Coherent X-ray Diffraction for mapping strains in ZnO Nanocrystals

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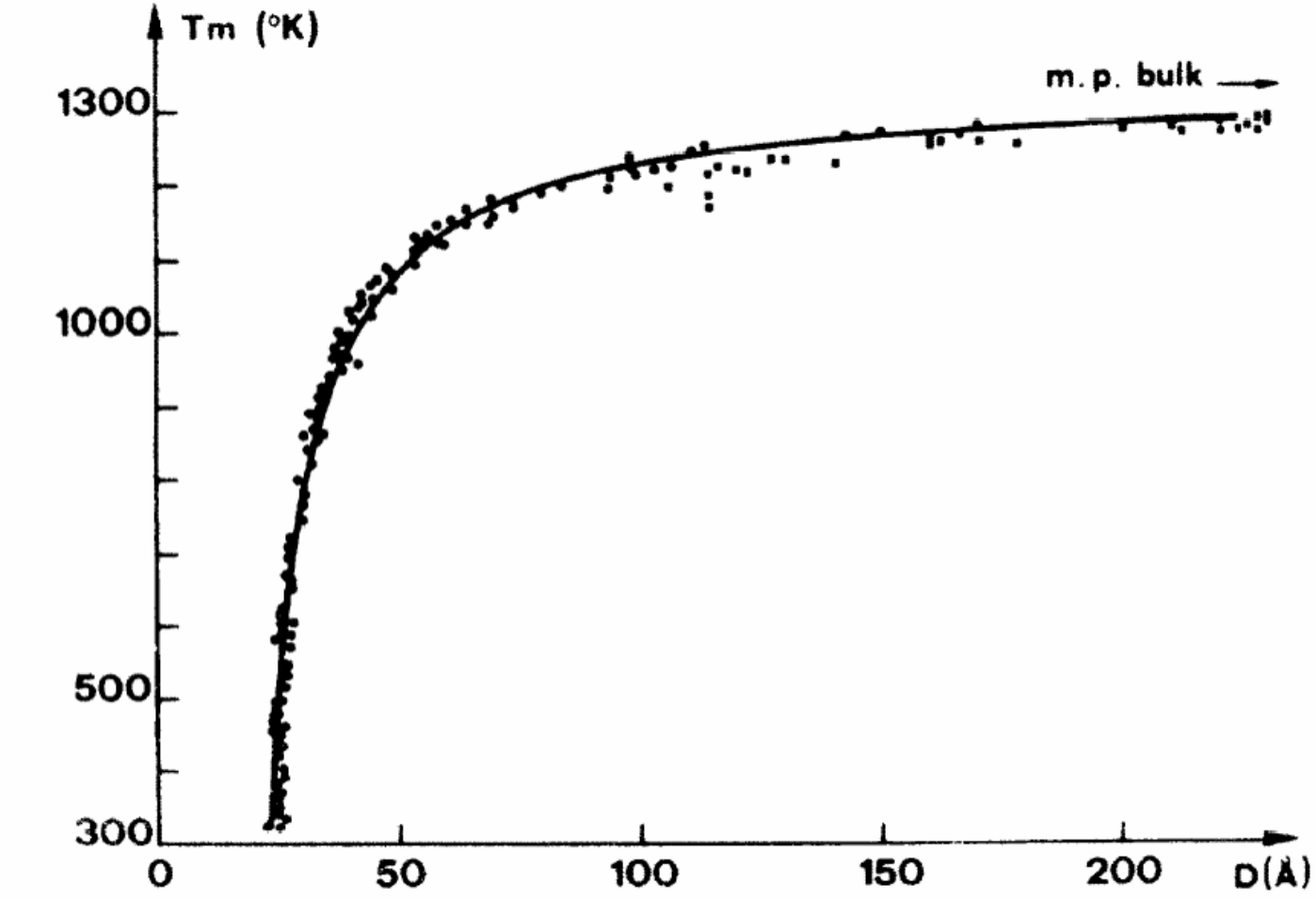
Outline

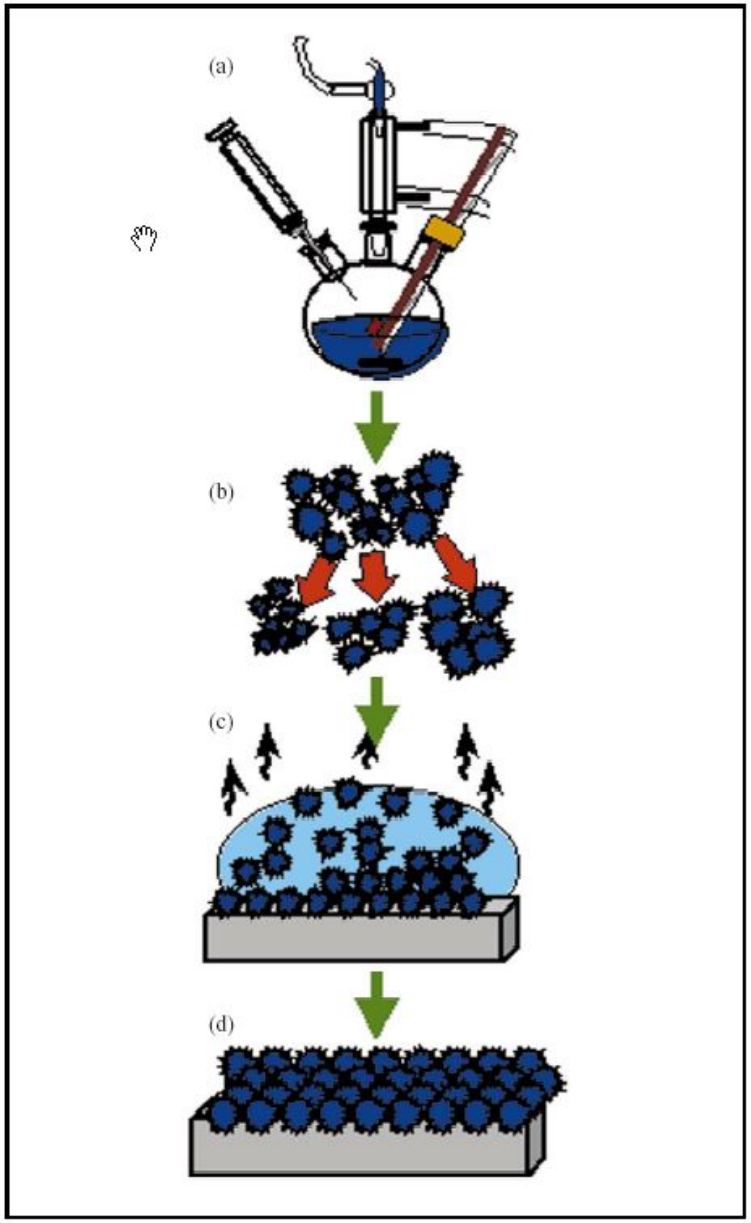
- Coherent x-ray diffraction
- Oversampling solves the phase problem
- Nanocrystal structures
- Exploration of crystal strain
- Effects of partial coherence

Size-dependent Melting of Au Particles

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

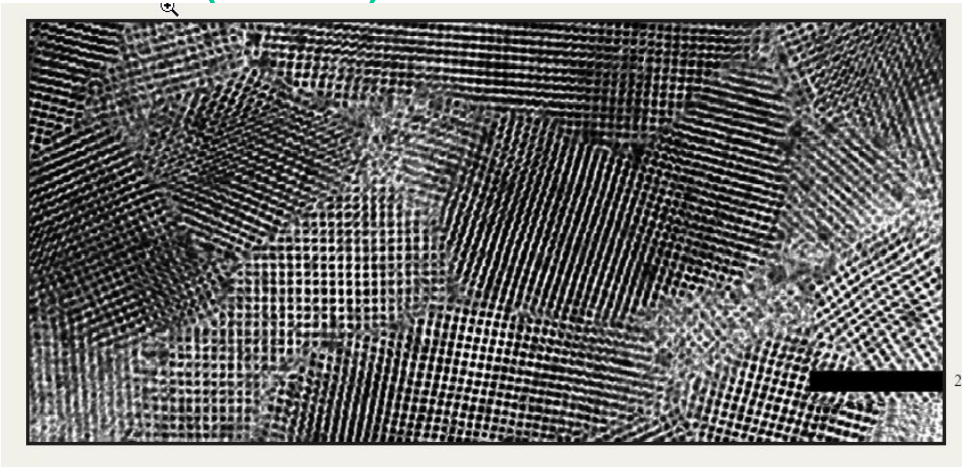


Chemical Synthesis of Nanocrystals



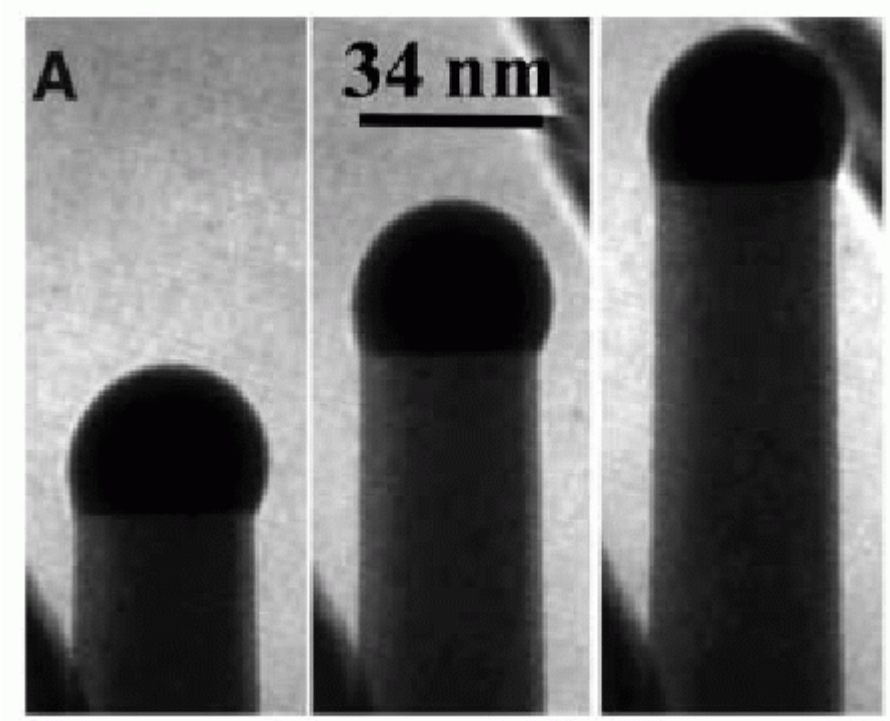
- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

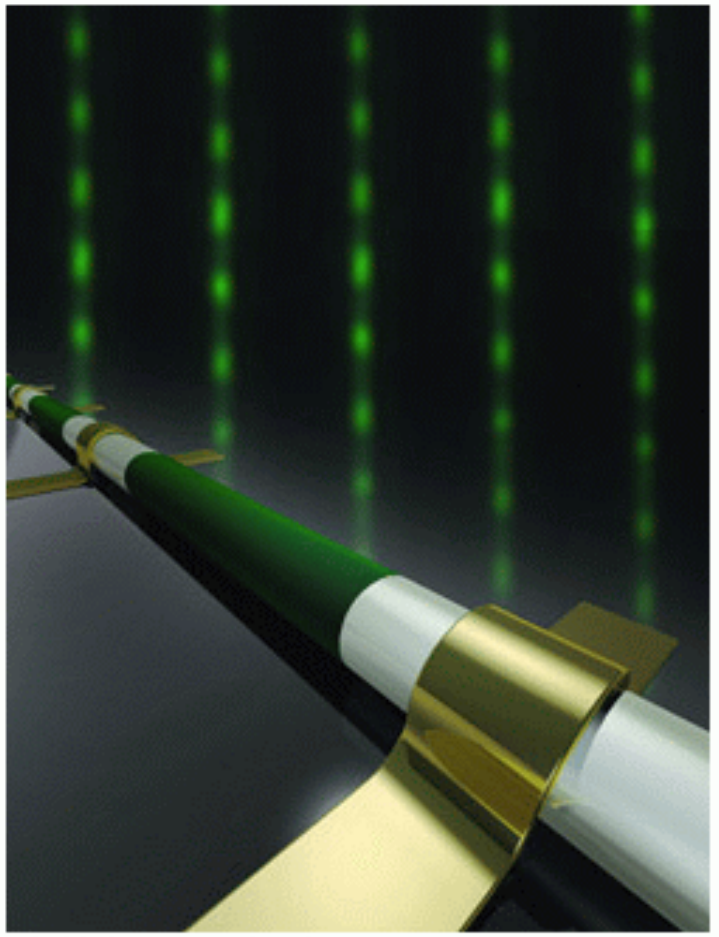
C. B. Murray, IBM J. Res. & Dev. **45** 47 (2001)



VLS growth of nanowires

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

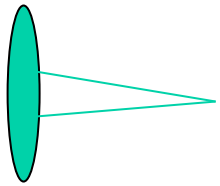




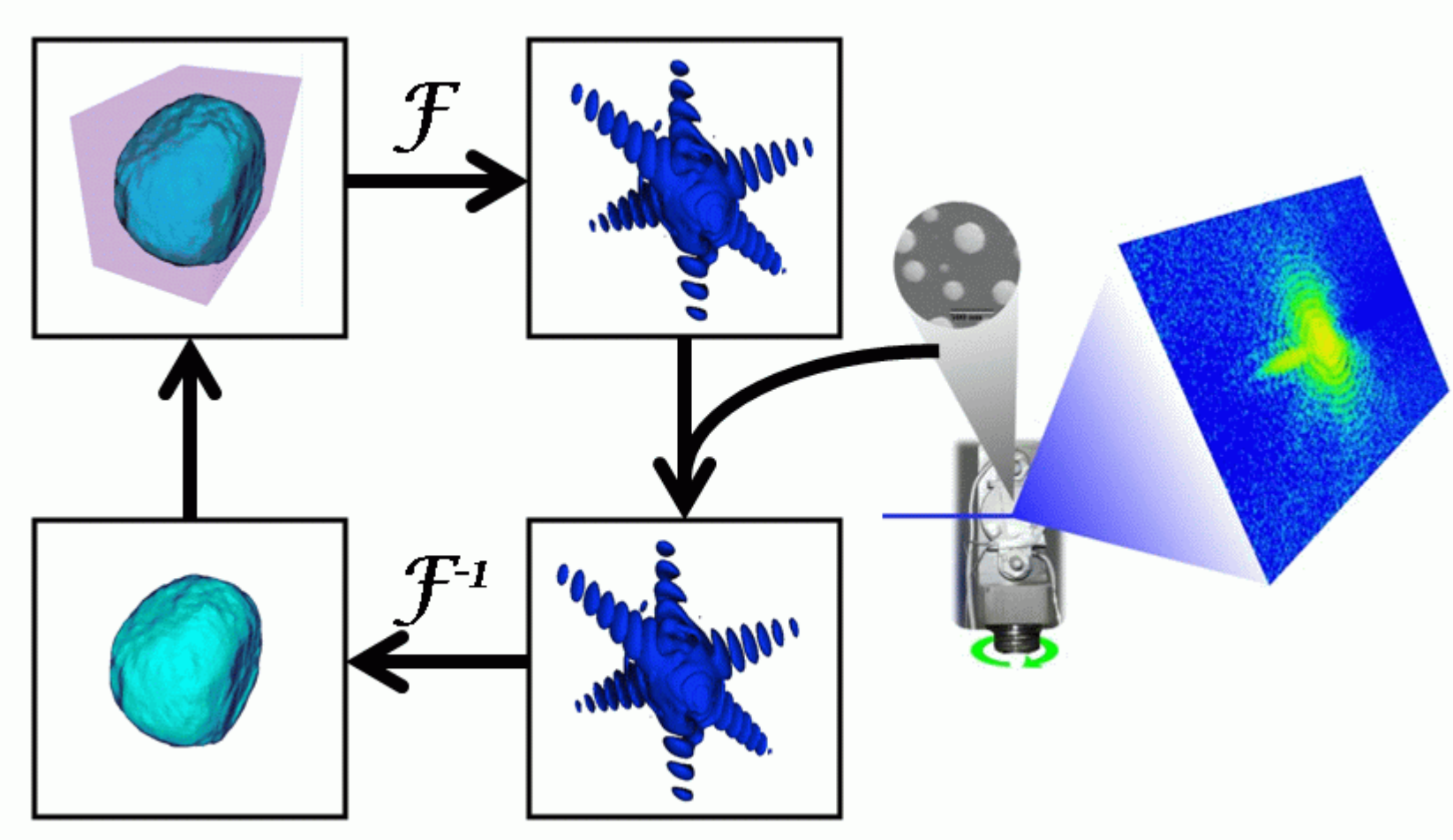
NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

I. K. Robinson, Regensb

Lensless X-ray Microscope, 2003



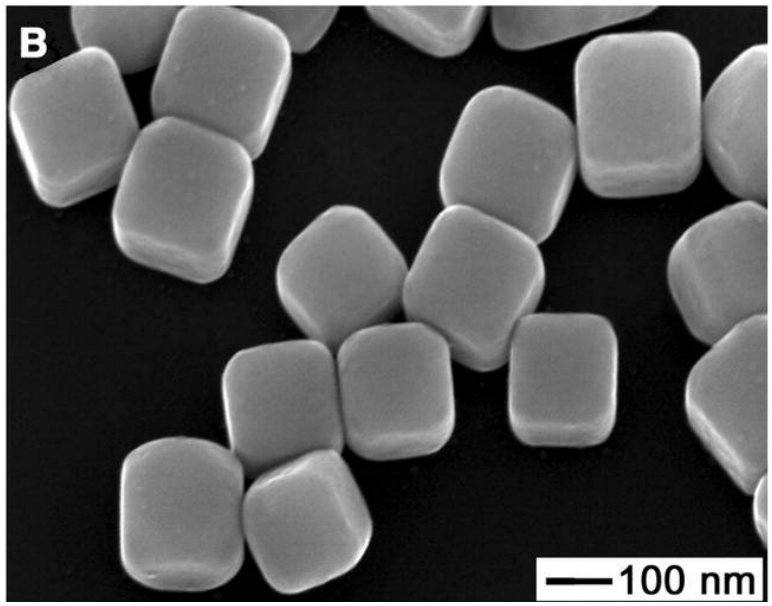
Generic "Error Reduction" method

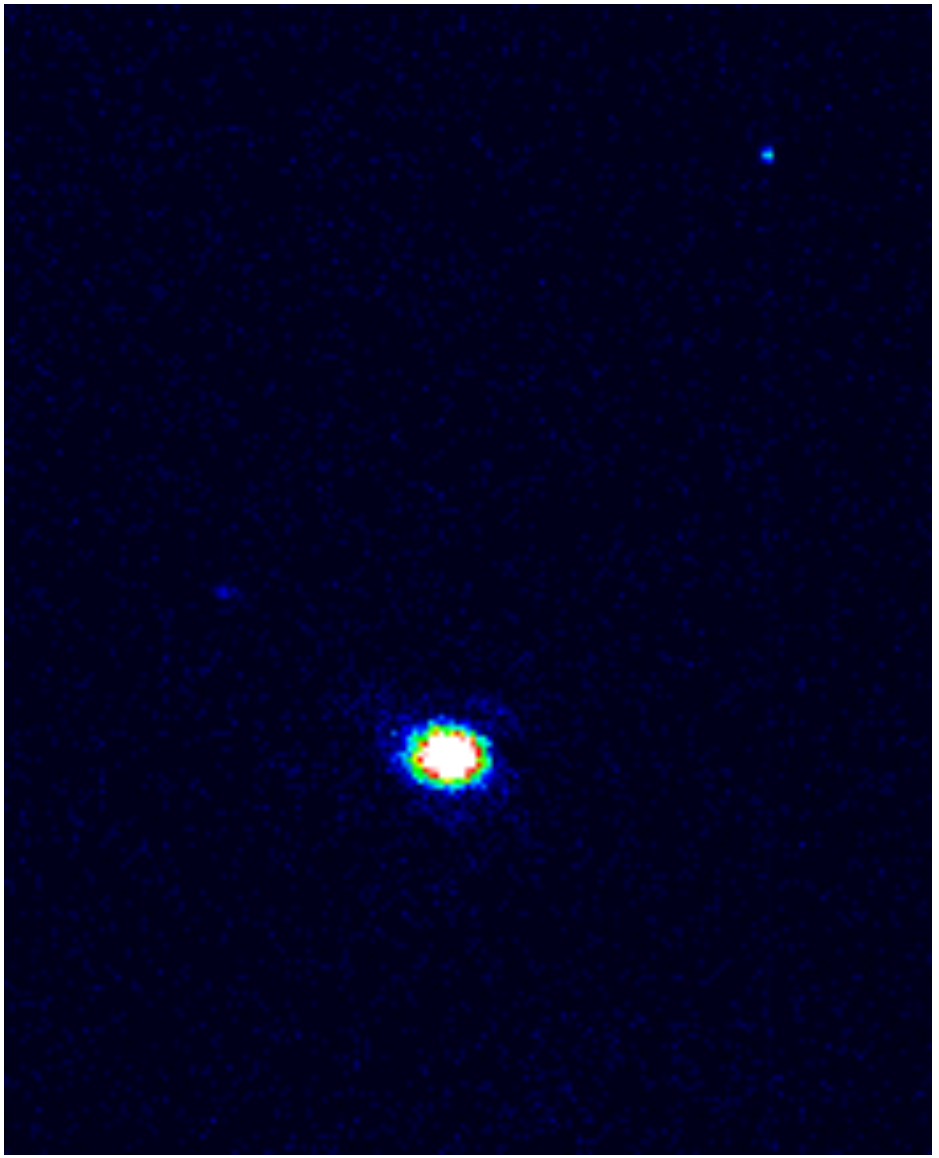


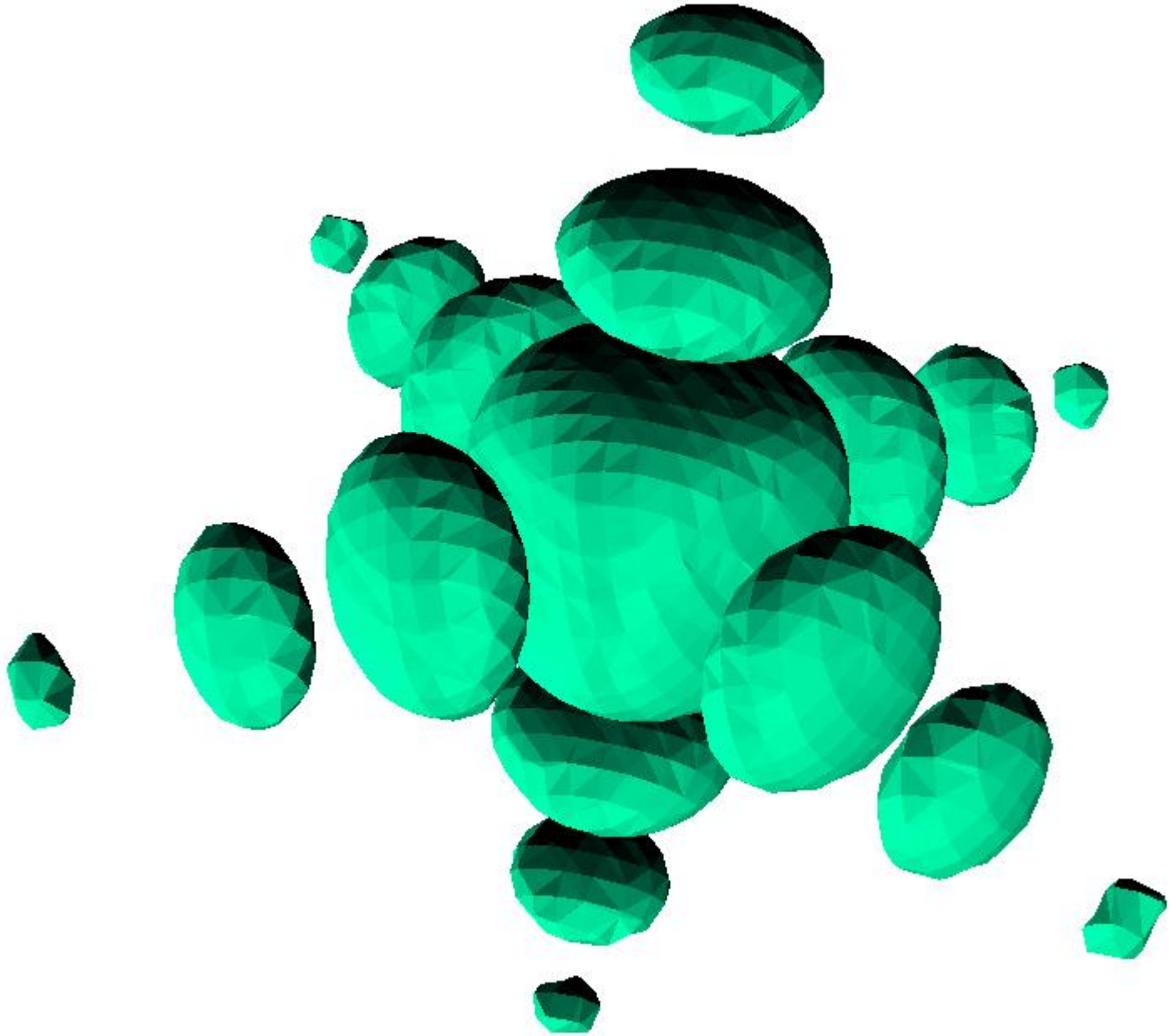
J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

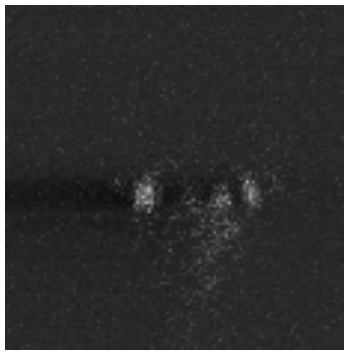
Chemically Synthesized Silver Nanocube Rock with 0.01° steps

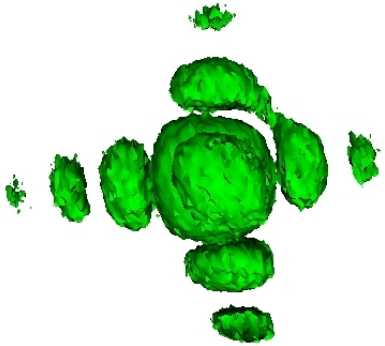
Yugang Sun and Younan Xia, Science 298 2177 (2003)

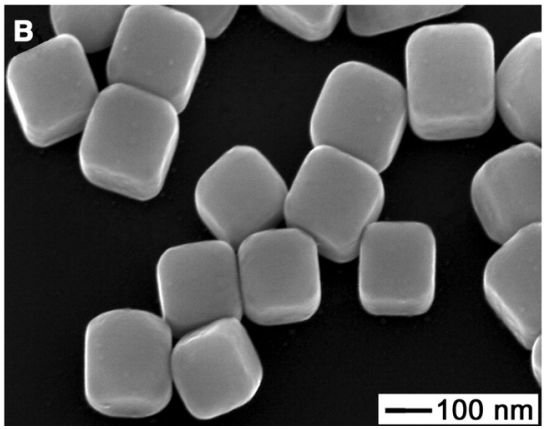


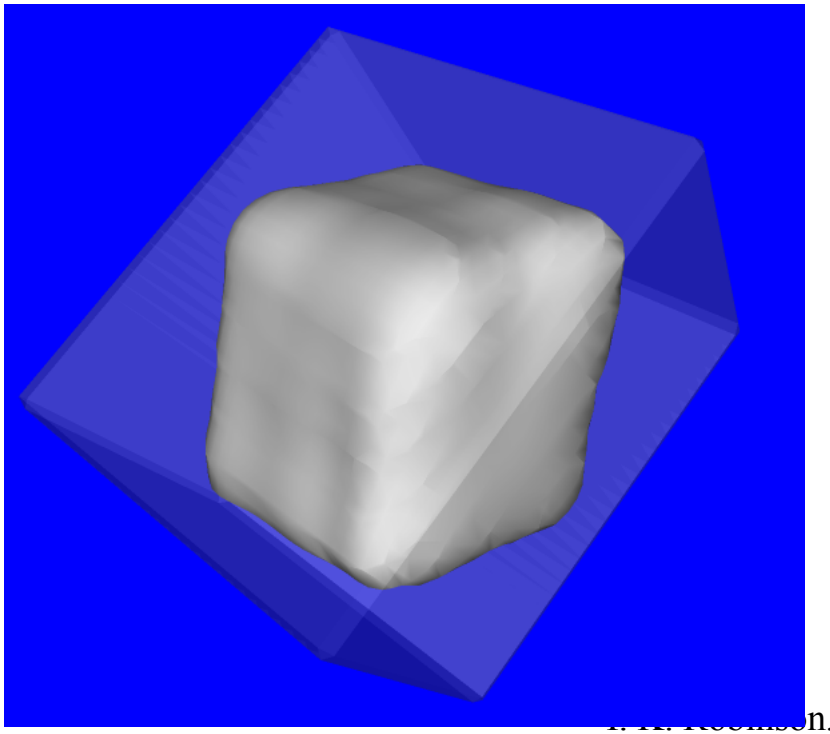


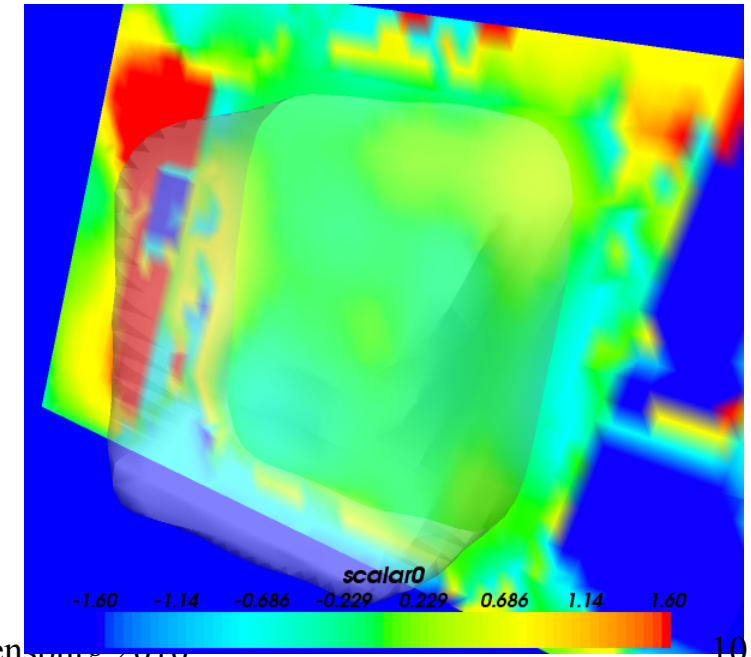




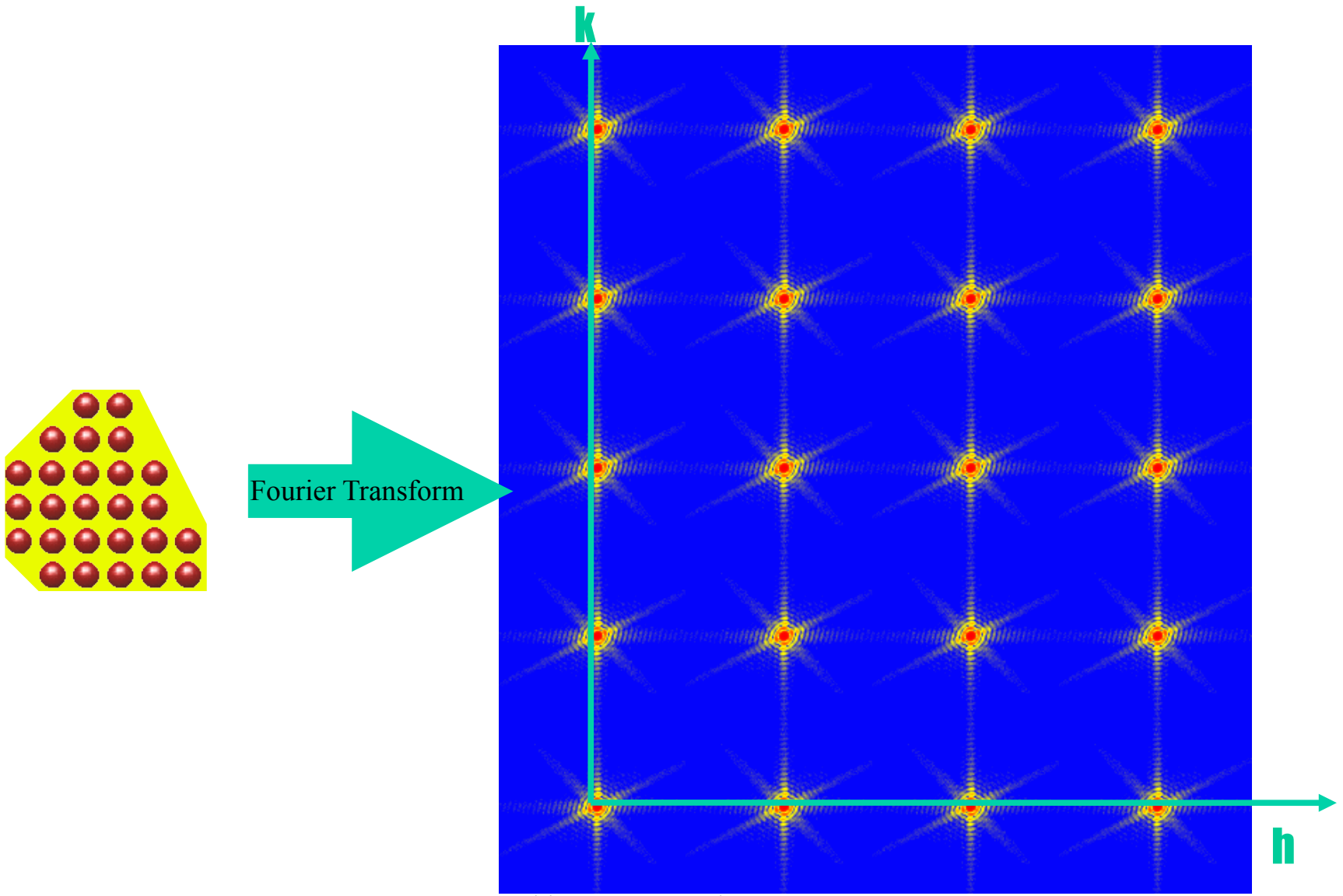



B
100 nm



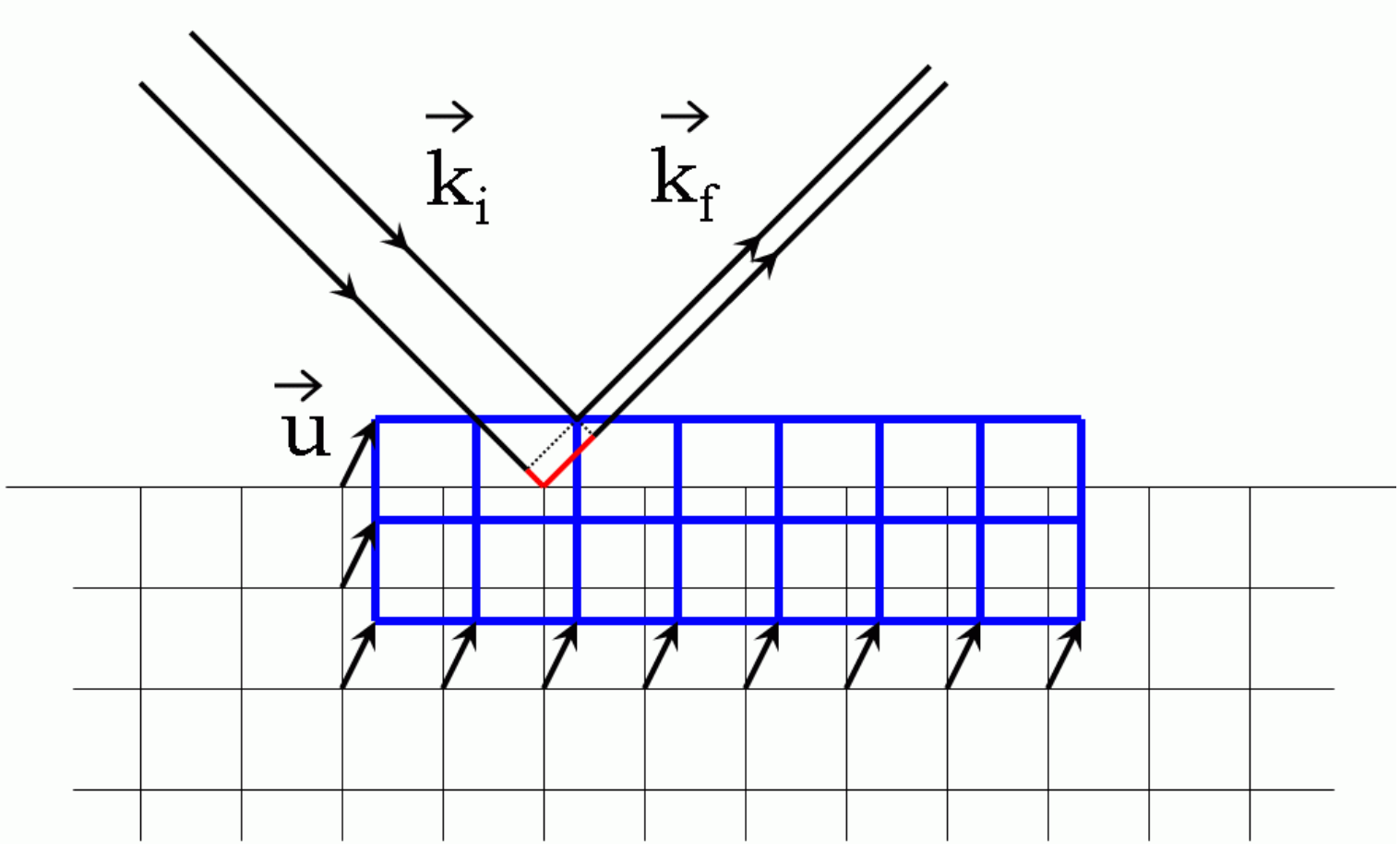

scalar0
-1.60 -1.14 -0.686 -0.229 0.229 0.686 1.14 1.60

Coherent Diffraction from Crystals

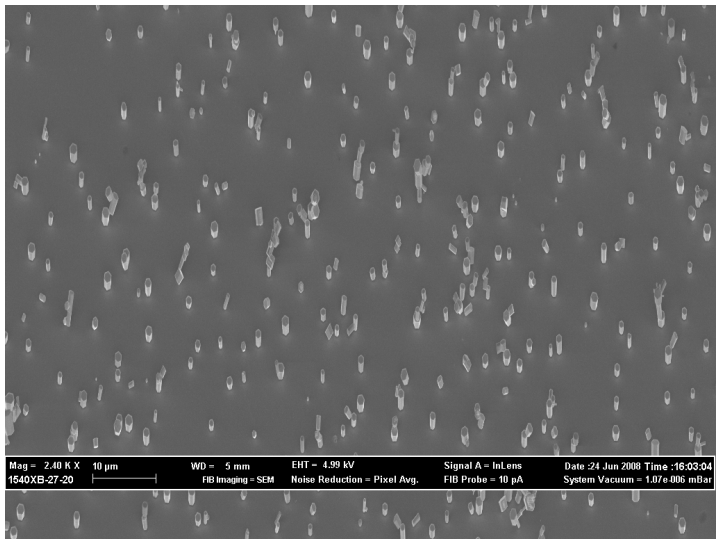


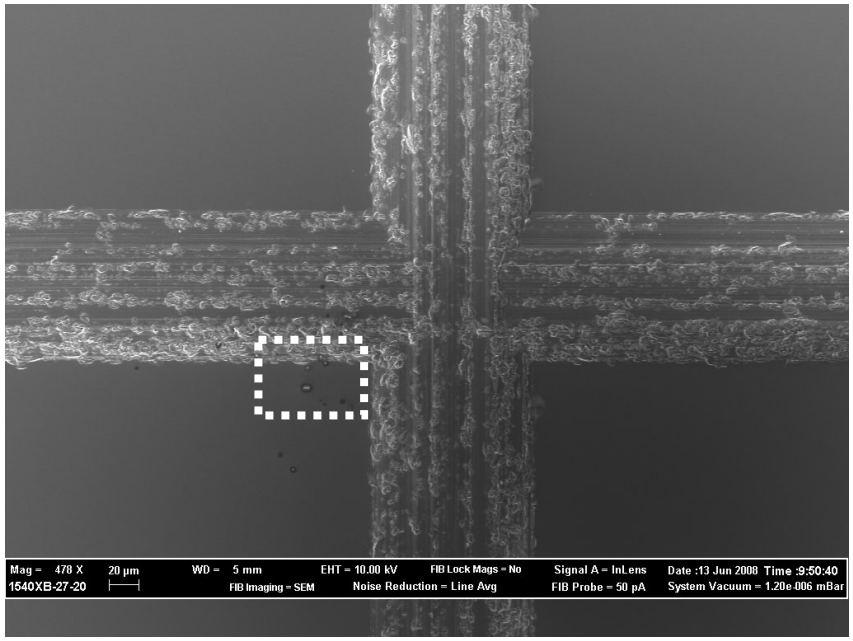
Sensitivity to strain

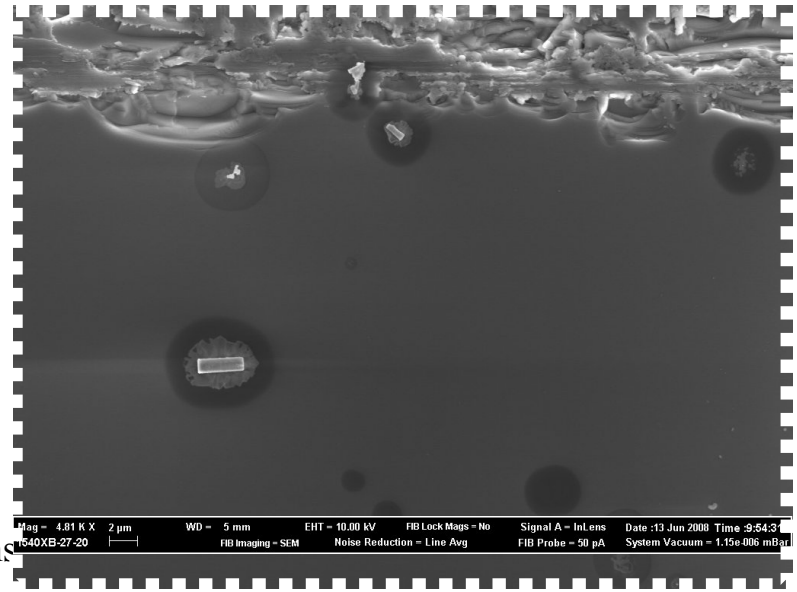
$$\Delta\varphi = \mathbf{k}_f \cdot \mathbf{u} - \mathbf{k}_i \cdot \mathbf{u} = \mathbf{Q} \cdot \mathbf{u}$$



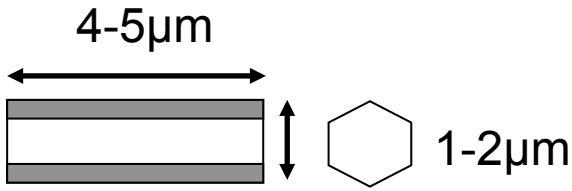
ZnO Sample Preparation







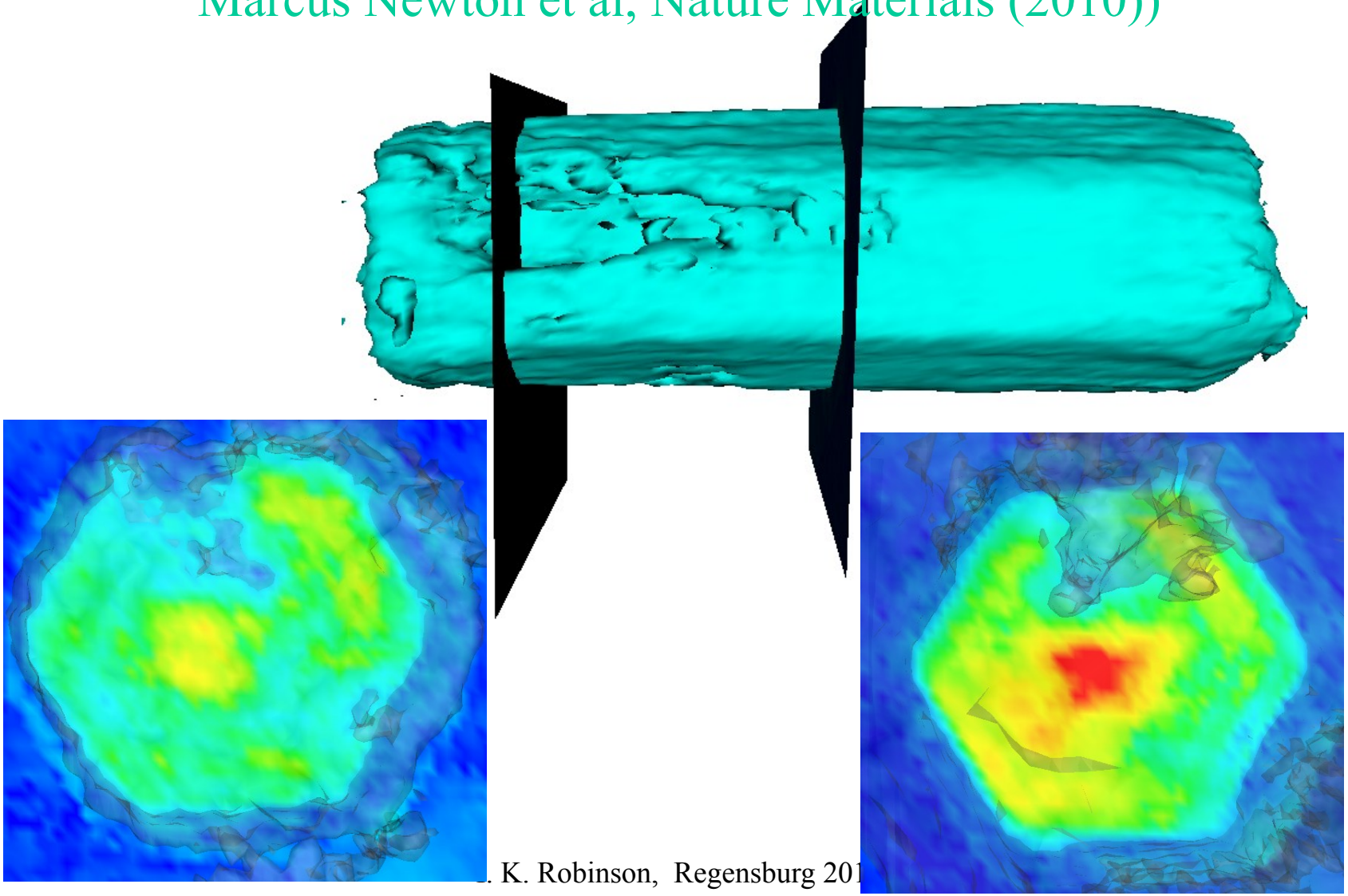
Dimensions:



I. K. Robinson, Regens

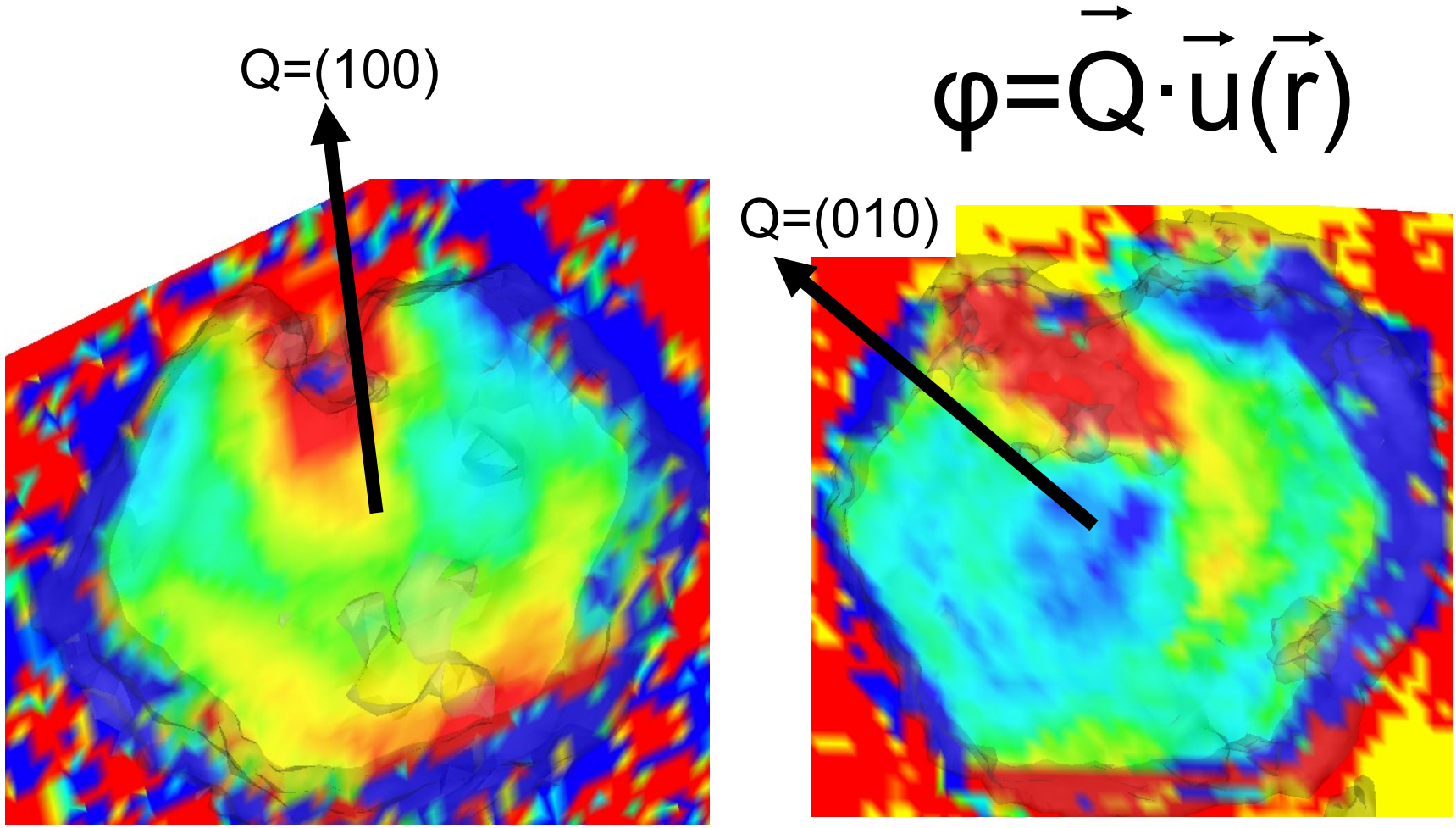
Density sections ZnO-39 (010)

Marcus Newton et al, Nature Materials (2010))

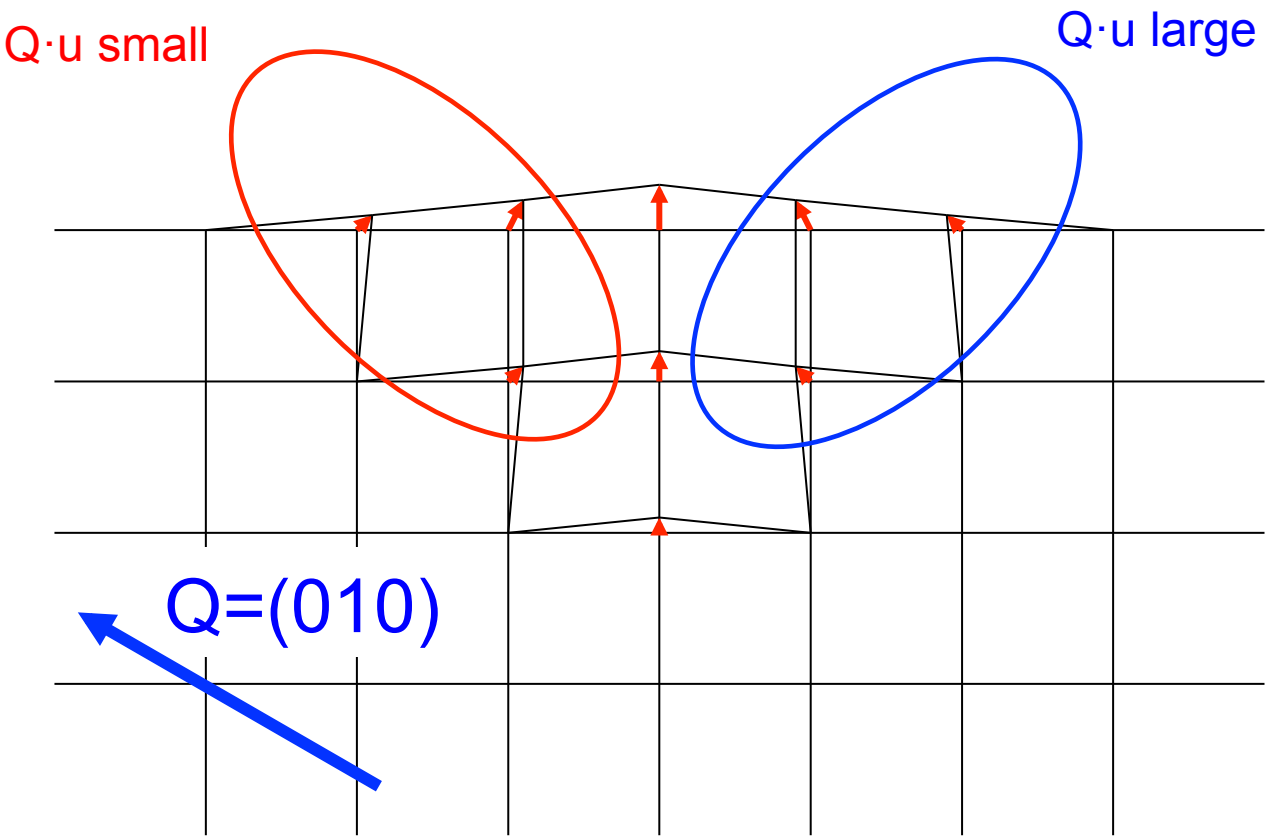


Phase maps from 2 Bragg peaks

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

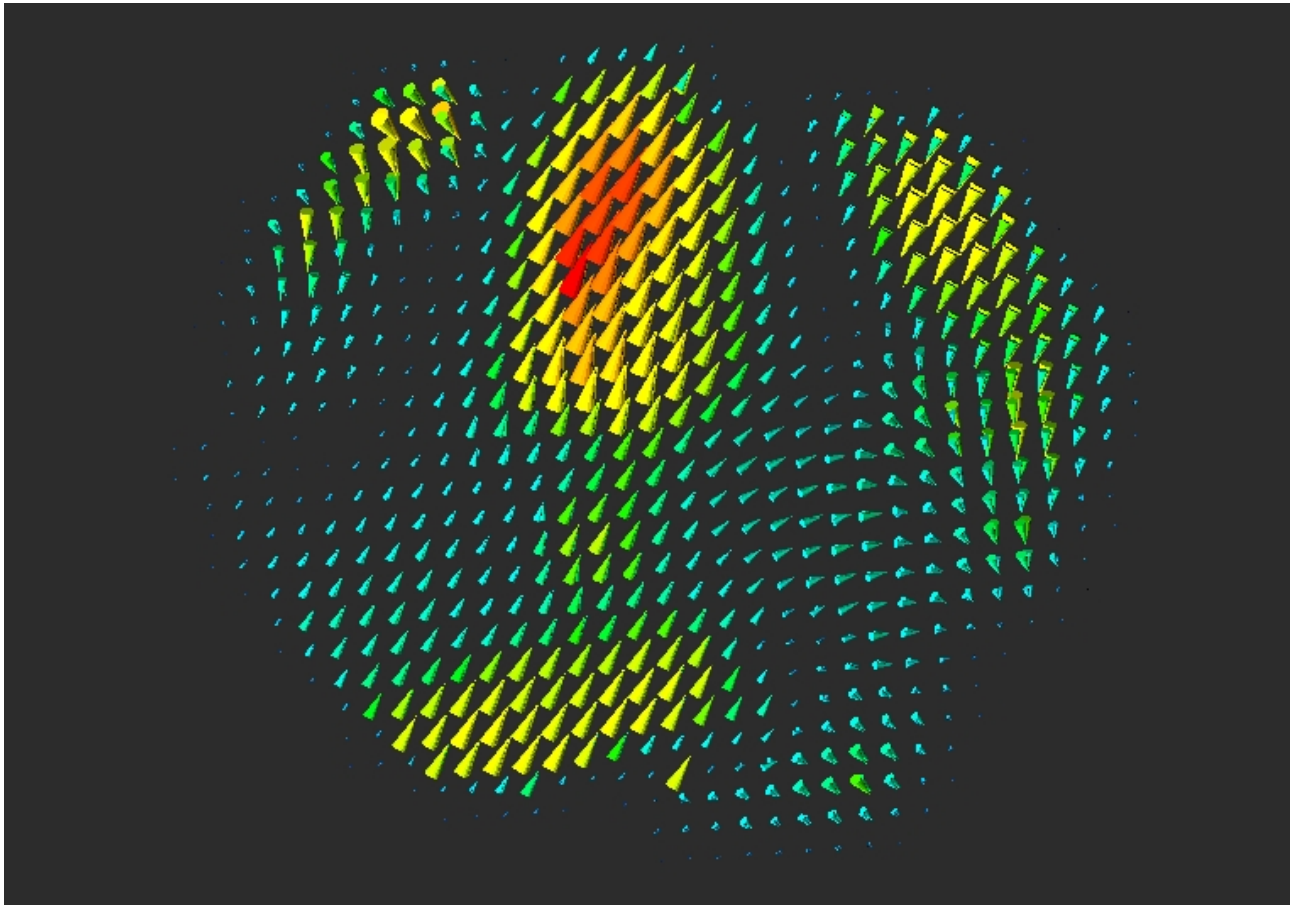


Typical displacement field

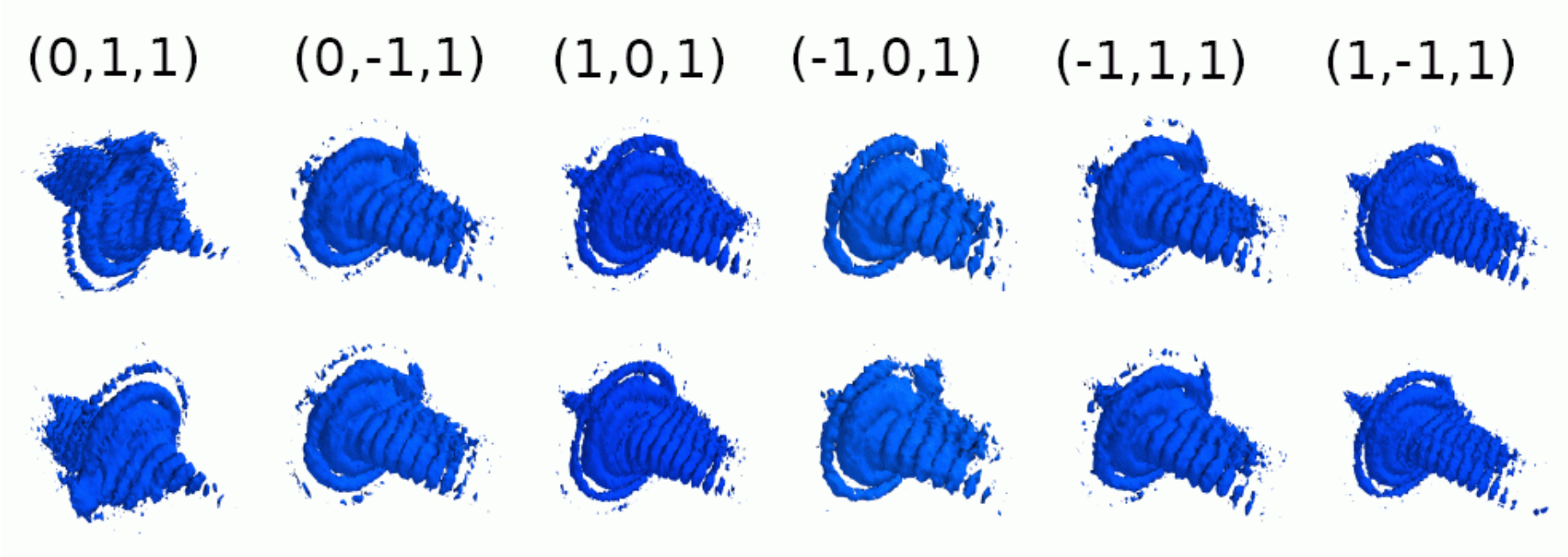


2D vector field of displacements

Marcus Newton et al, Nature Materials (2010)

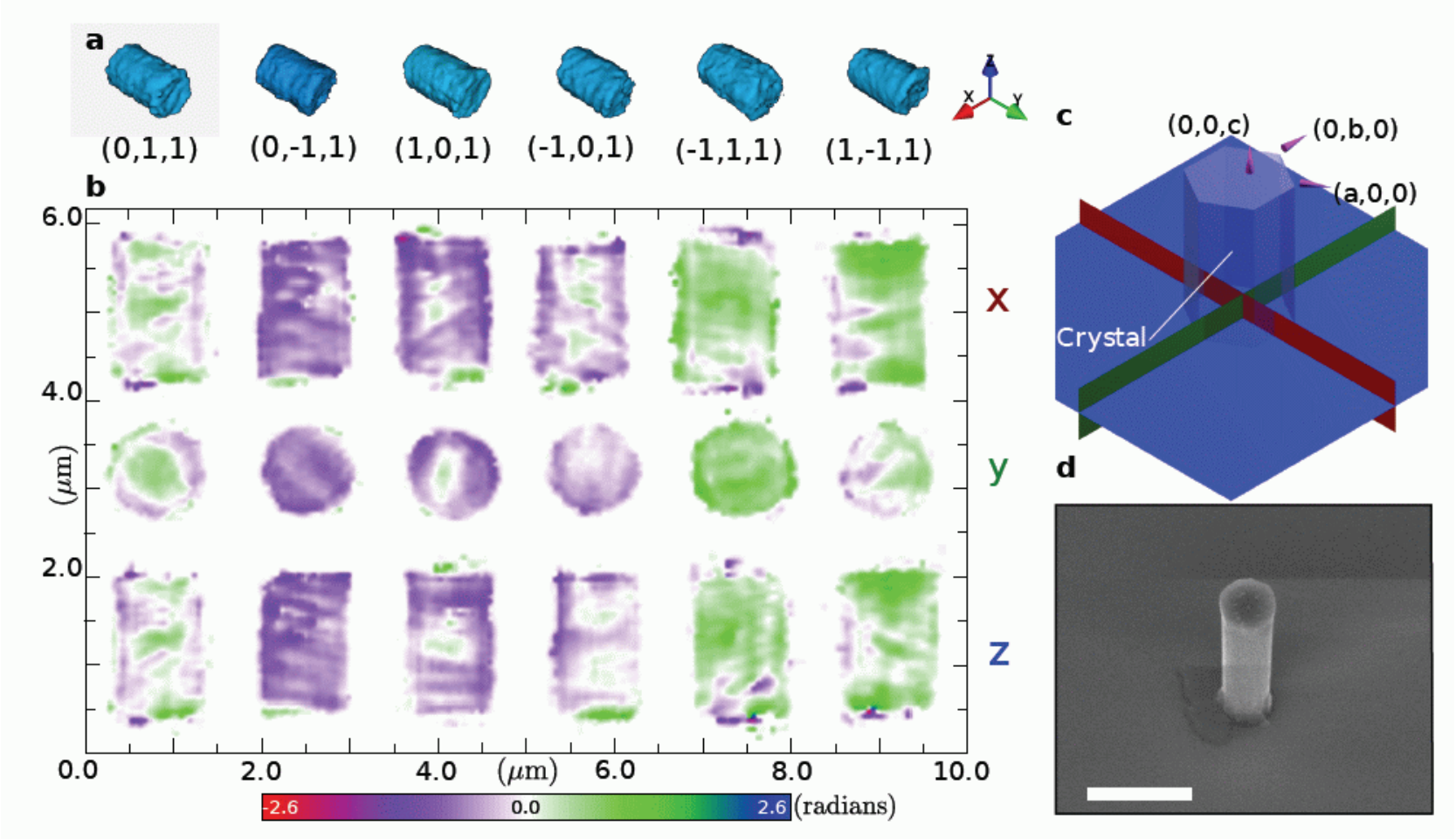


Extension to 6 Bragg Peaks



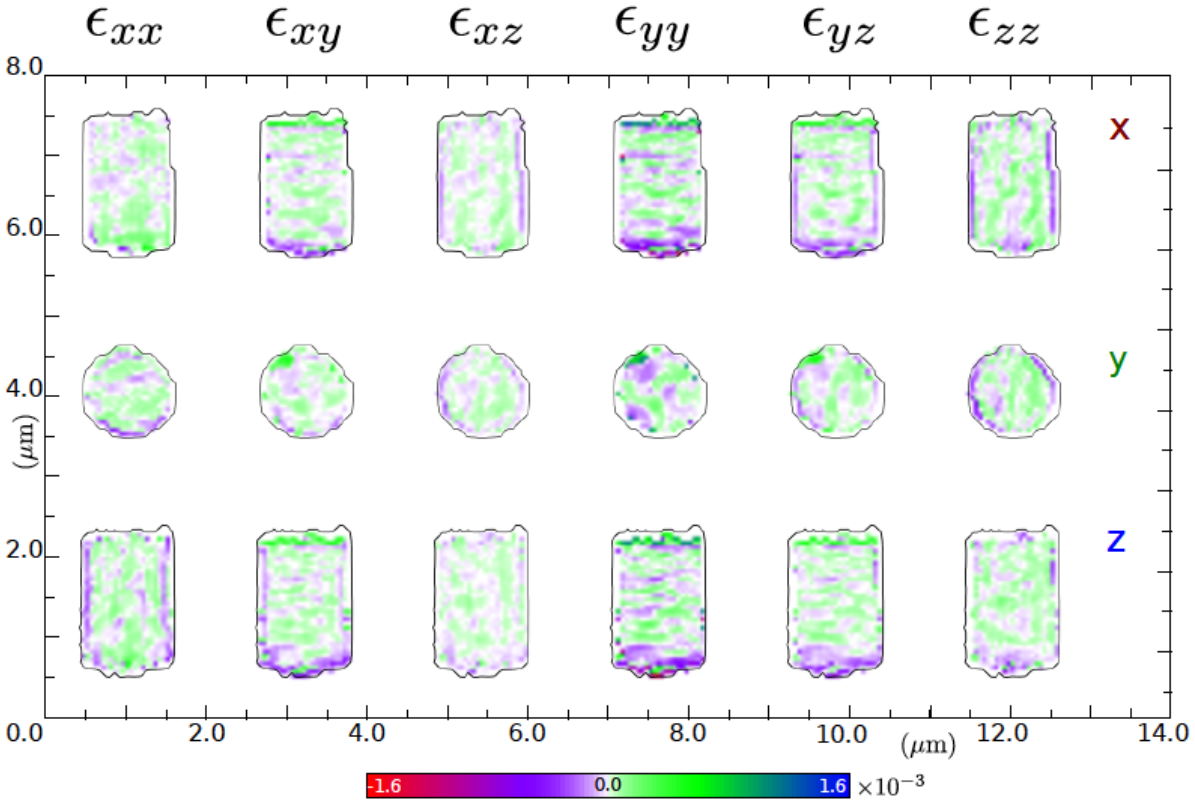
Extension to 6 Bragg Peaks

Marcus Newton et al, Nature Materials (2010)

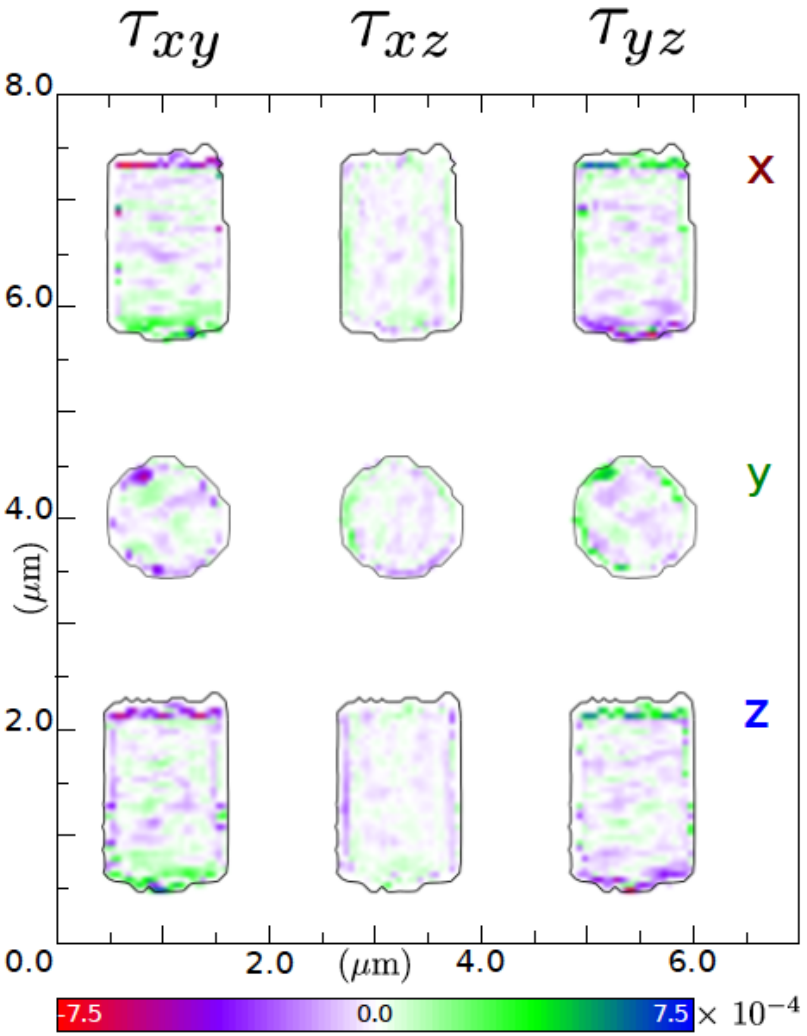


Full Strain Tensor

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

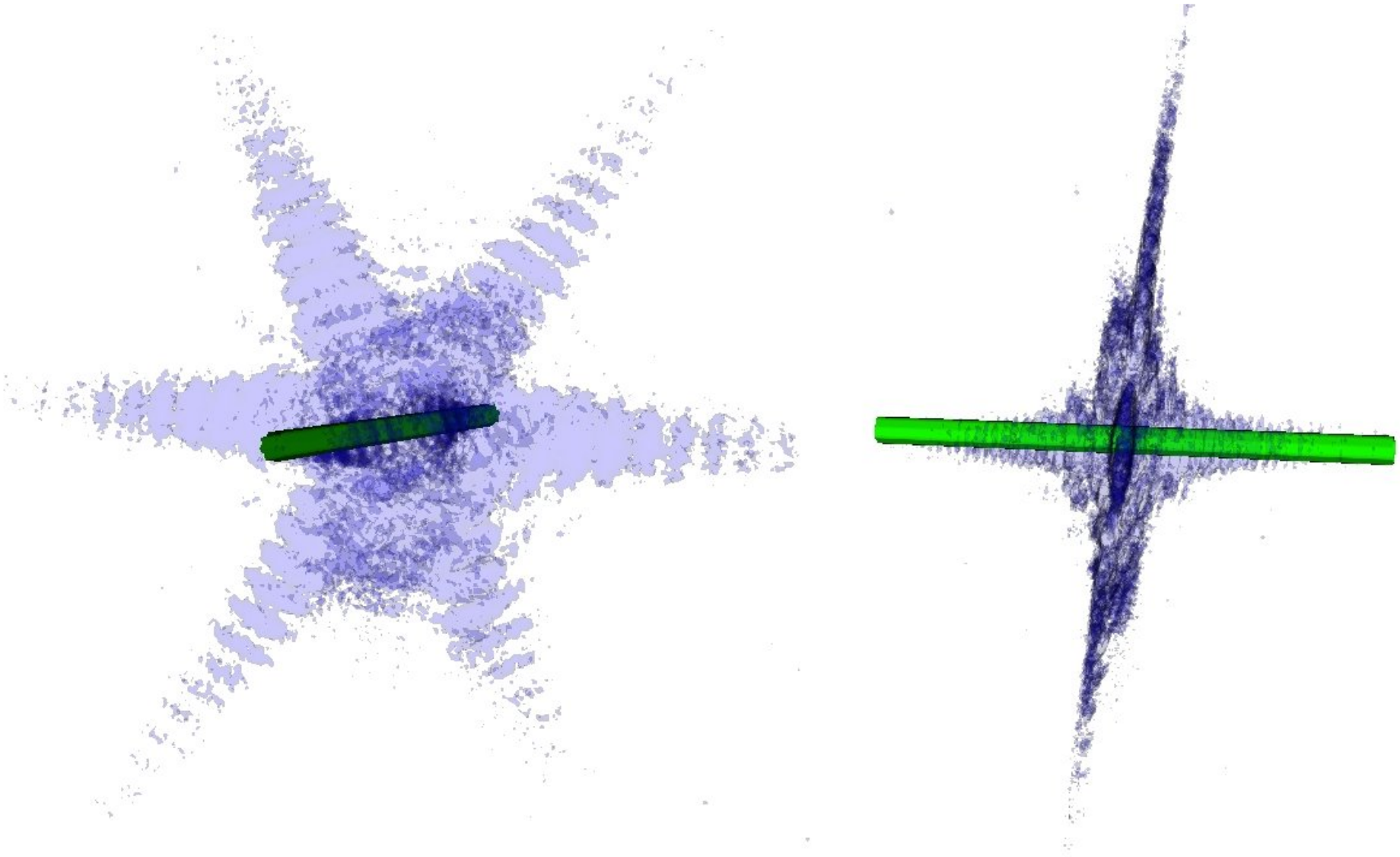


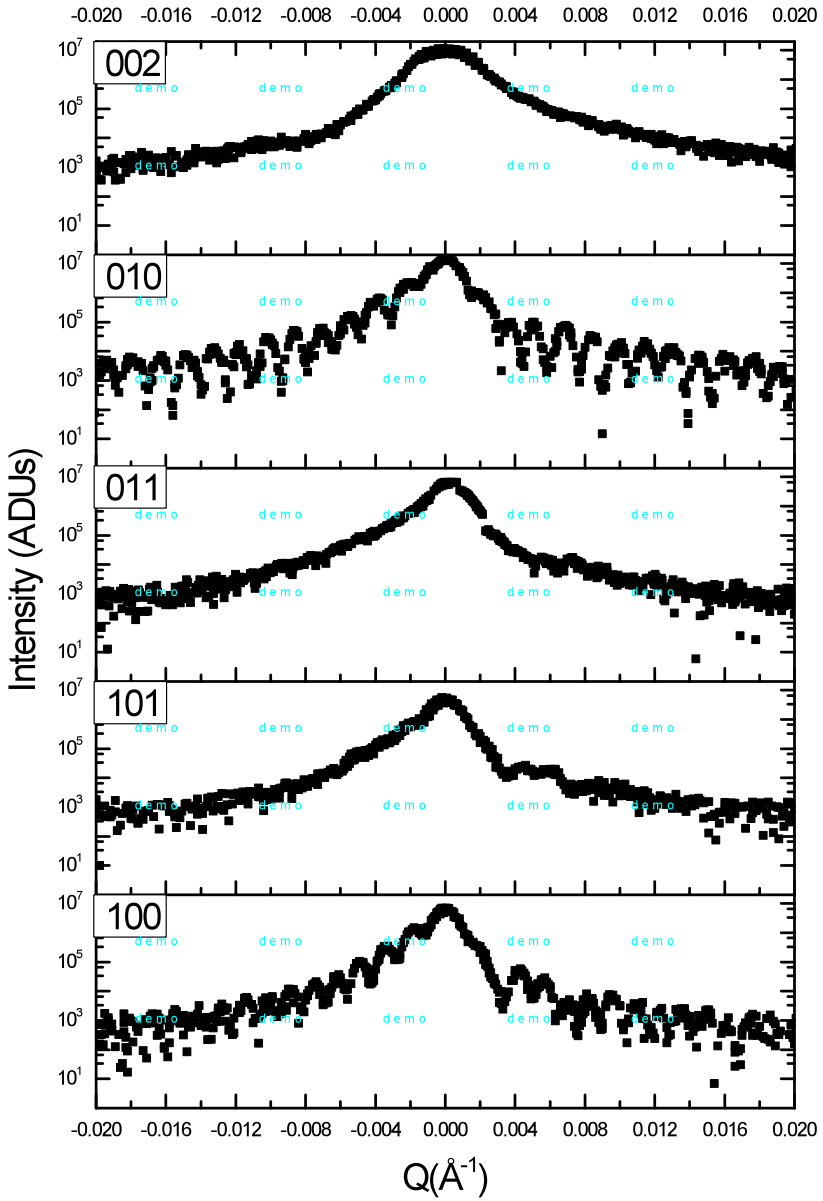
ZnO Rigid-body Rotations



Partial Beam Coherence

Line scan to extract the contrast visibility





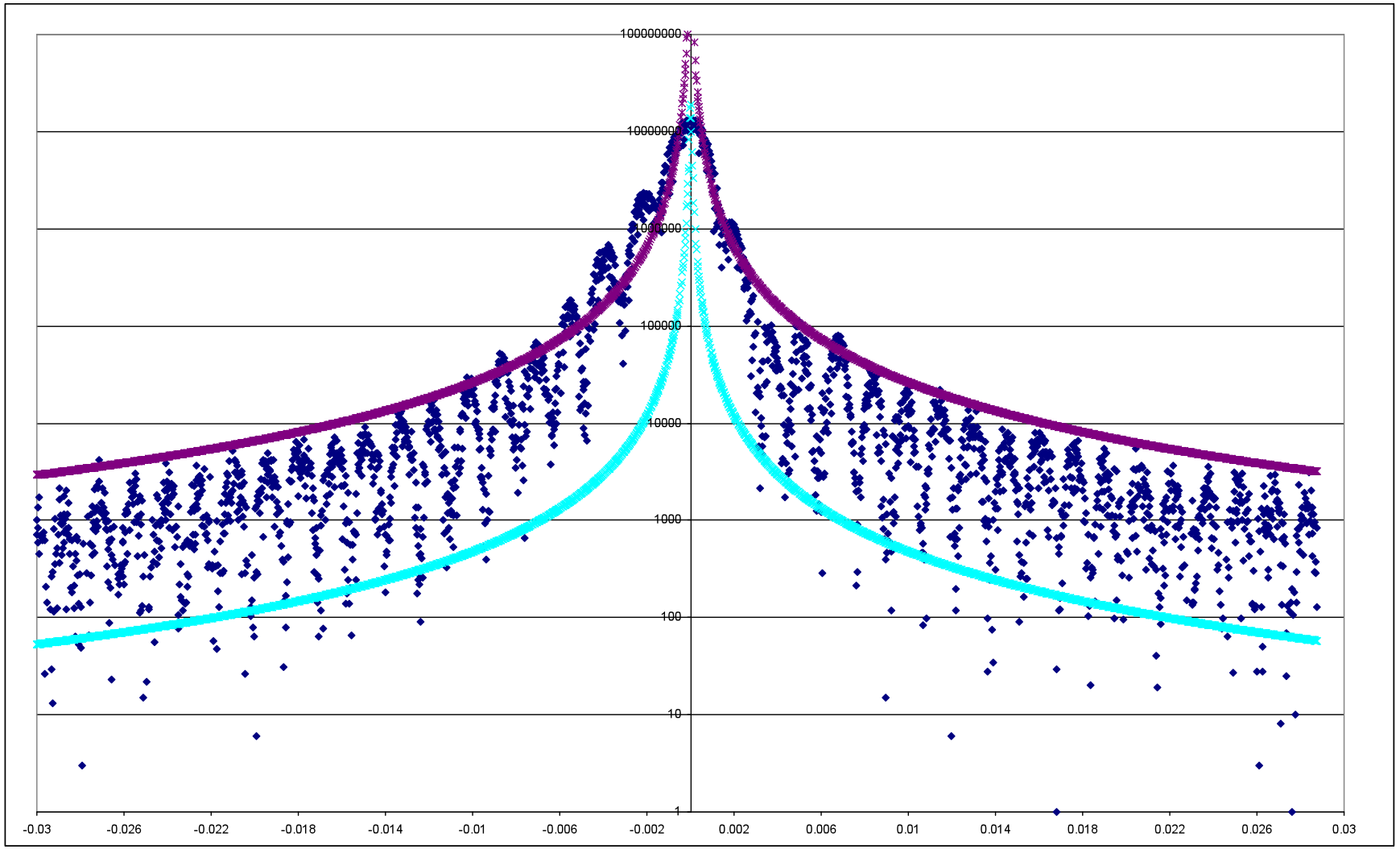
Five Bragg peaks

002 no fringe visibility

010 & 100 good fringe visibility

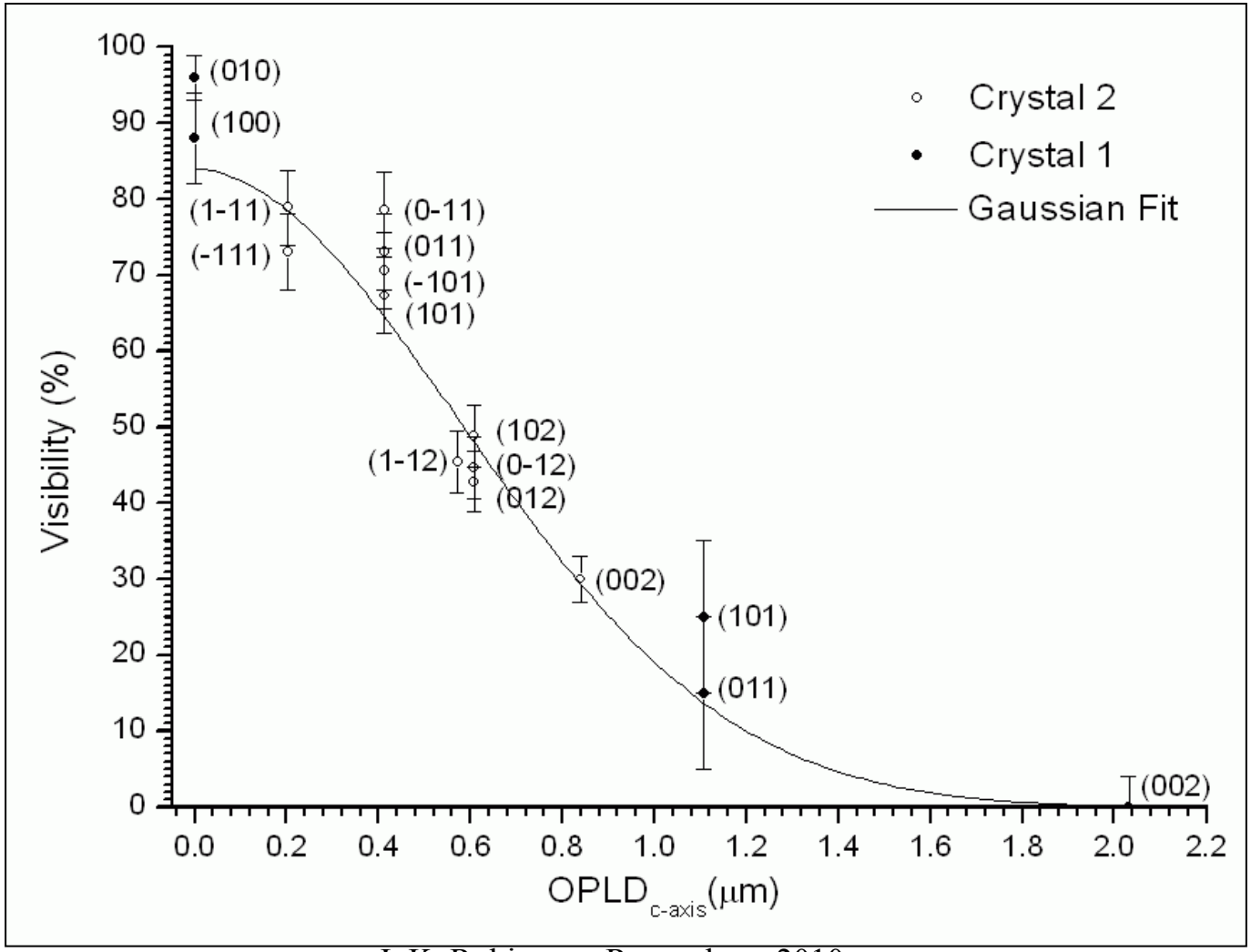
101 & 011 diminished fringe visibility but fringes still evident

Fringe Visibility 96±2% @010



Measured Longitudinal Coherence

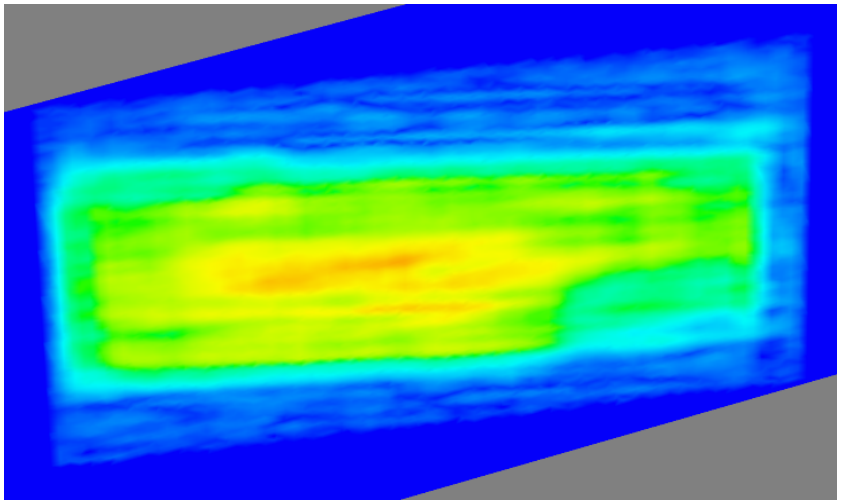
Steven Leake, Optics Express 17 15853 (2009)

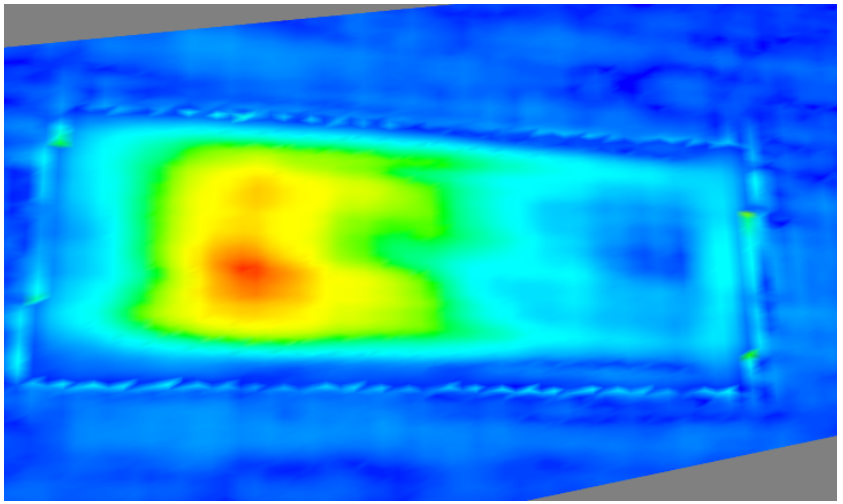


Density Section of Reconstruction using 100 and 101 reflections

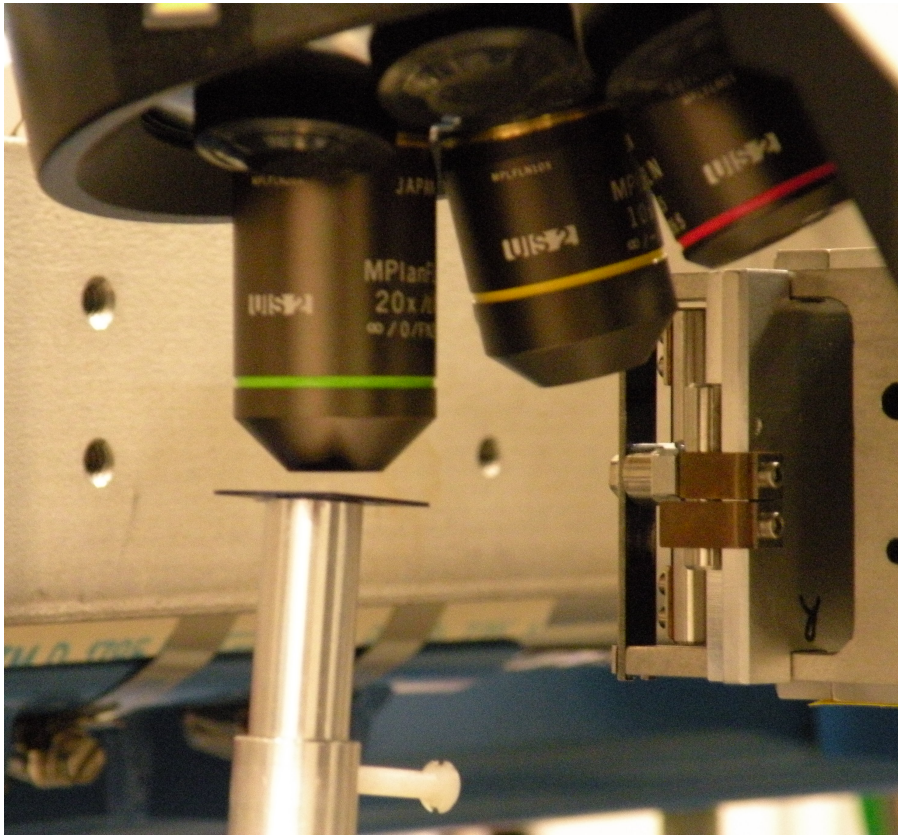
"hot spot" more developed for limited coherence

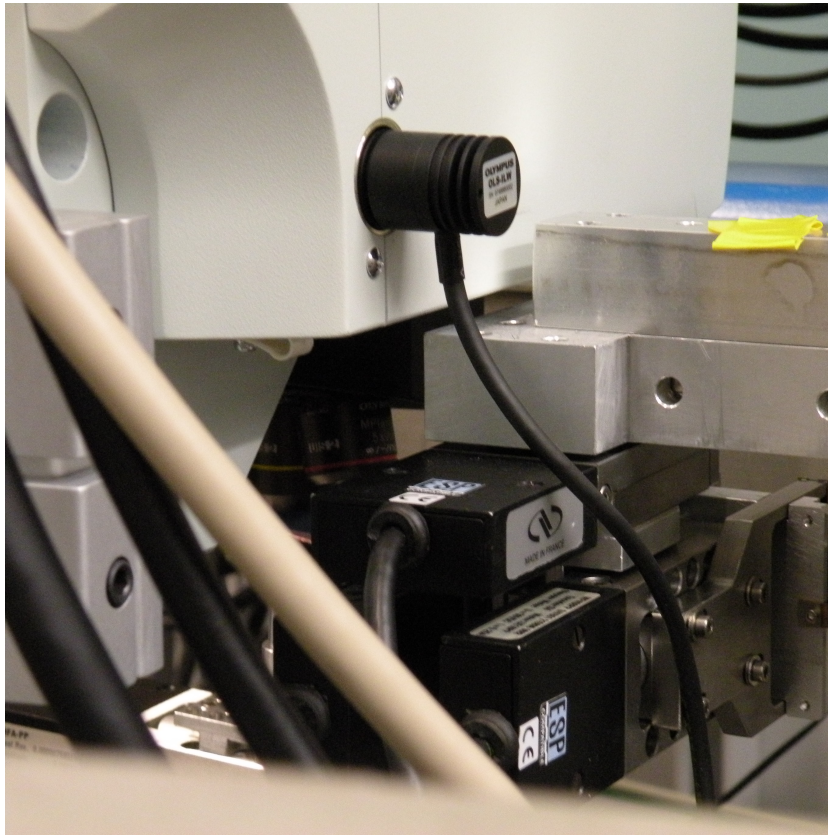
Steven Leake, Optics Express 17 15853 (2009)



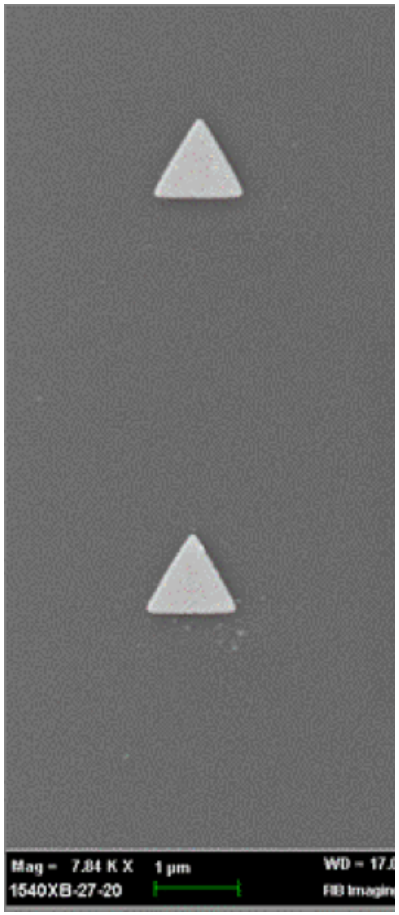


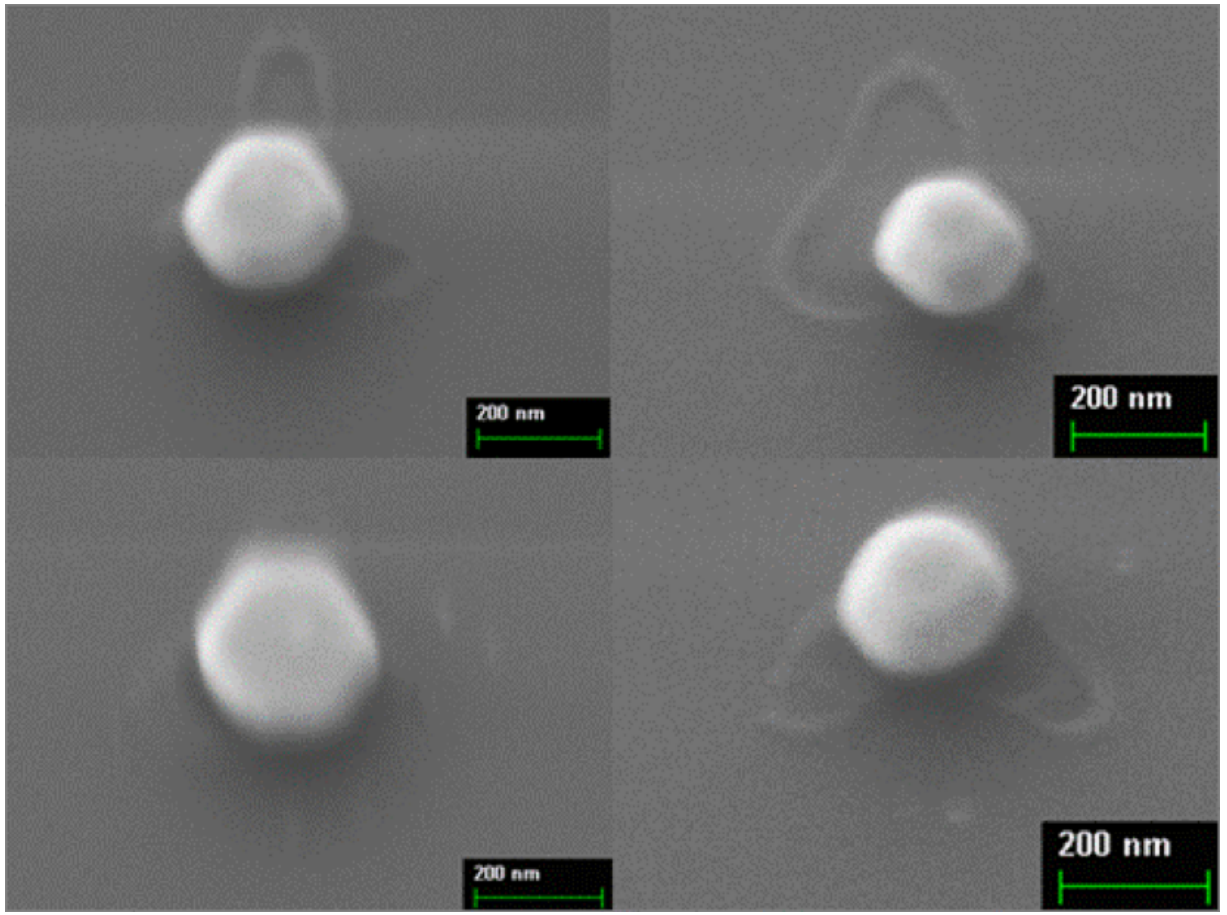
Confocal Alignment Microscope





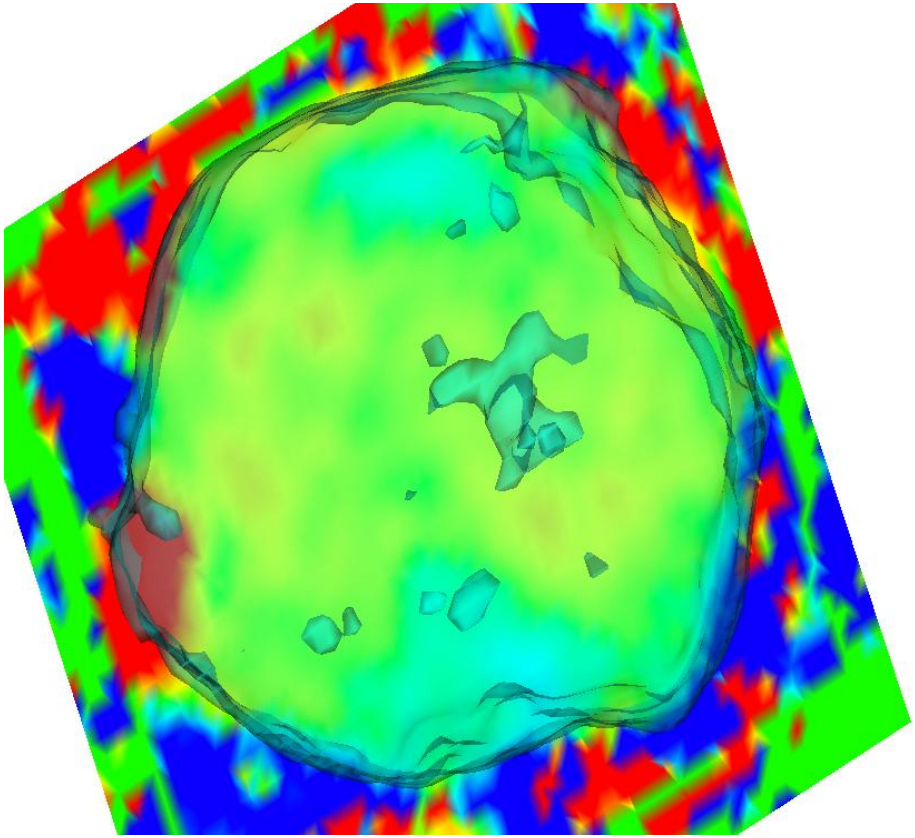
Single Au nanocrystal synthesis

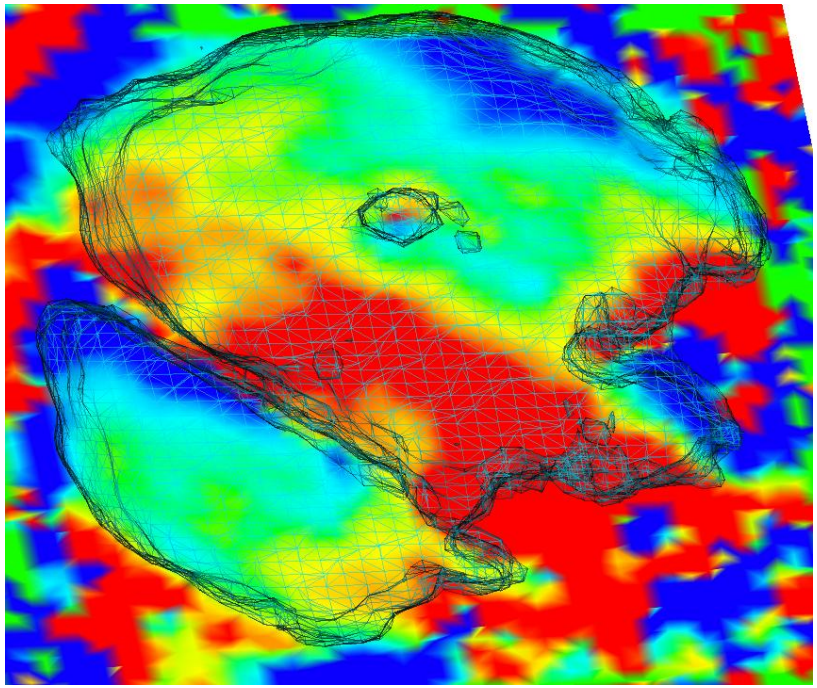


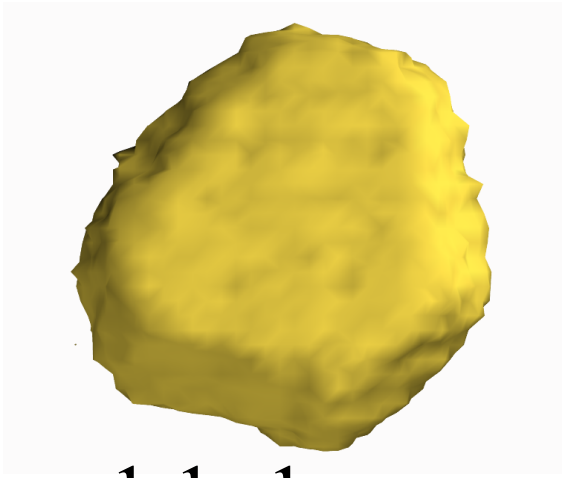


Two views of strain in Au NC

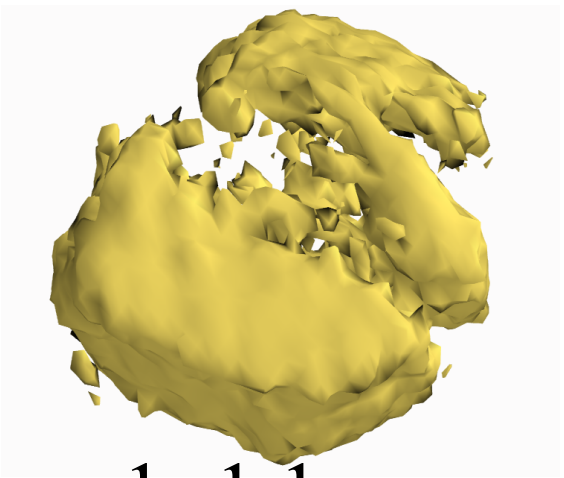
Au409B-52 (11-1) and Au409B-60 (200)



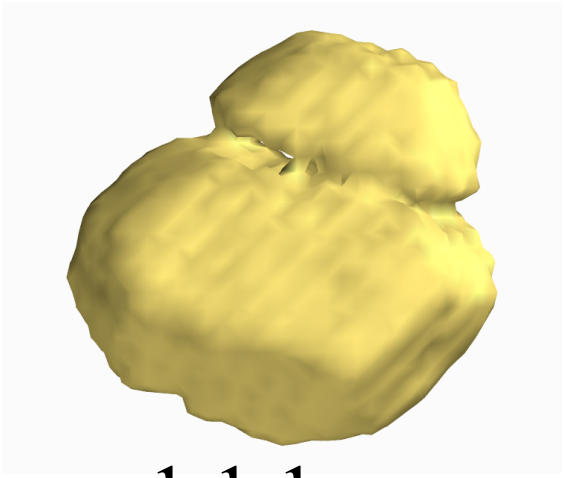




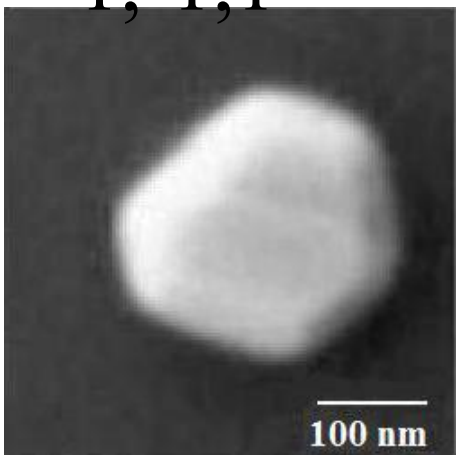
1,1,-1



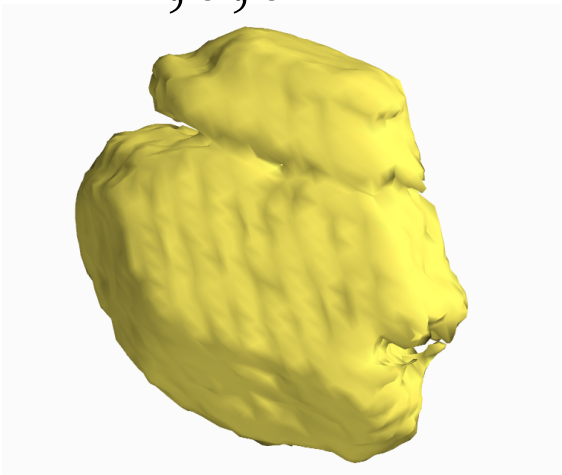
1,-1,1

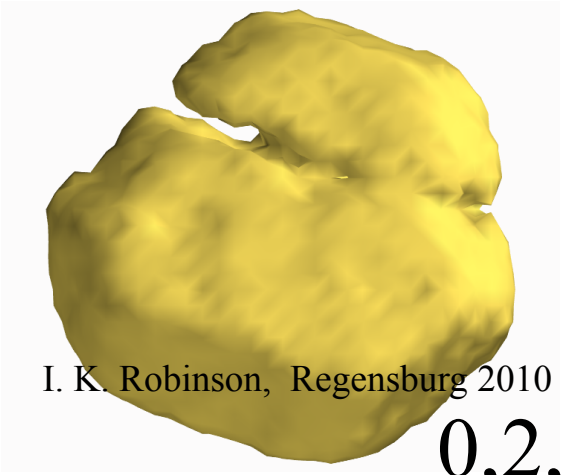


-1,1,1



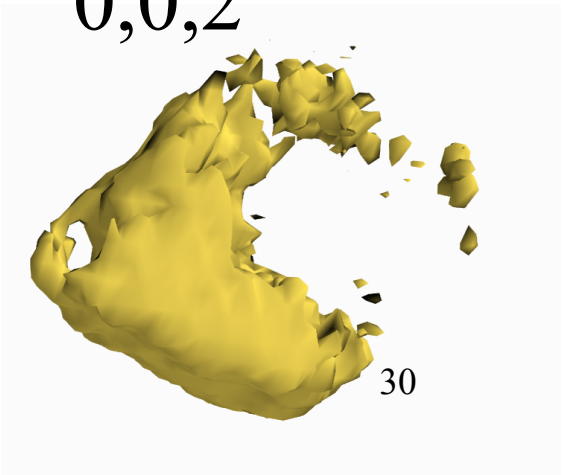
2,0,0





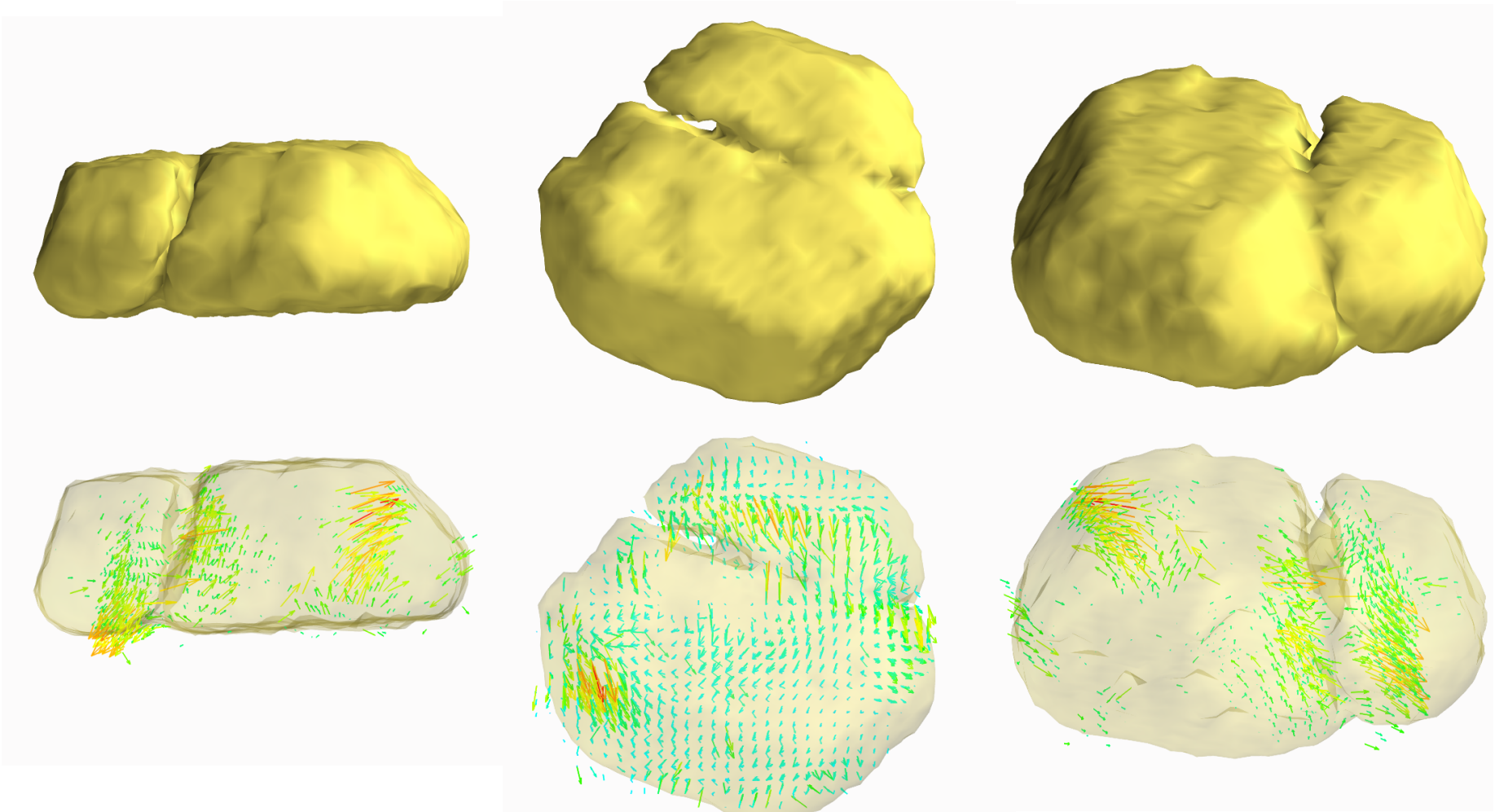
0,2,0

0,0,2



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
- Full Strain Tensor accessible
- Partial Coherence affects Image Quality