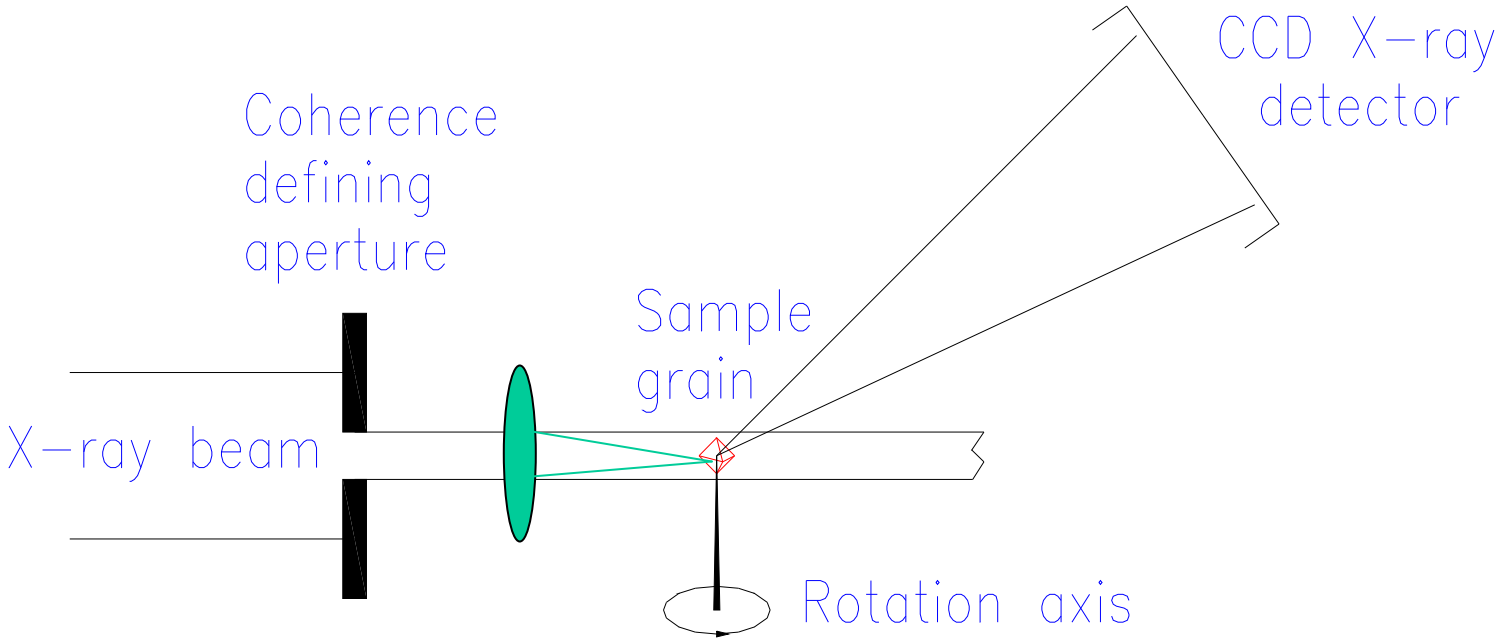


Diamond in-vacuum X-ray Undulator

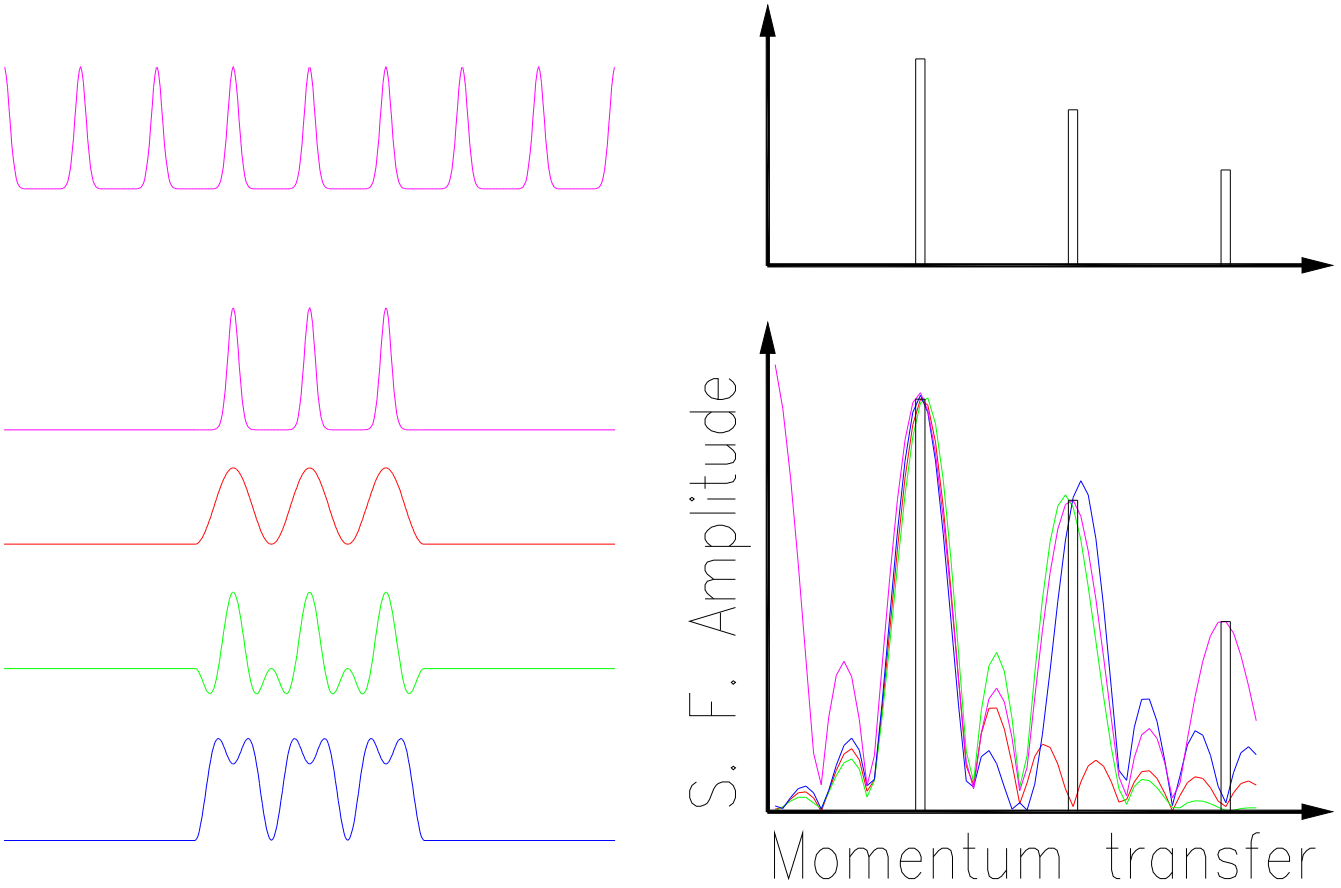


I.

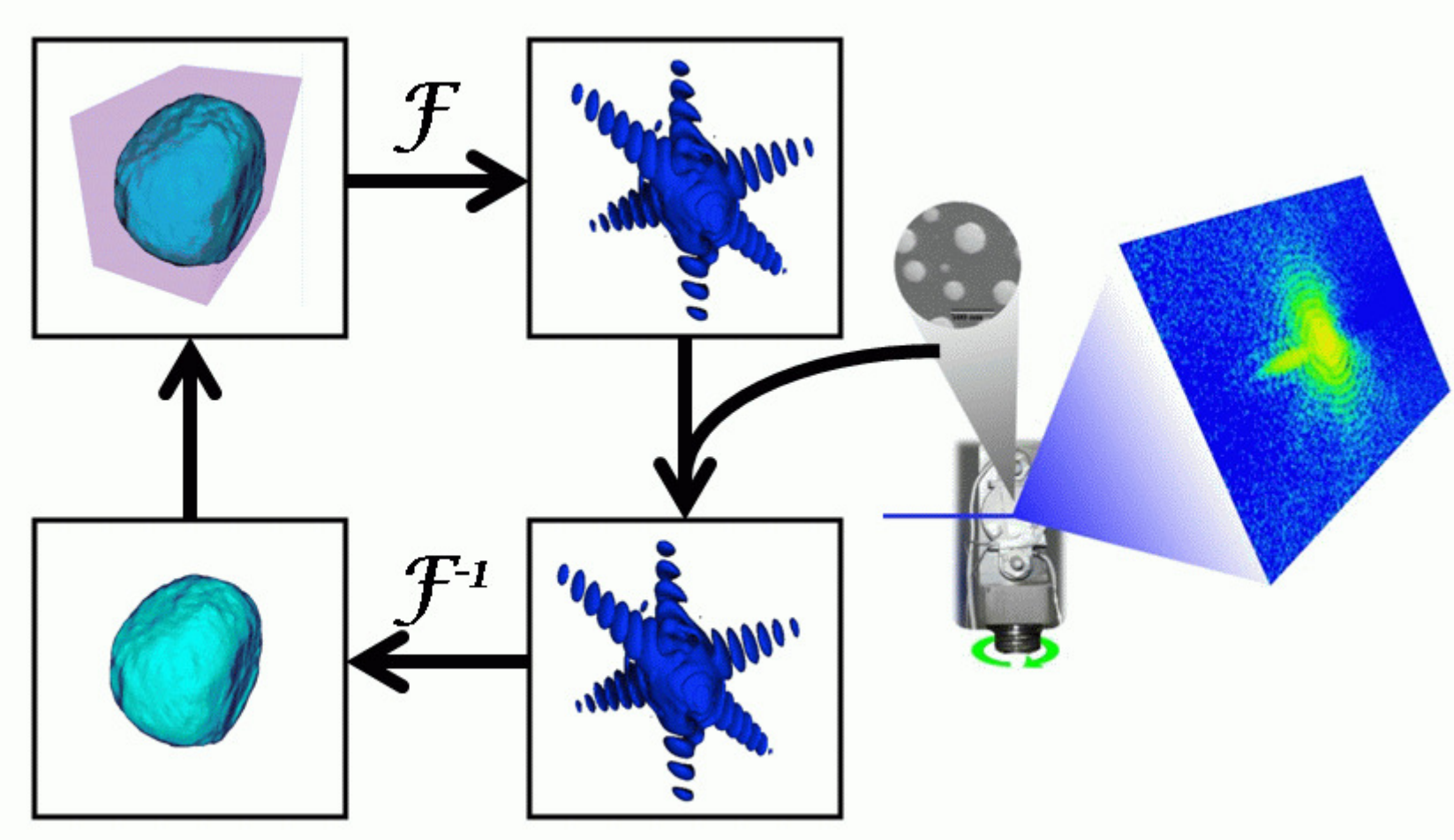
Lensless X-ray Microscope, 2003



Oversampling solves Phase Problem



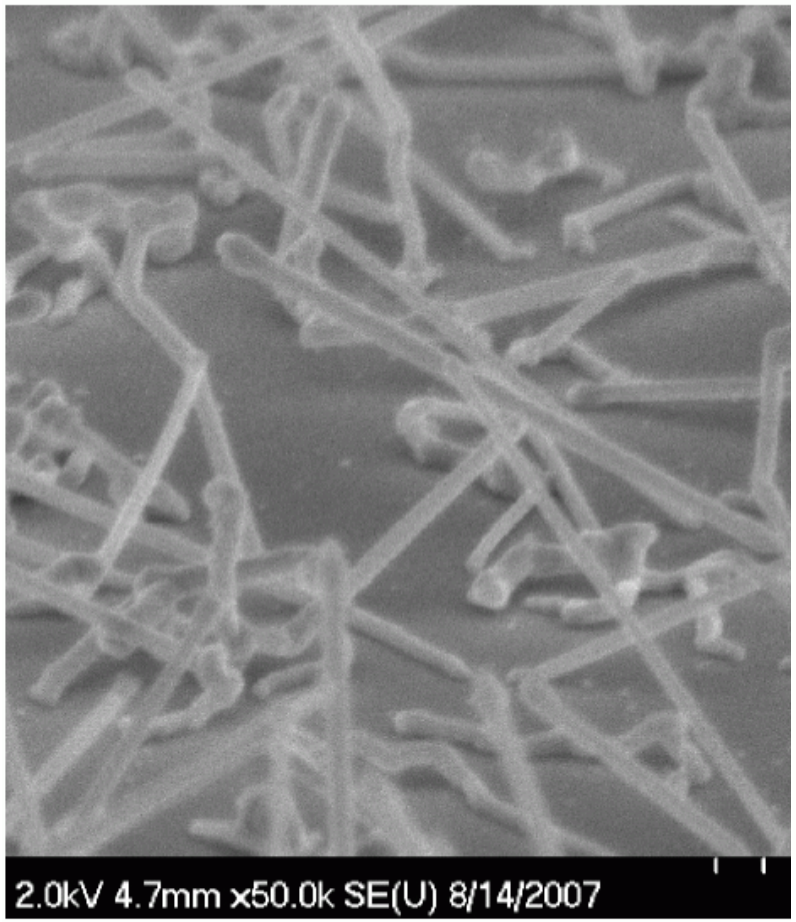
Generic "Error Reduction" method



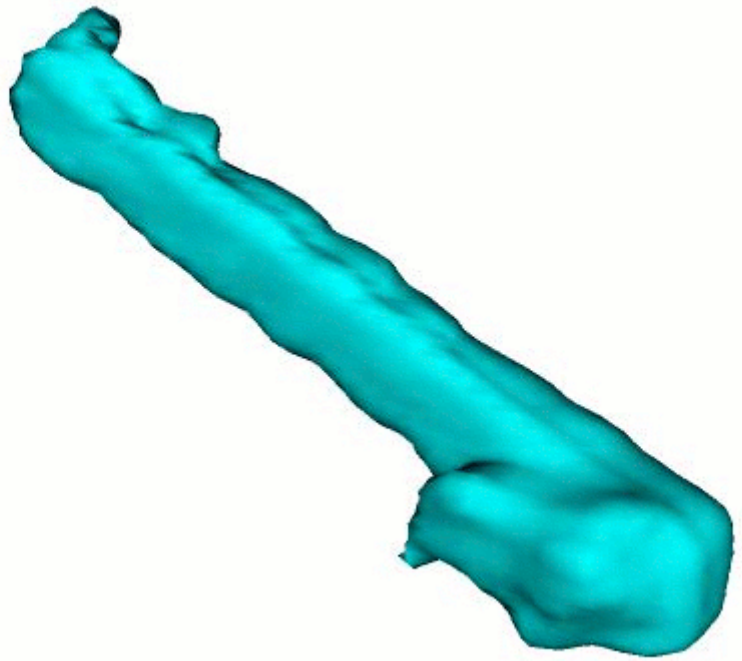
J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

Reconstruction of InP nanowire

CVD on Si, Suneel Kodambaka, UCLA

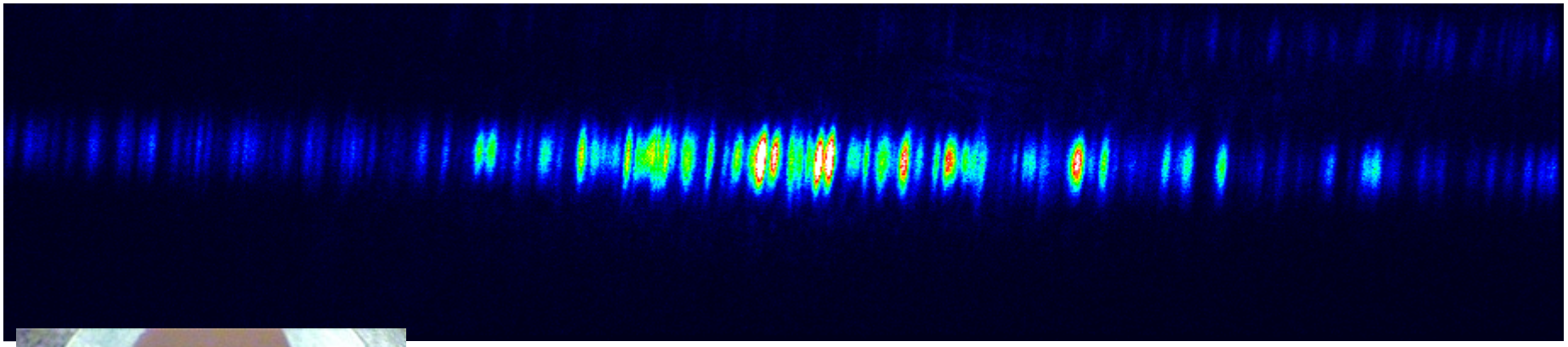


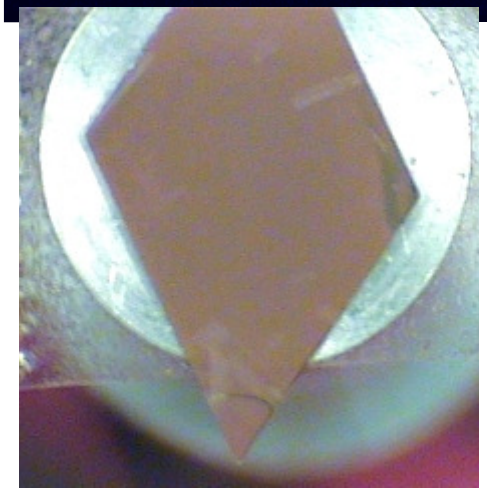
InP nanowires grown on Si (111)

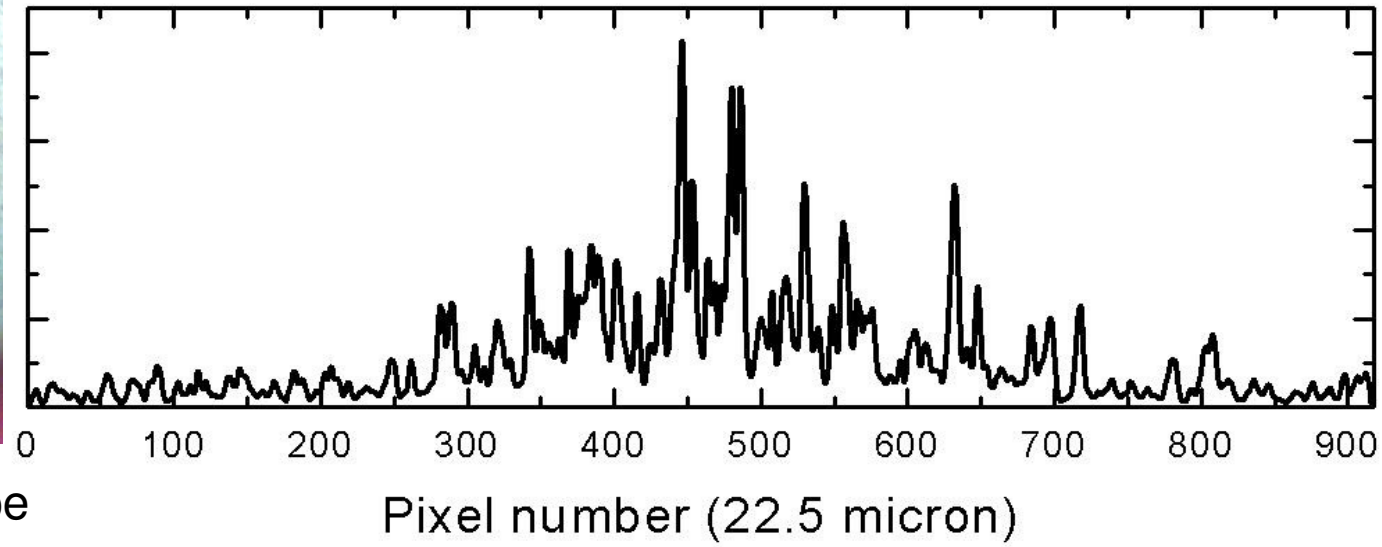


GaAs Nanowire "Barcode"

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





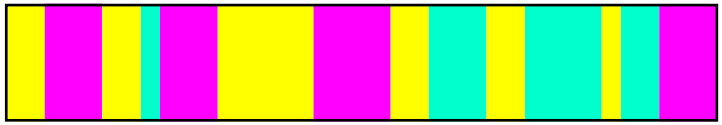


GaAsNW1106-22.spe
B9348 from Philips

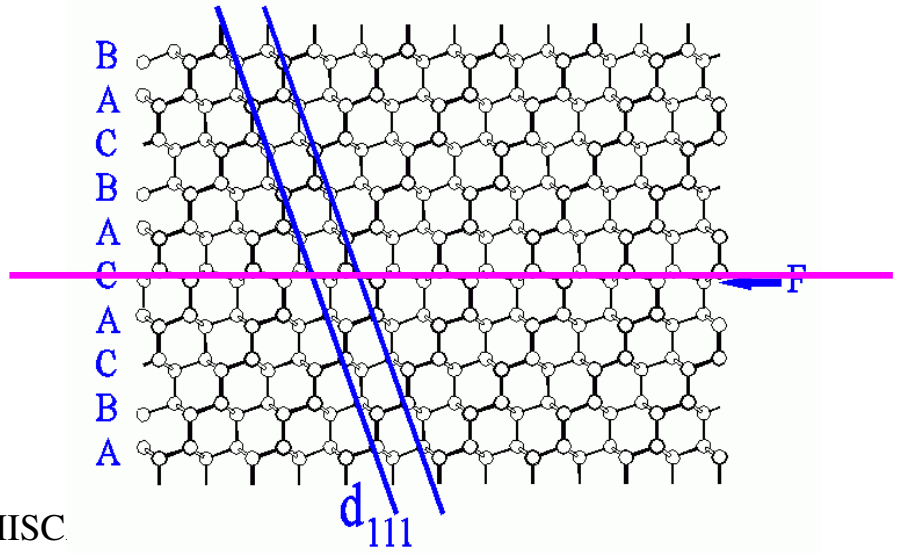
Models of Barcode Diffraction

(111) wires at (11-1) reflection

- Twinned stacking sequence

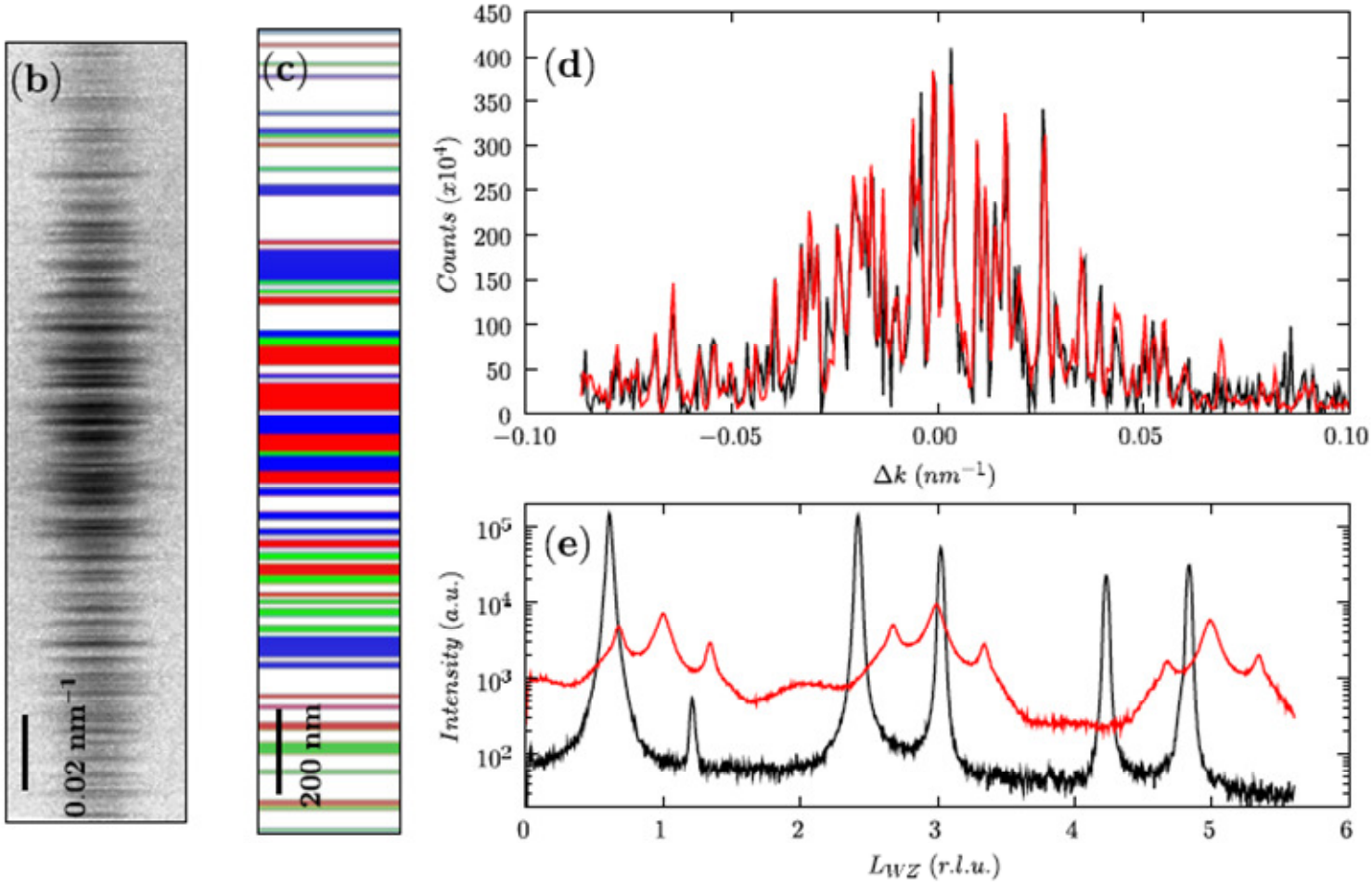


- Deformation faults



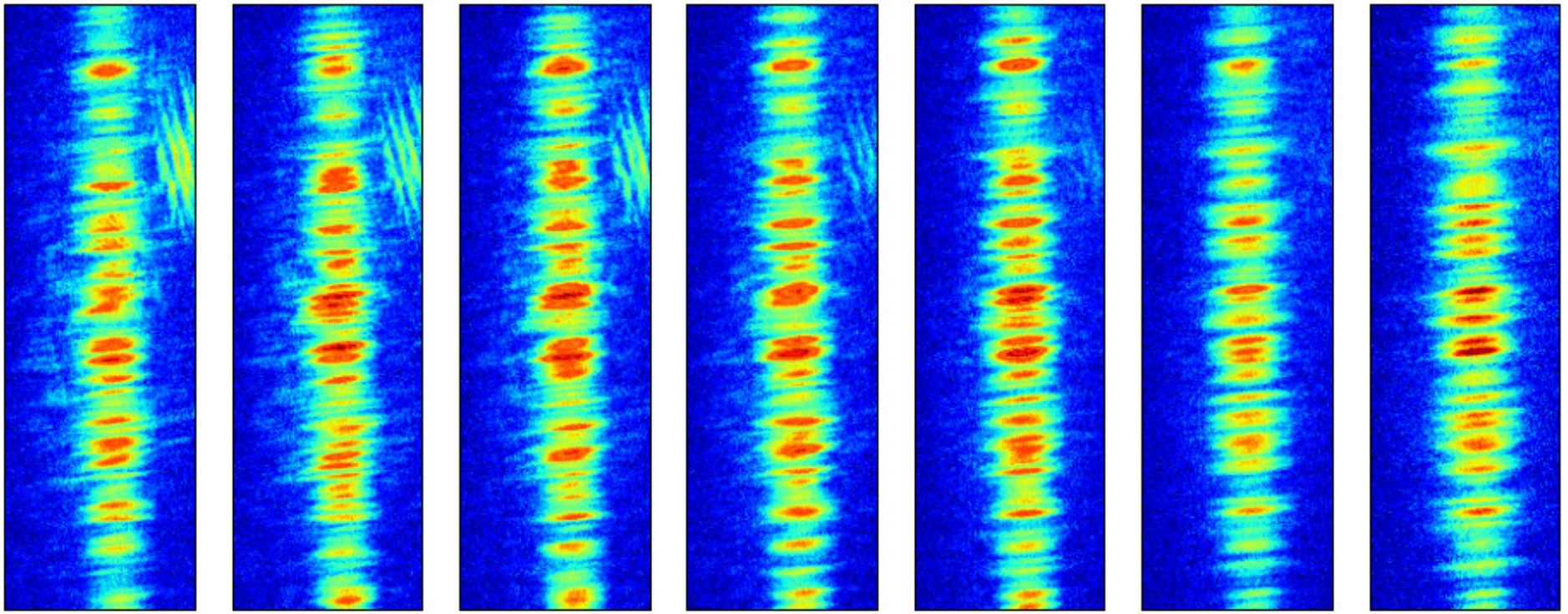
Barcode Modelling (biased MC)

V. Favre-Nicolin, New Journal of Physics 12 035013 (2010)



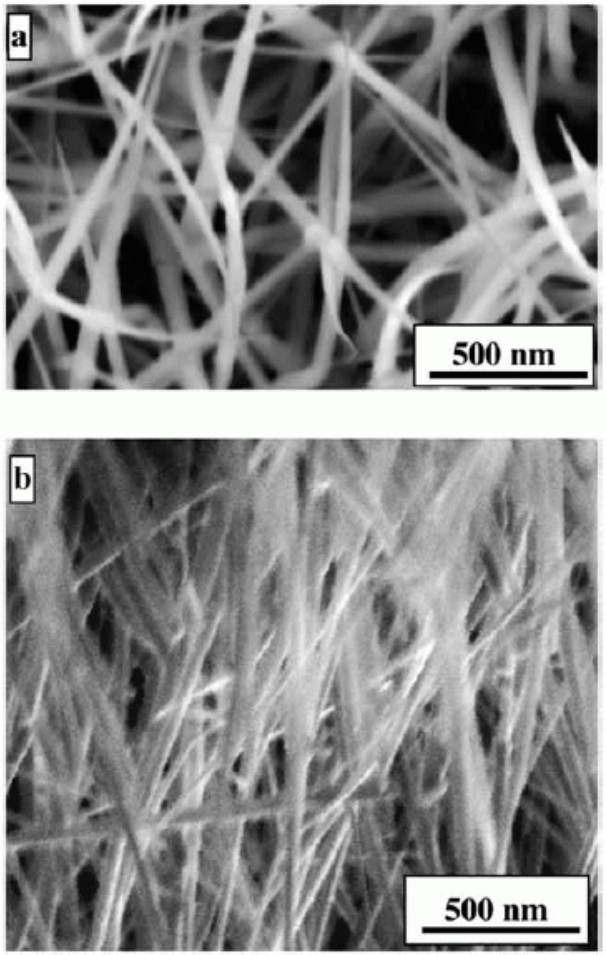
Barcode Ptychography

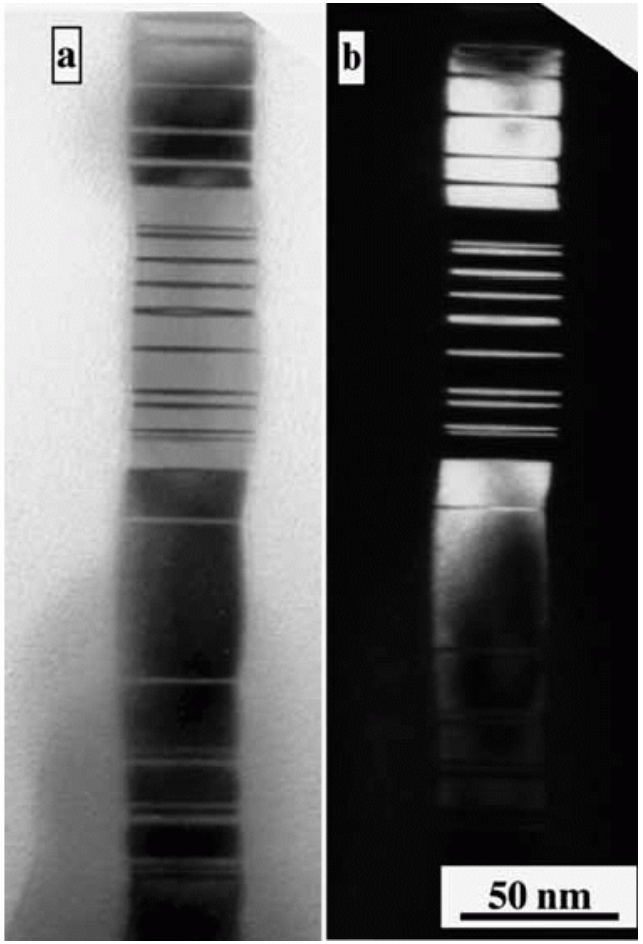
V. Favre-Nicolin, New Journal of Physics 12 035013 (2010)



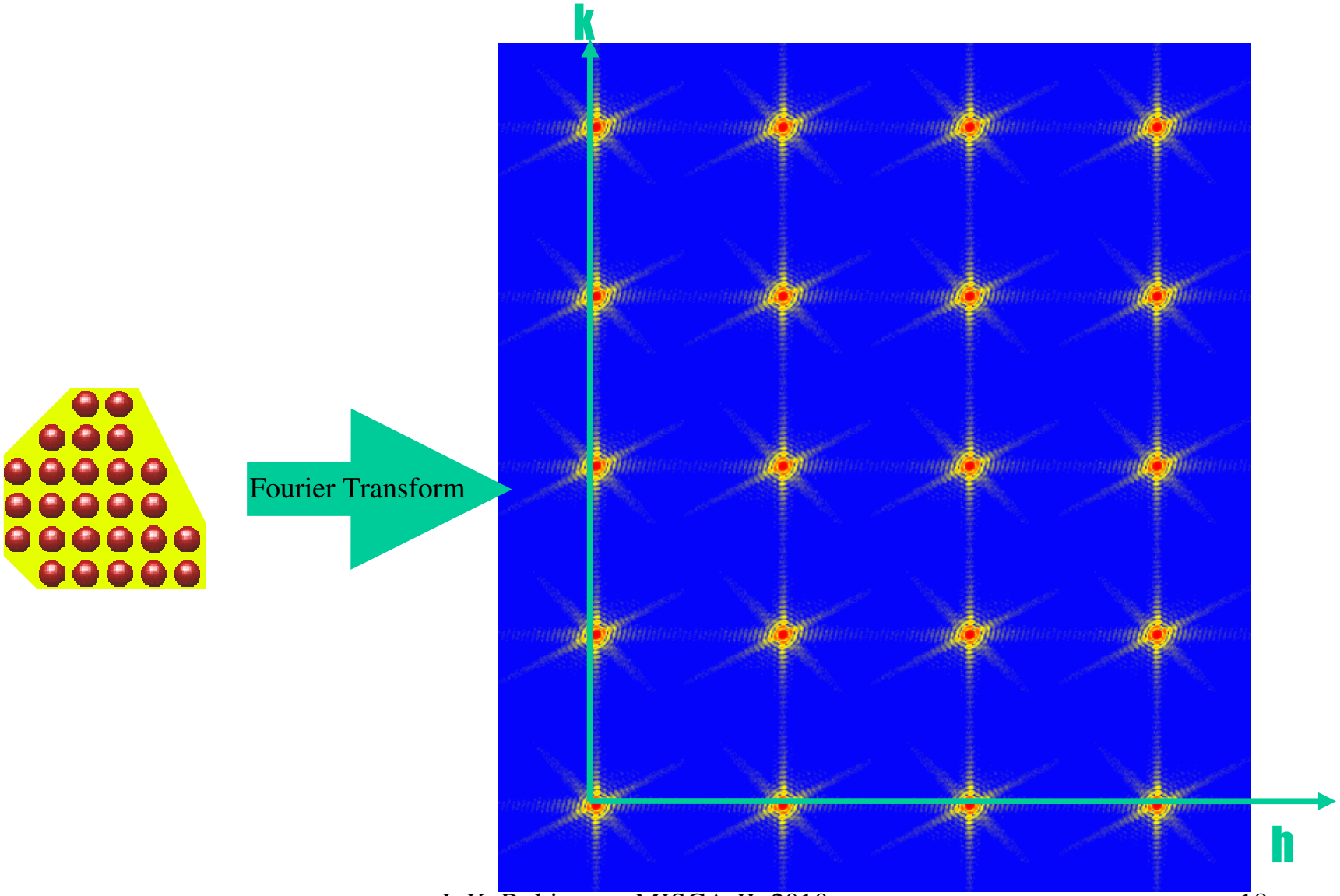
Dark Field TEM of GaAs Nanowires

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



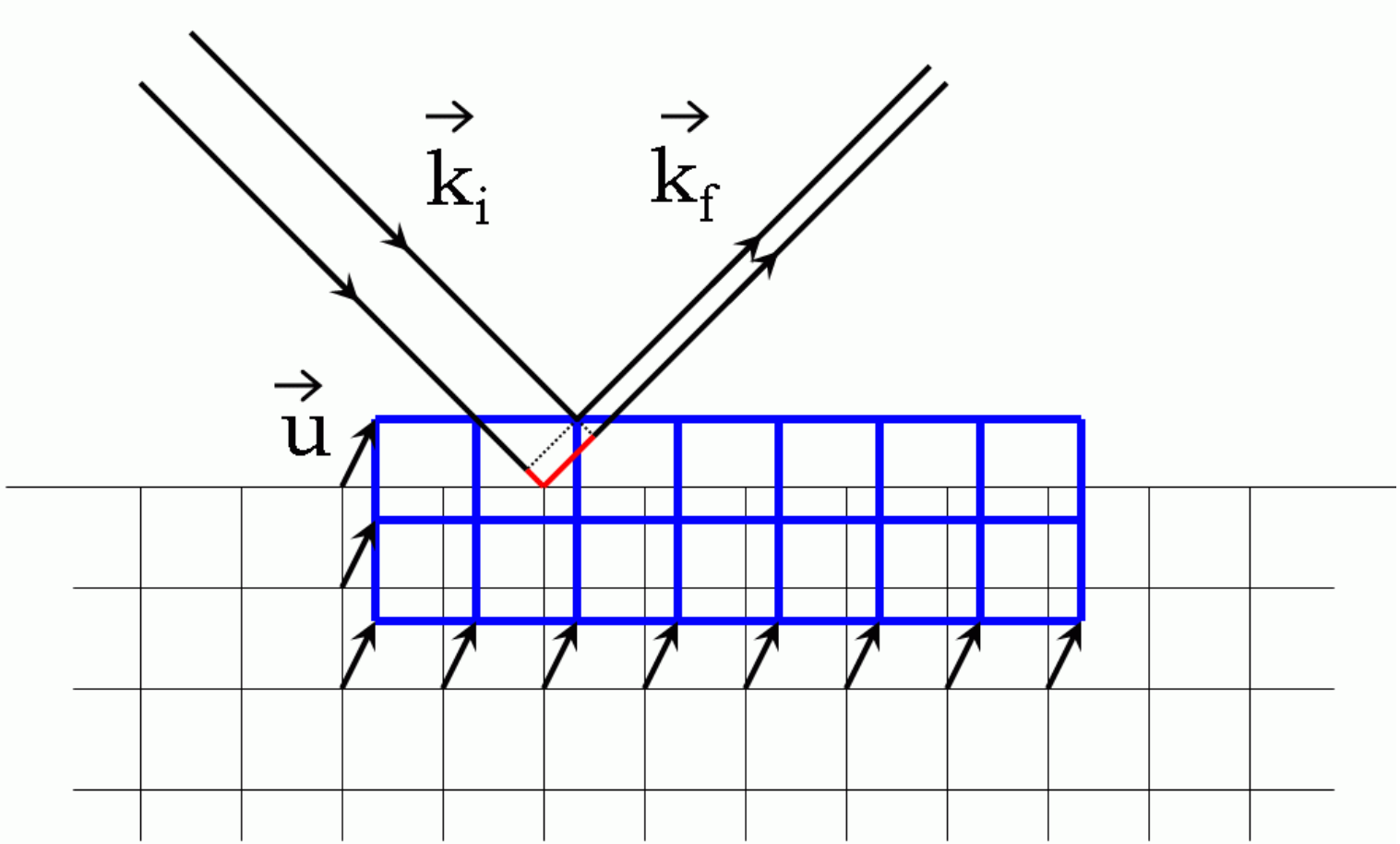


Coherent Diffraction from Crystals

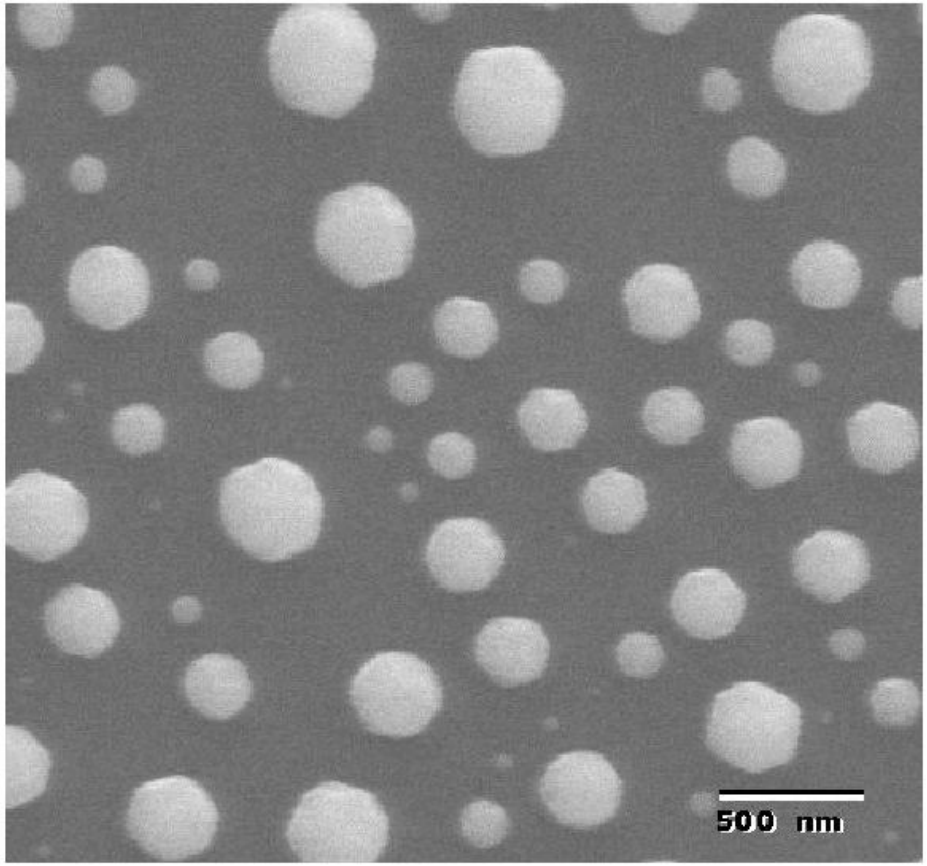


Sensitivity to strain

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



In situ growth of Pb crystals



Good statistics, 3D diffraction data

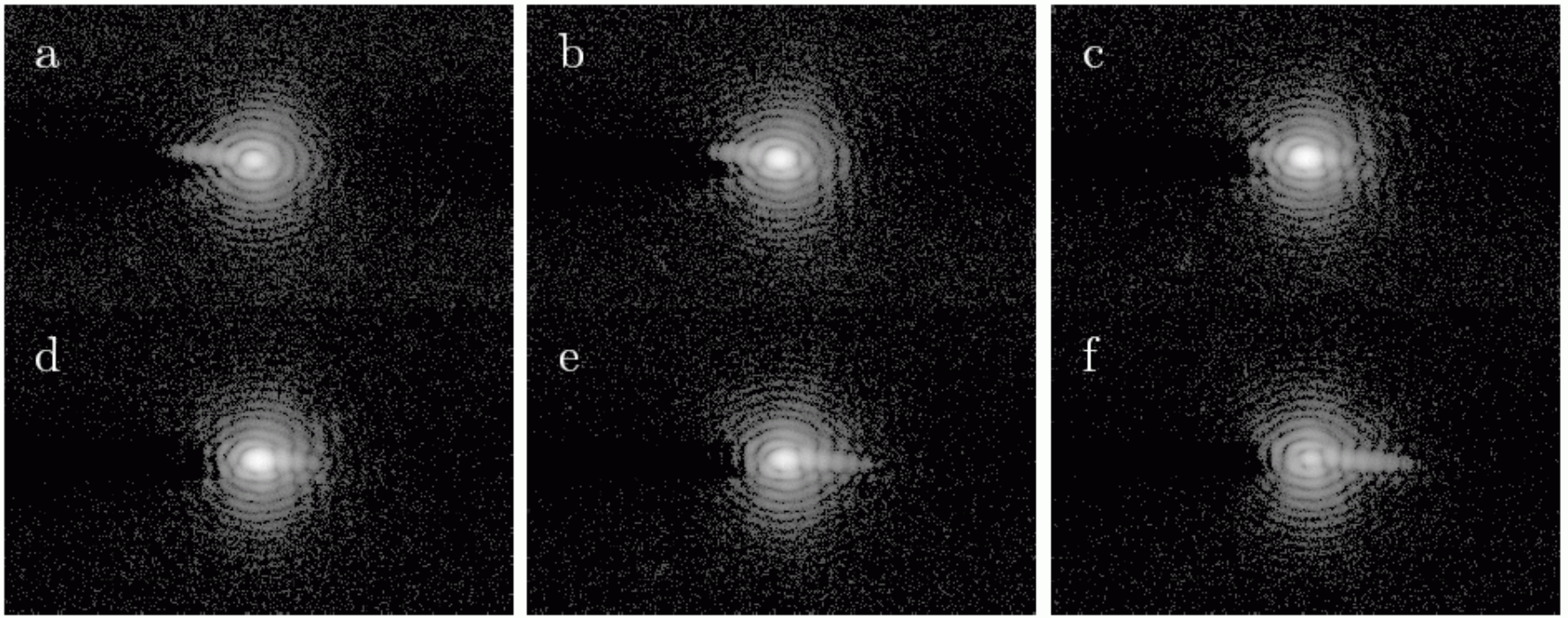
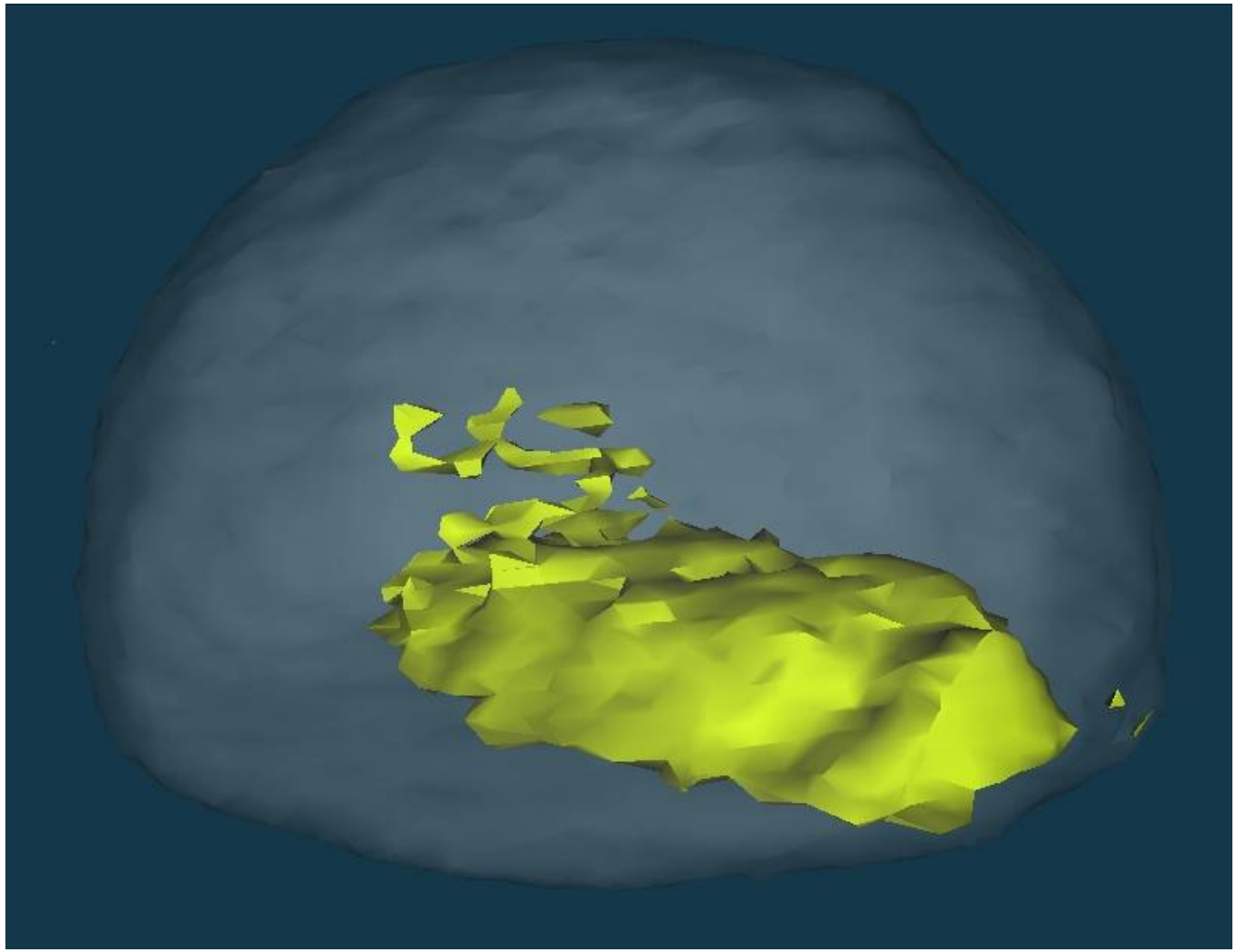
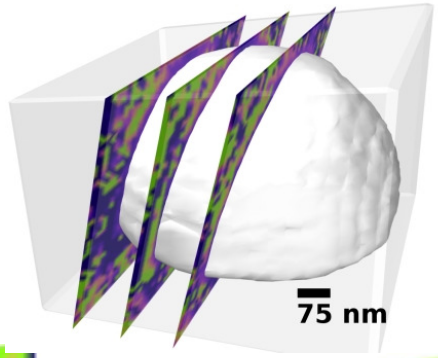


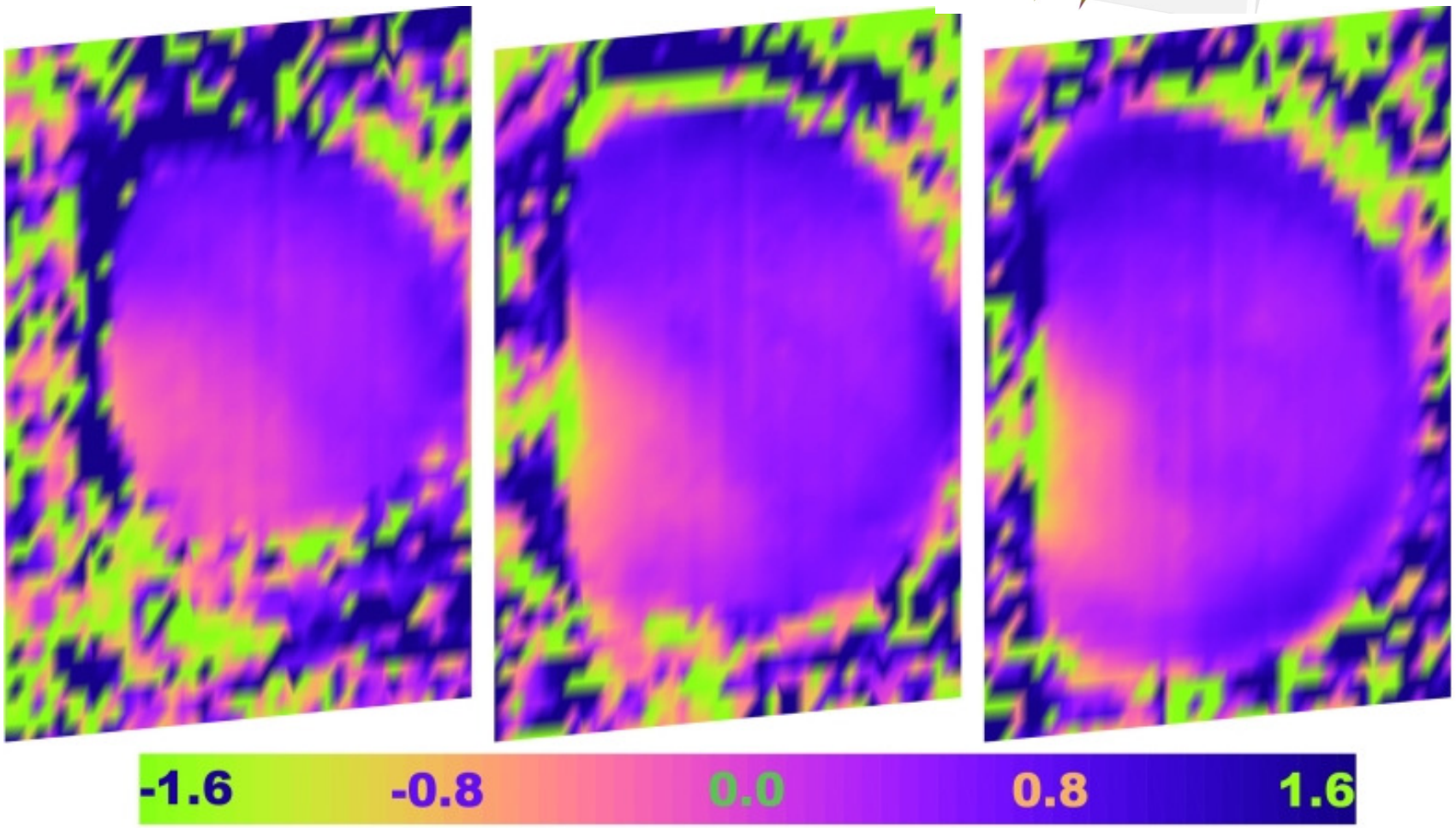
Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

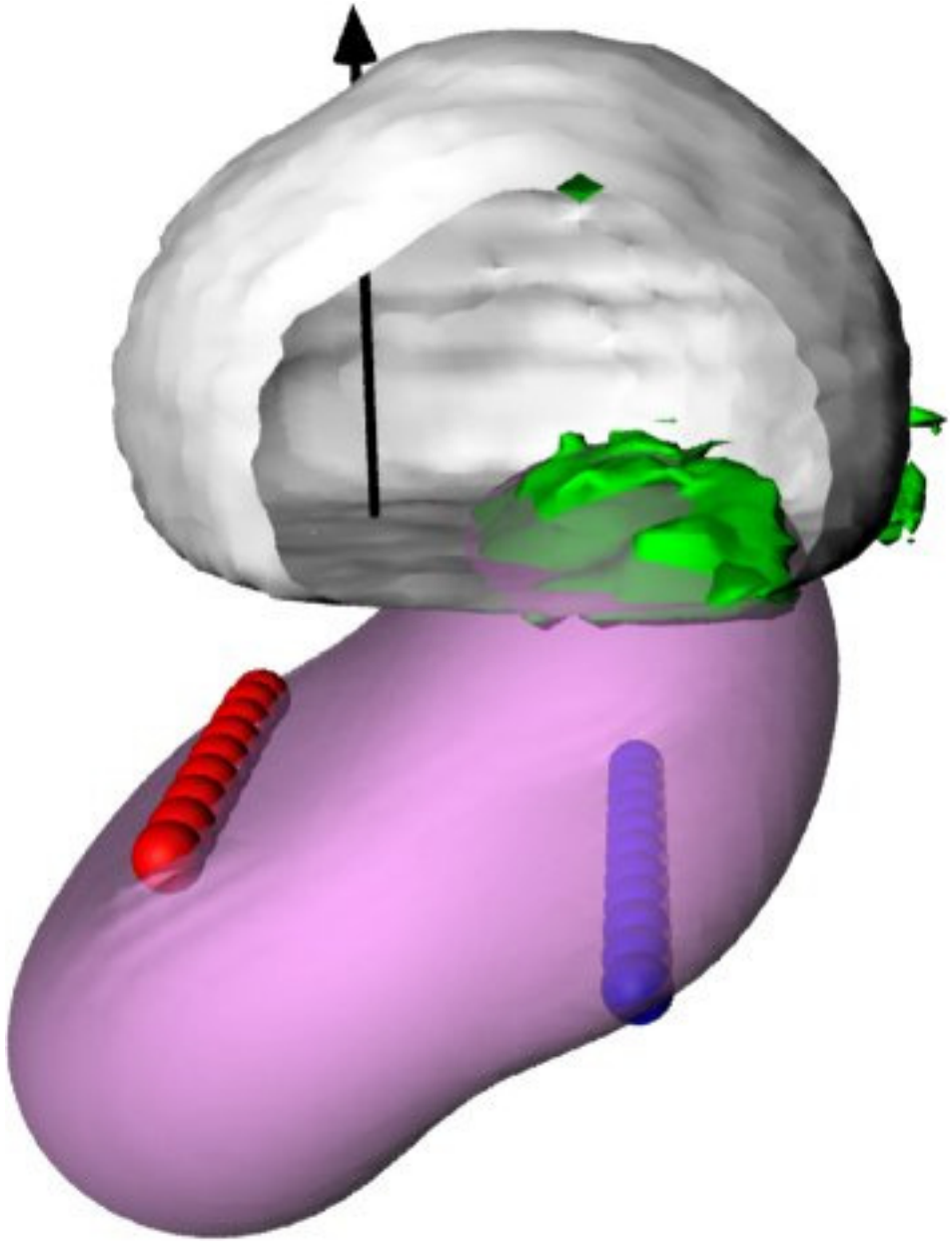
Modeling of 3D Phase Bump



3D phase map sections





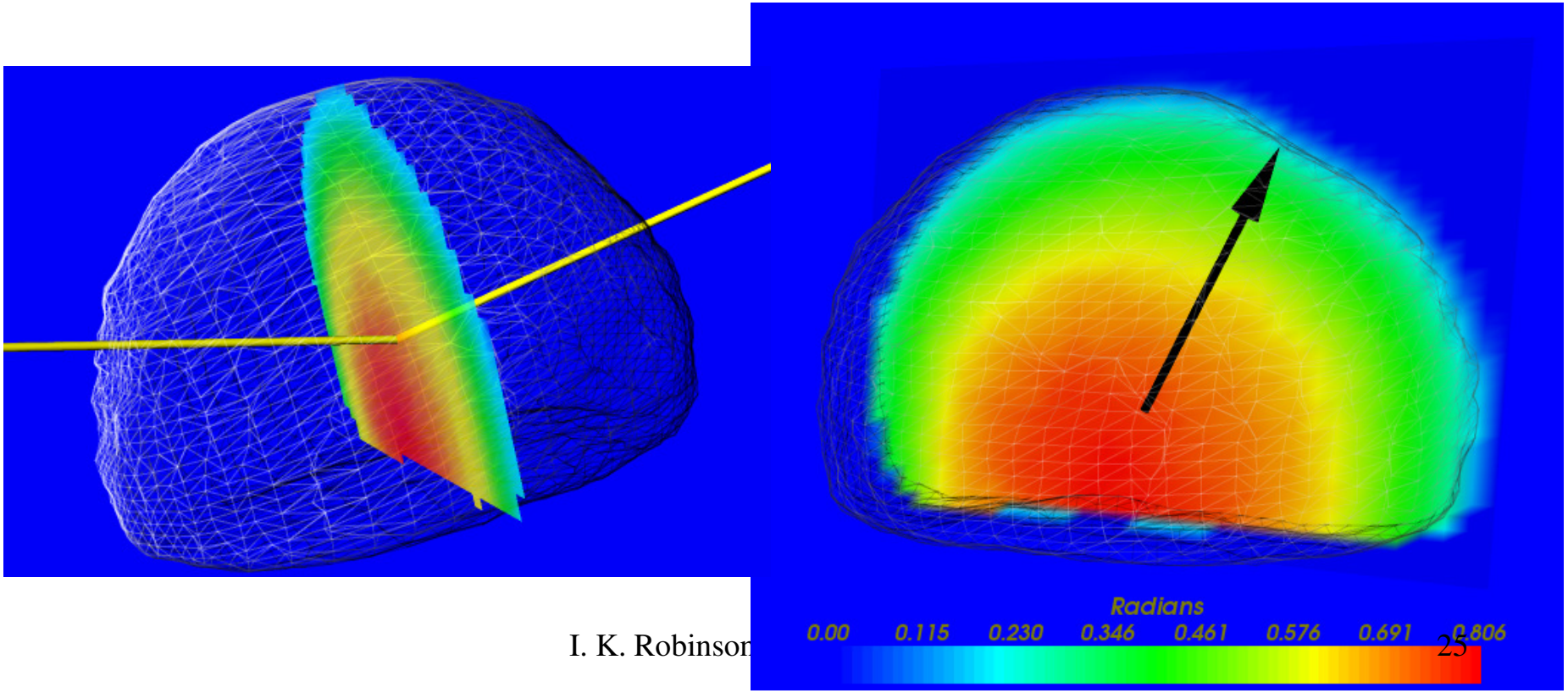


Refraction effects in Lead at 8.9keV

Phase accumulation due to refraction along scattering path

$$n=1-\delta+i\beta$$

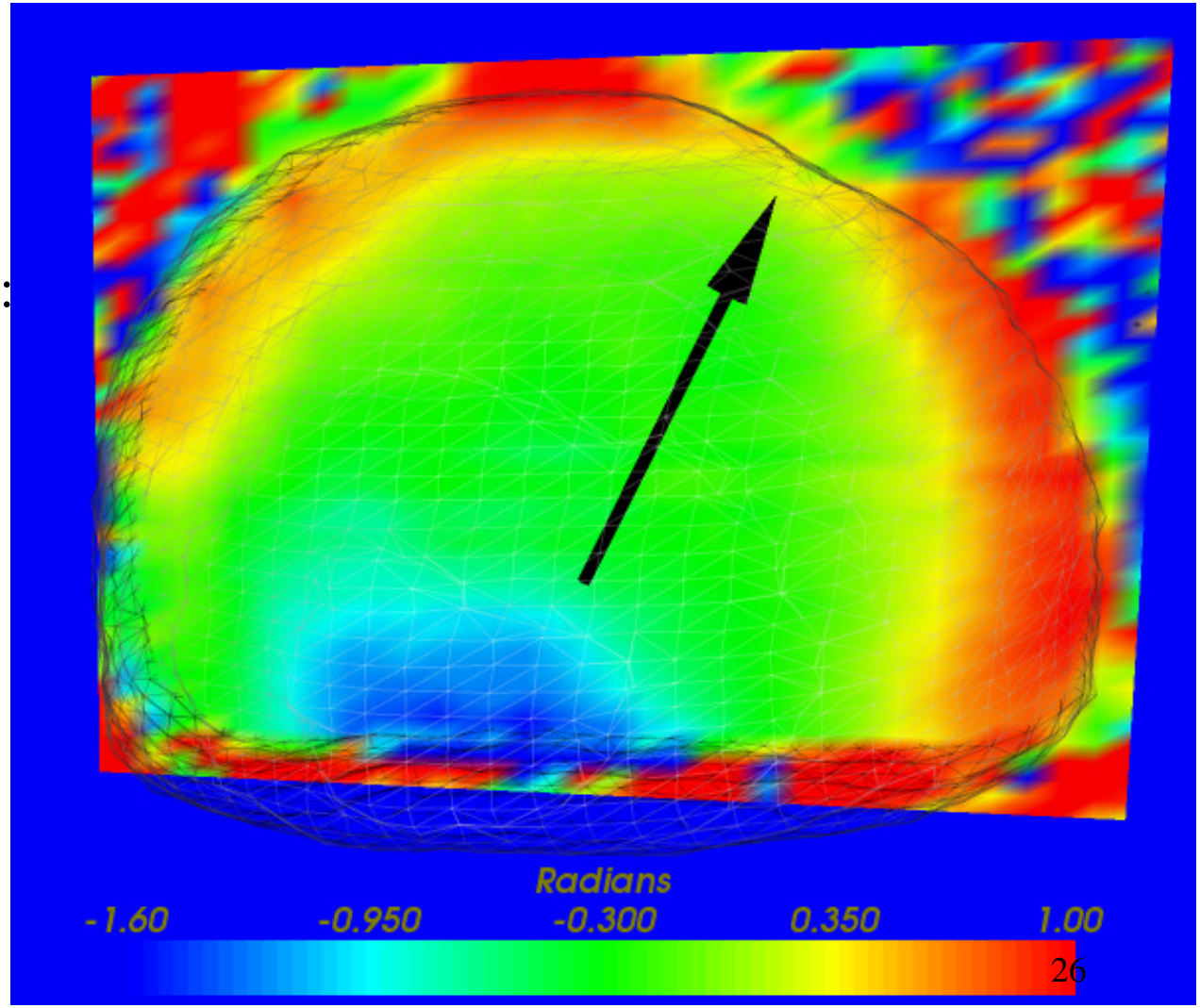
$$\delta=2.23\text{x}10^{-5}$$
$$\beta=2.19\text{x}10^{-6}$$



Refraction corrected phase map

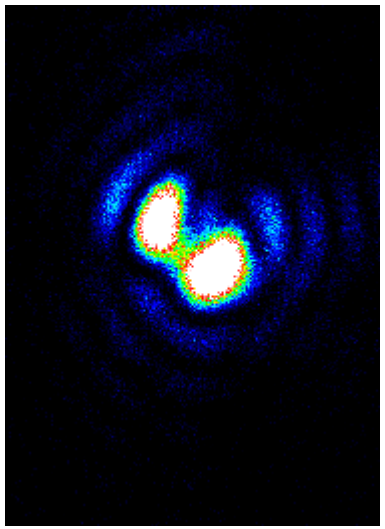
Max phase = 1.15rad
= 0.052nm

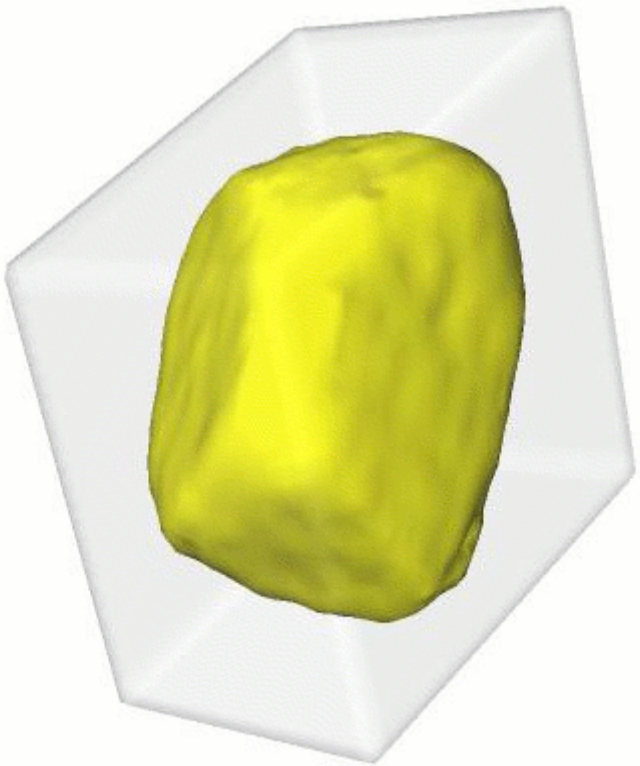
Phase on the (111) facet:
= 0.47 rad
= 0.02nm



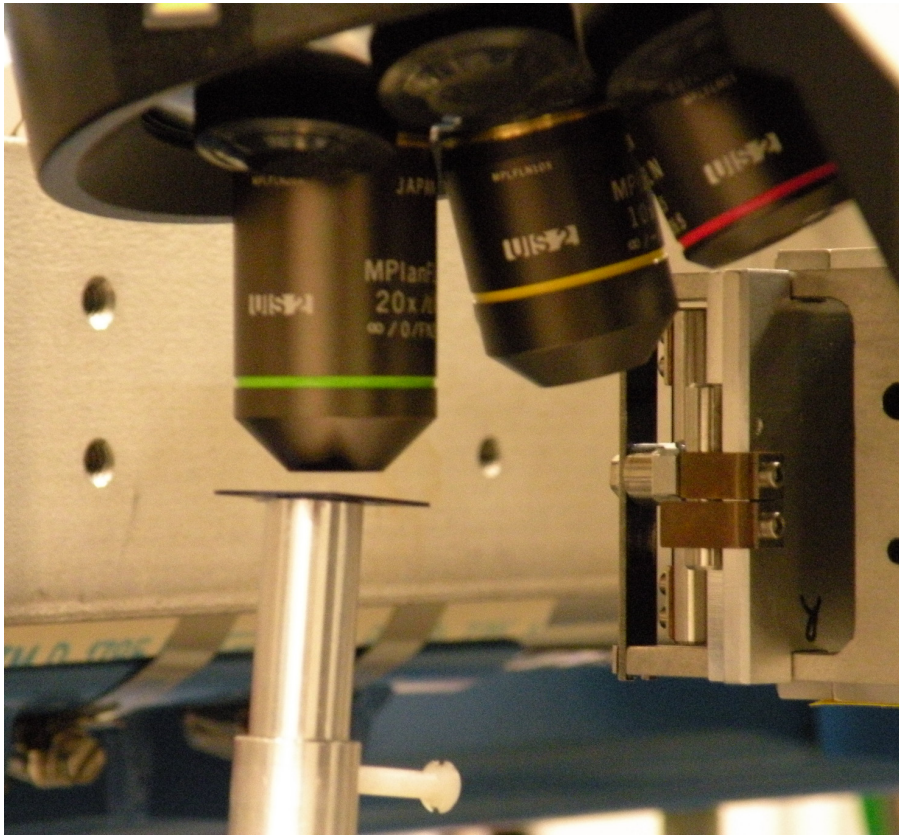
Gold nanocrystal reconstruction

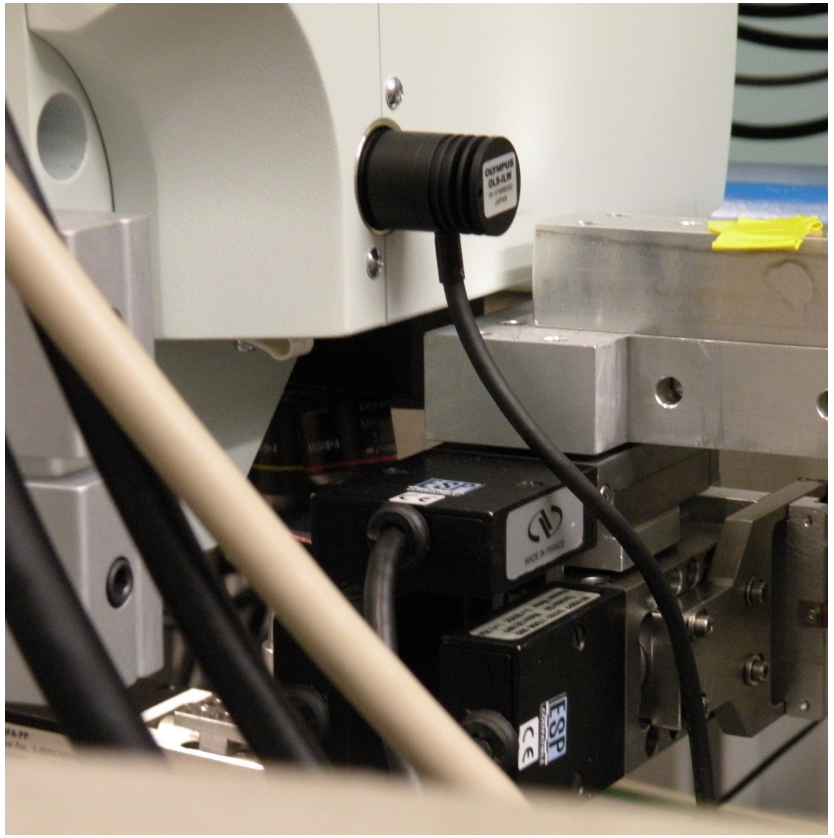
showing support used for 20 HIO followed by 10 ER



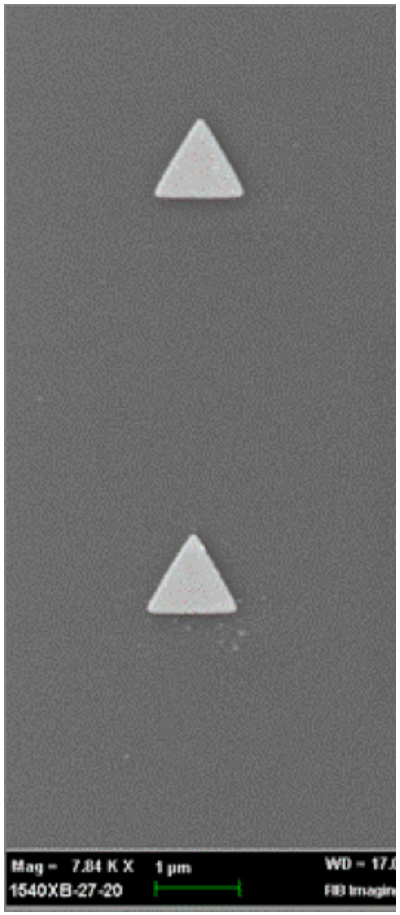


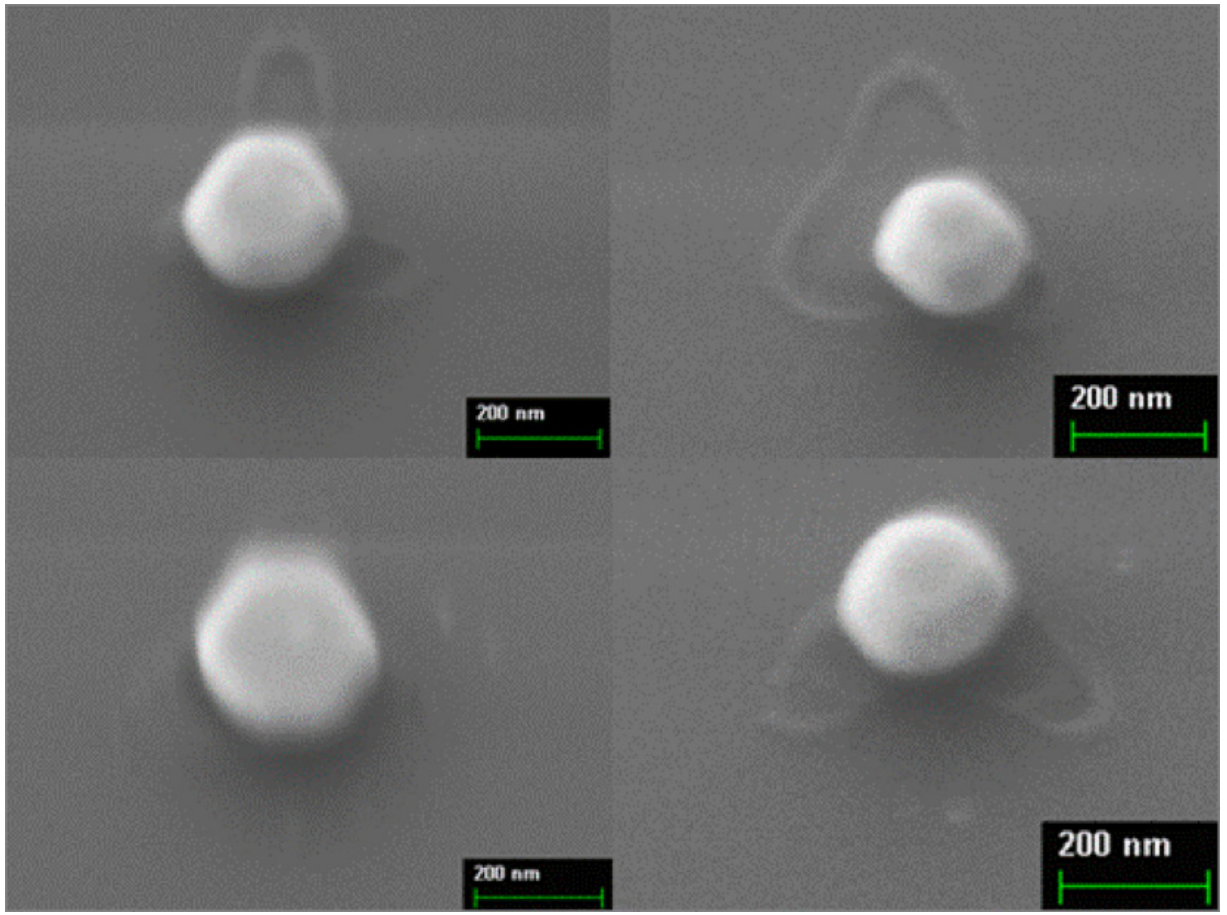
Confocal Alignment Microscope





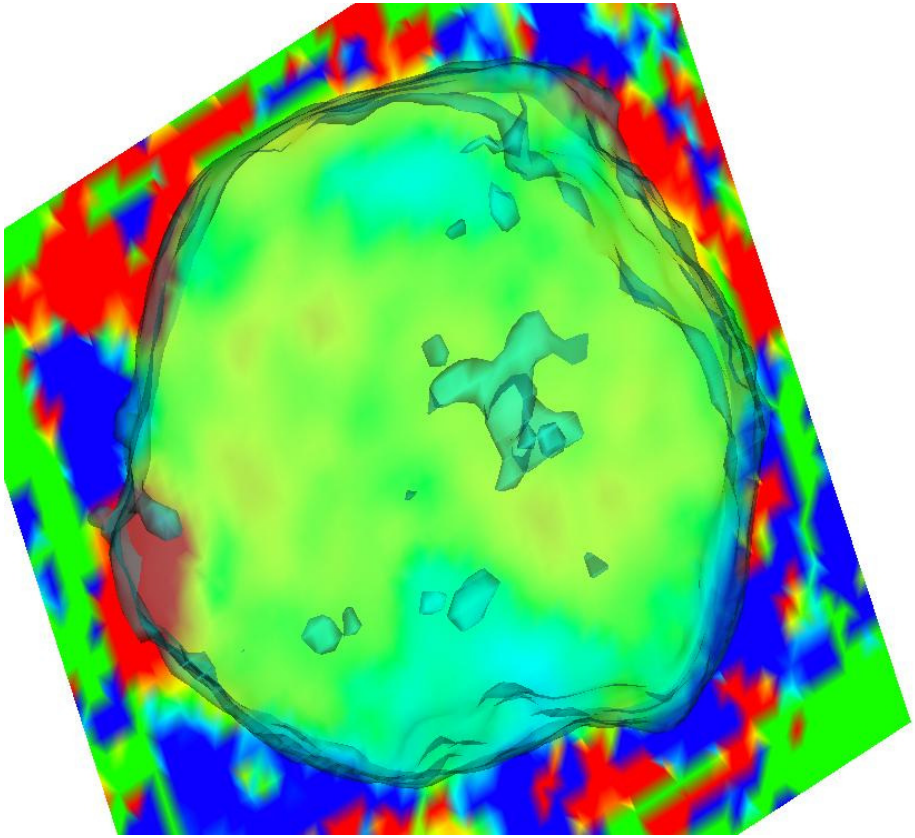
Single Au nanocrystal synthesis

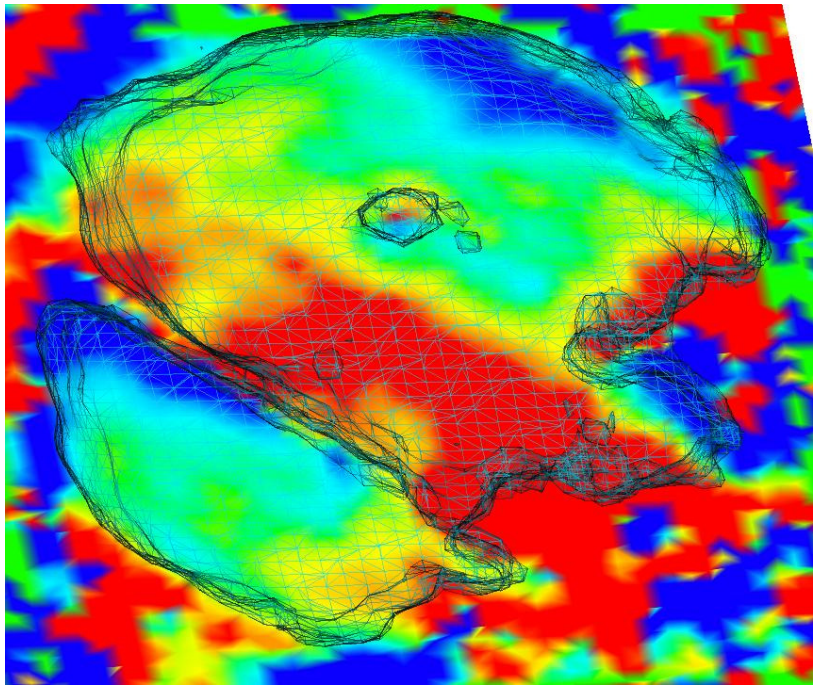




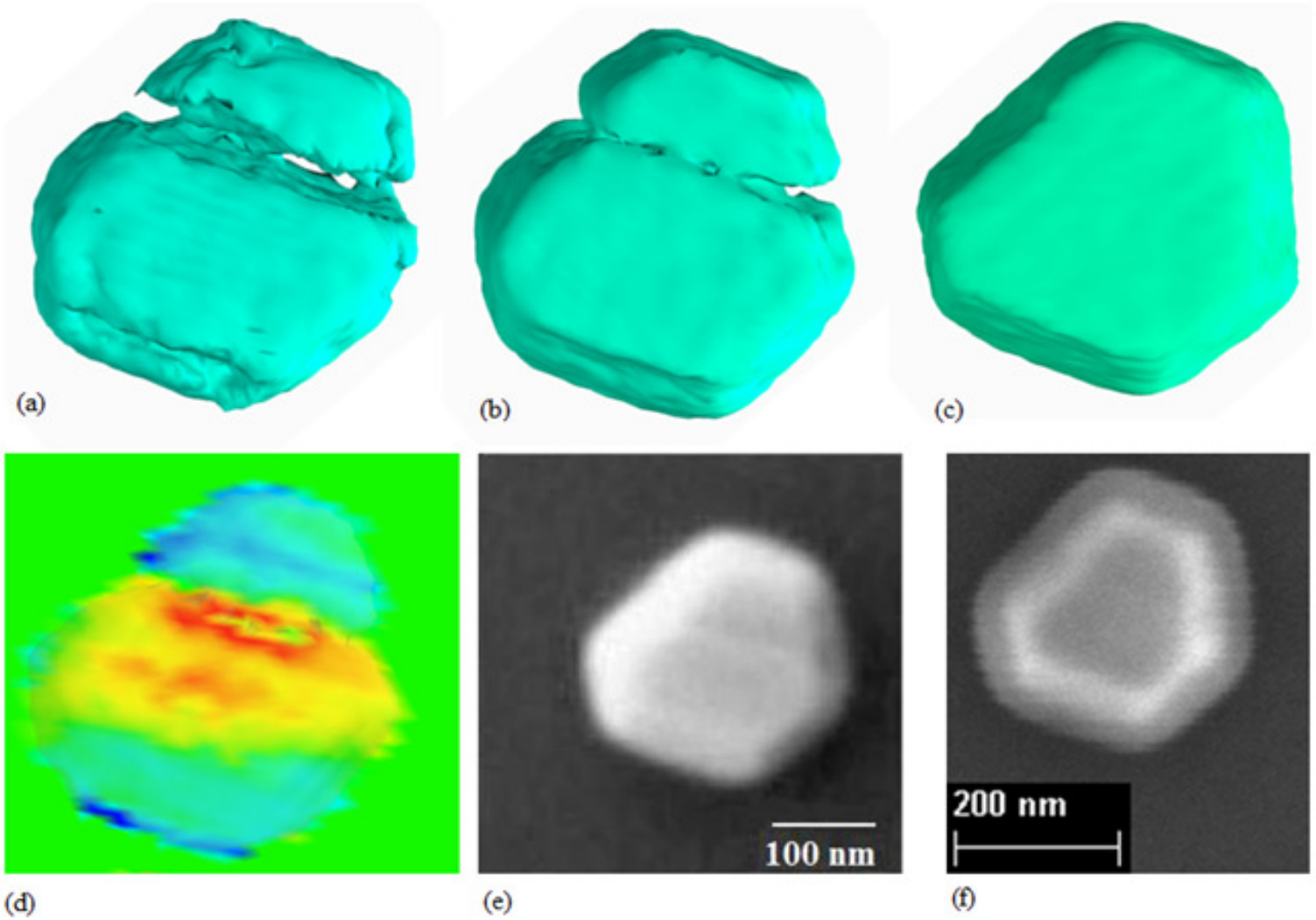
Two views of strain in Au NC

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



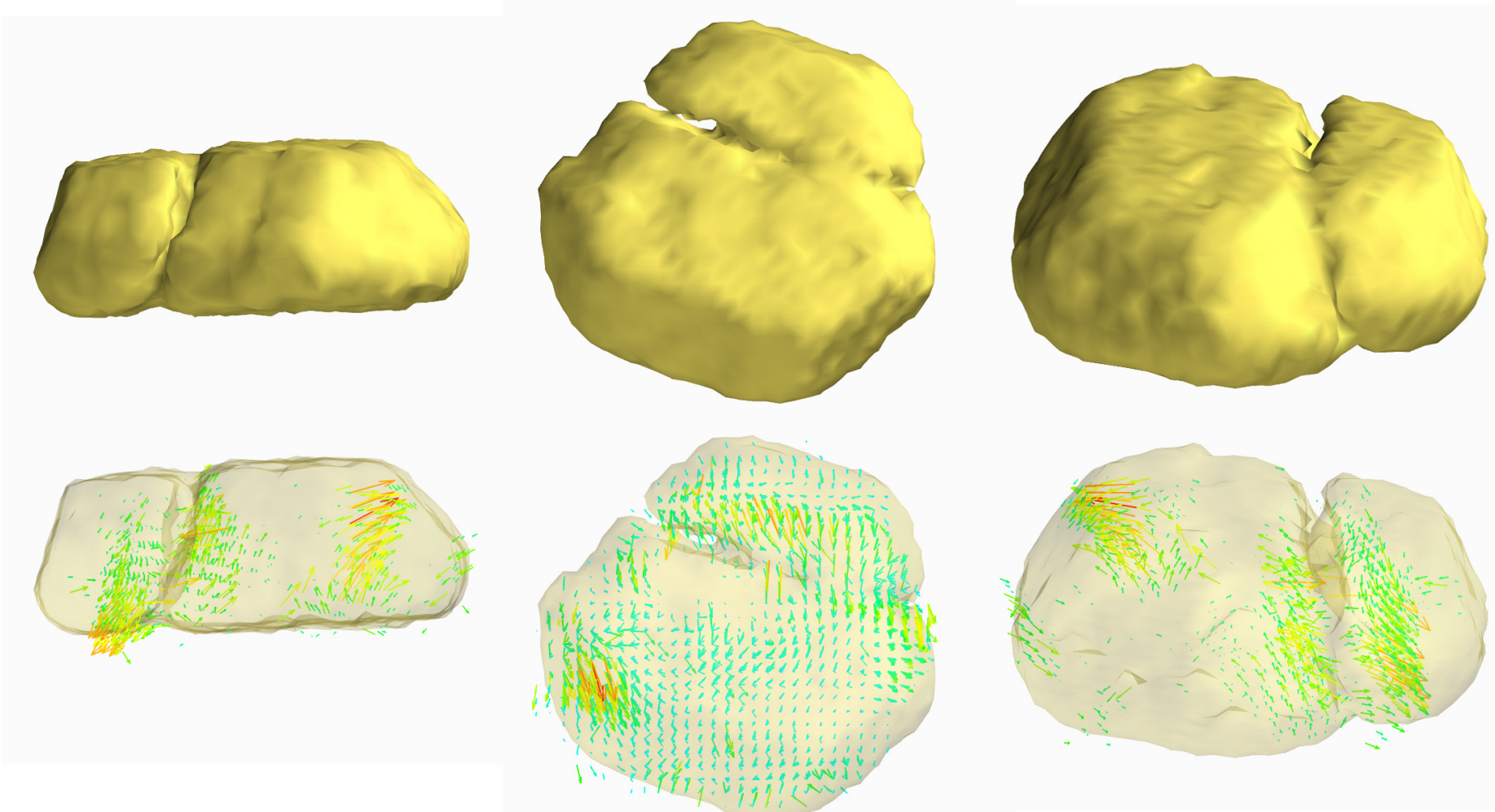


Different Bragg Peaks

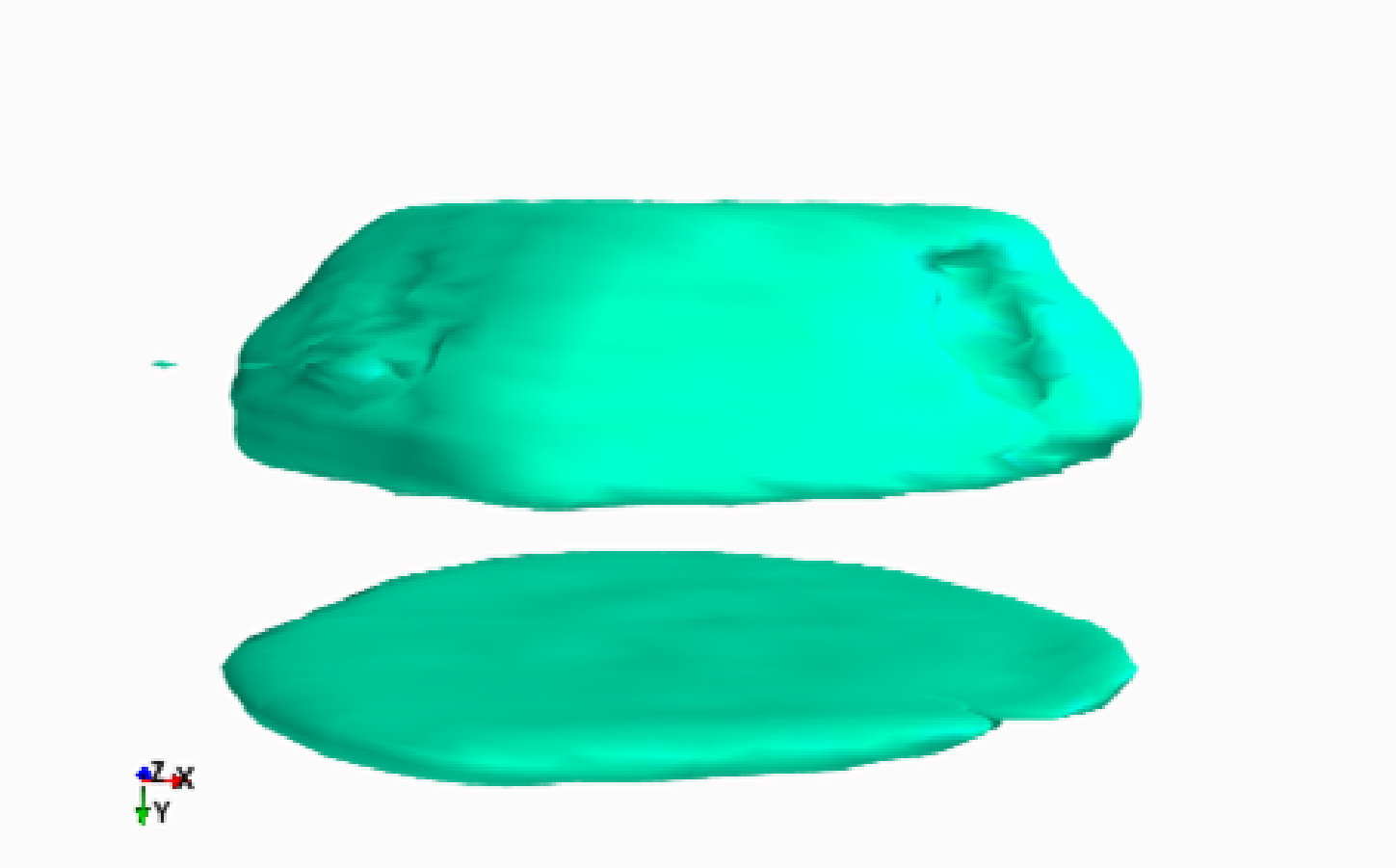


Vector displacement field

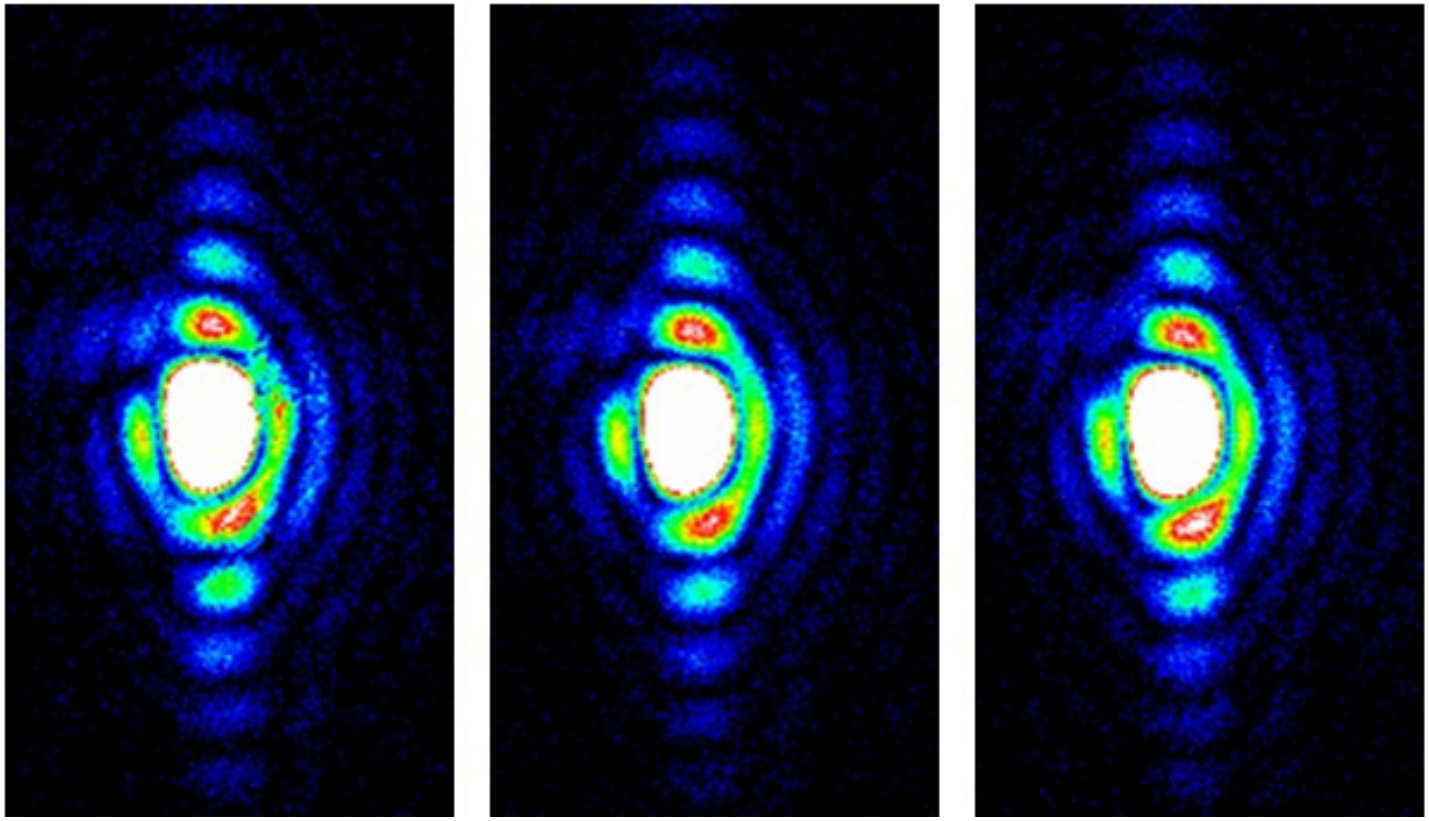
Merged reconstructions from (11-1) (020) and (-111)



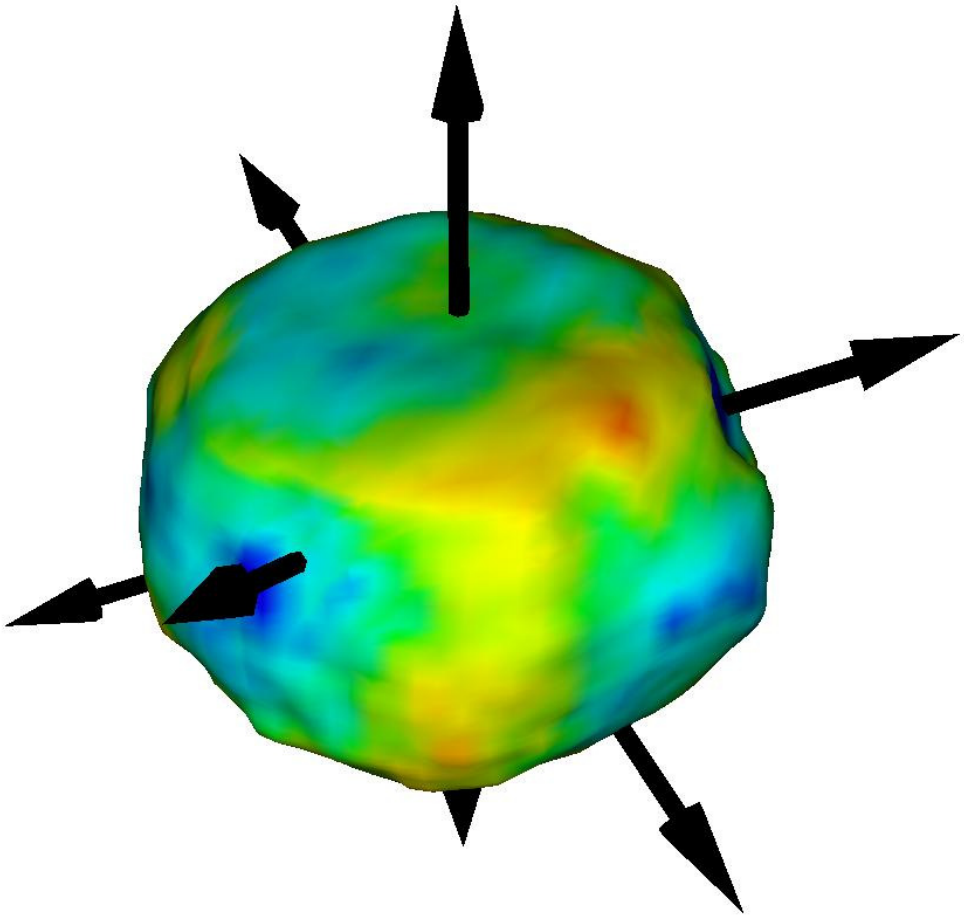
Horizontally Faulted Slab



Typical Au nanocrystal CXD

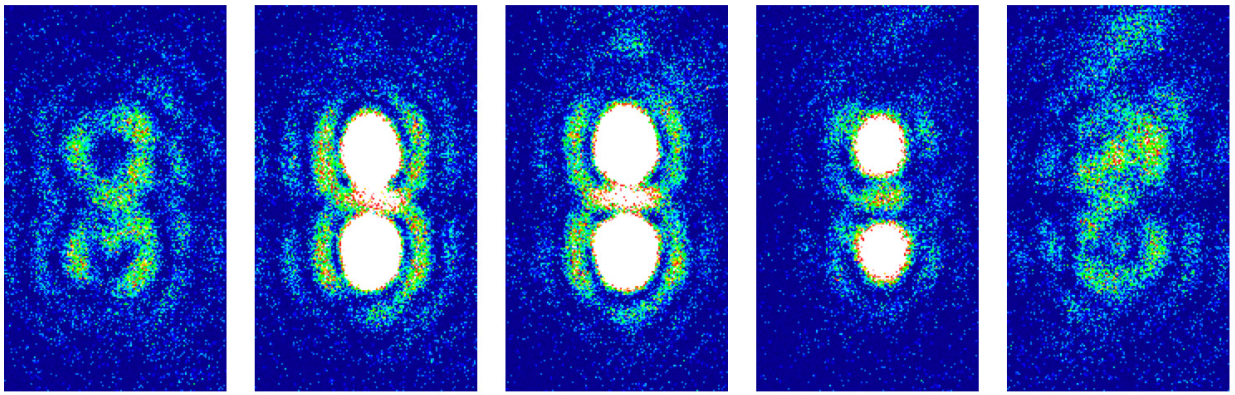


Phase isosurface of residual strain



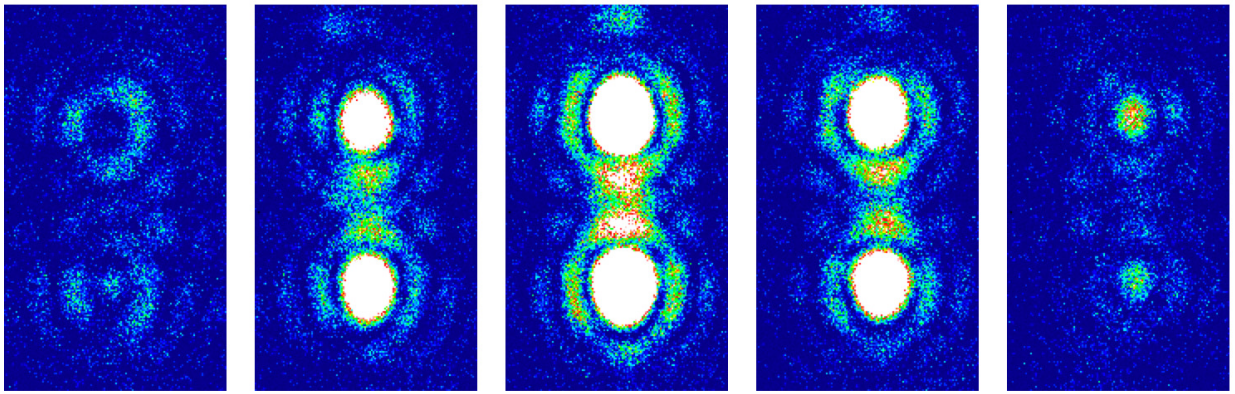
Au nanocrystal, doubled CXD

Au606-49, αi = 0.1°



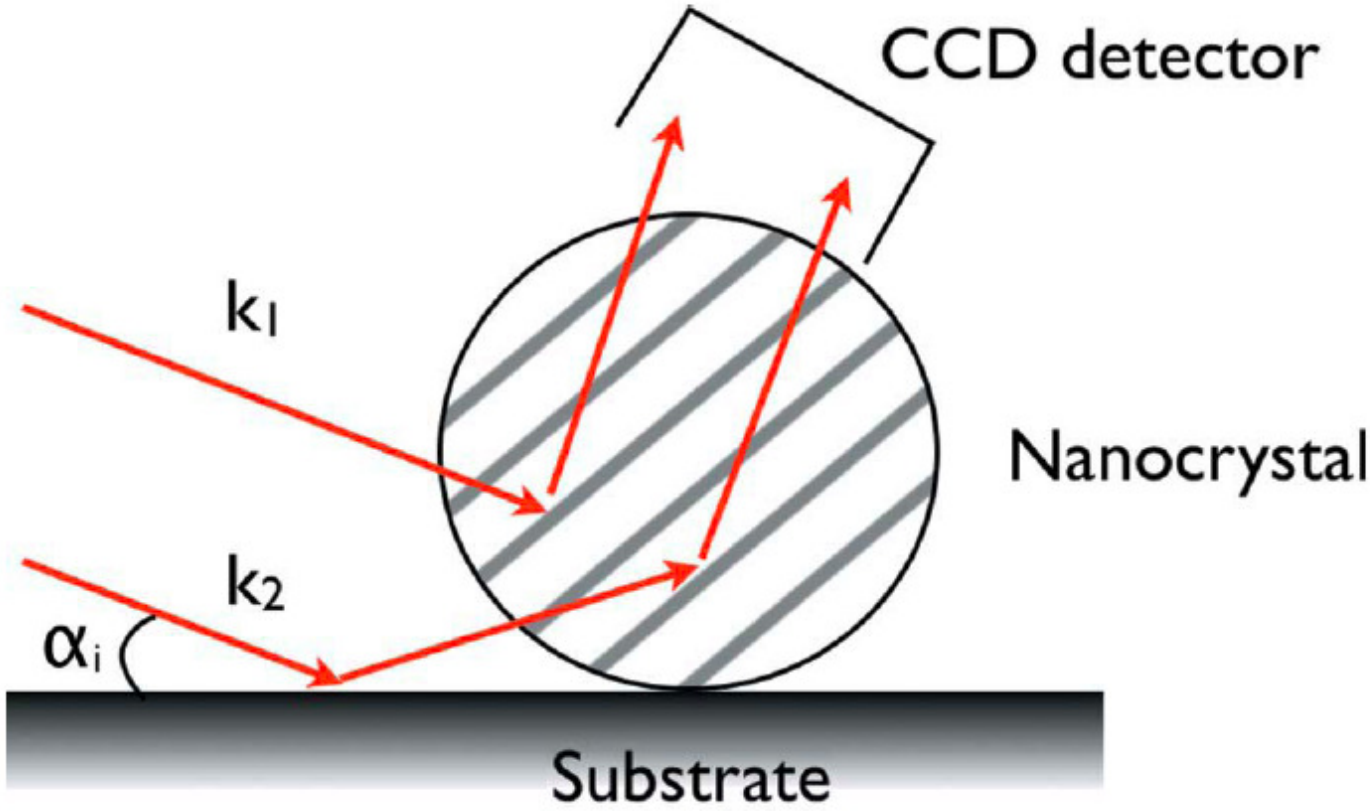
-0.2° -0.1° 0° +0.1° +0.2°

Au606-51, αi = 0.15°

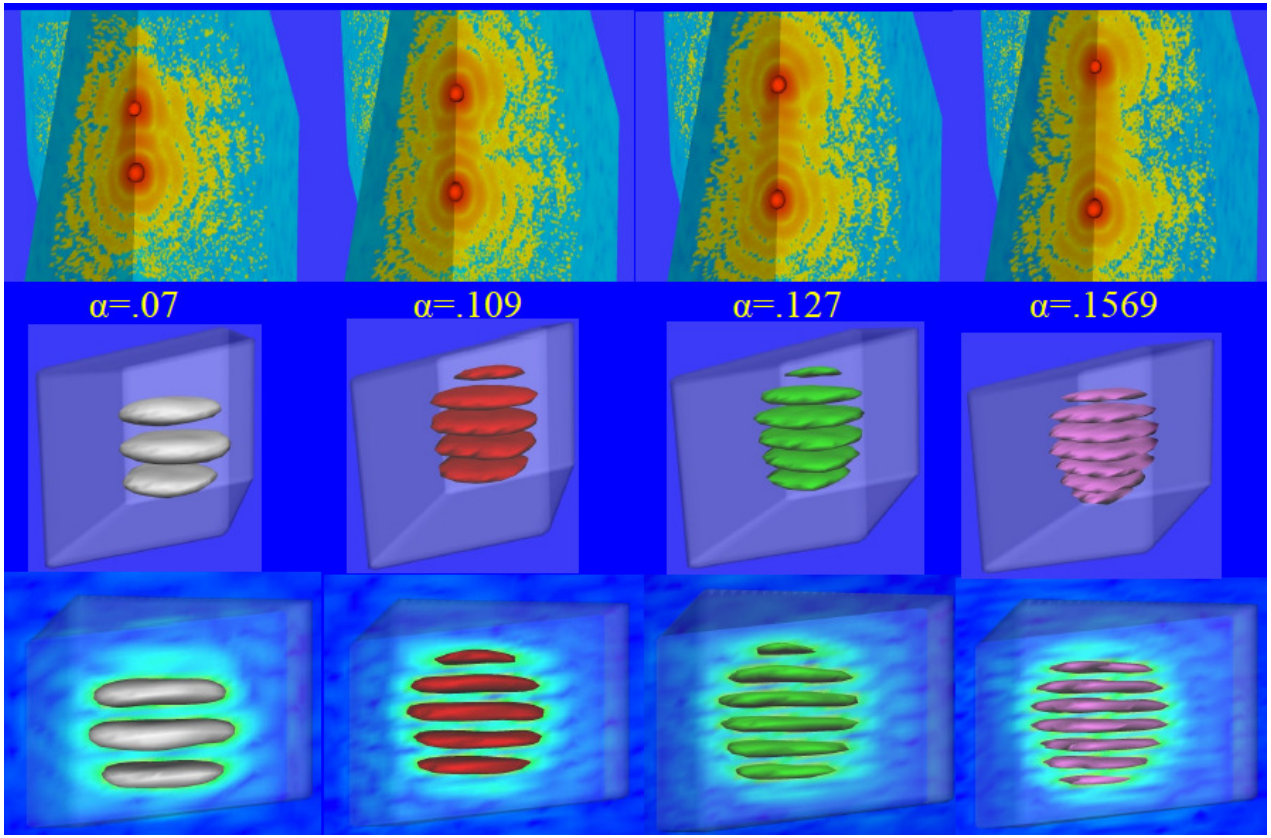


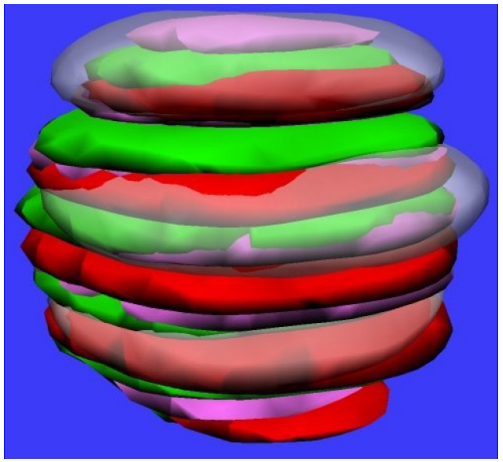
-0.2° -0.1° 0° +0.1° +0.2°

Standing Wave Illumination



Reconstructed Au images
$\alpha_i = 0.07, 0.11, 0.13, 0.16$





Conclusions

- Internal structure of Nanocrystals
- 3D imaging of faults in Nanowires
- Phasing by computation instead of lens
- Strain fields imaged from asymmetric patterns
- Contact Forces and Surface Strains
- Standing Wave effects directly imaged