X-ray Coherence methods for LCLS

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Diamond Light Source

LCLS Coherence Workshop
October 2008

Discussion Questions

- Coherent x-ray diffraction imaging
- How much information in a single shot?
- 3D solution from a single shot?
- XPCS or Imaging approach?
- Real or Reciprocal space view?
- Planning for initial LCLS experiments

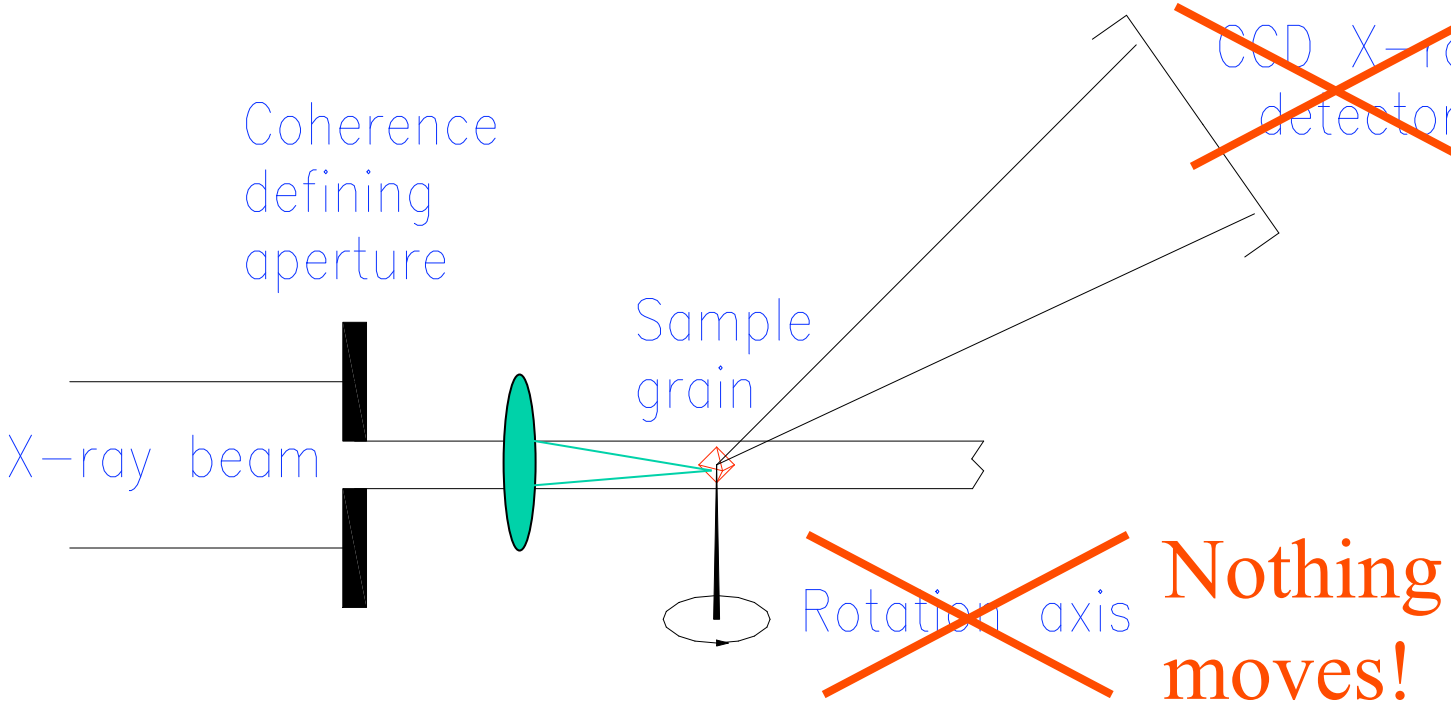
Diamond in-vacuum X-ray Undulator

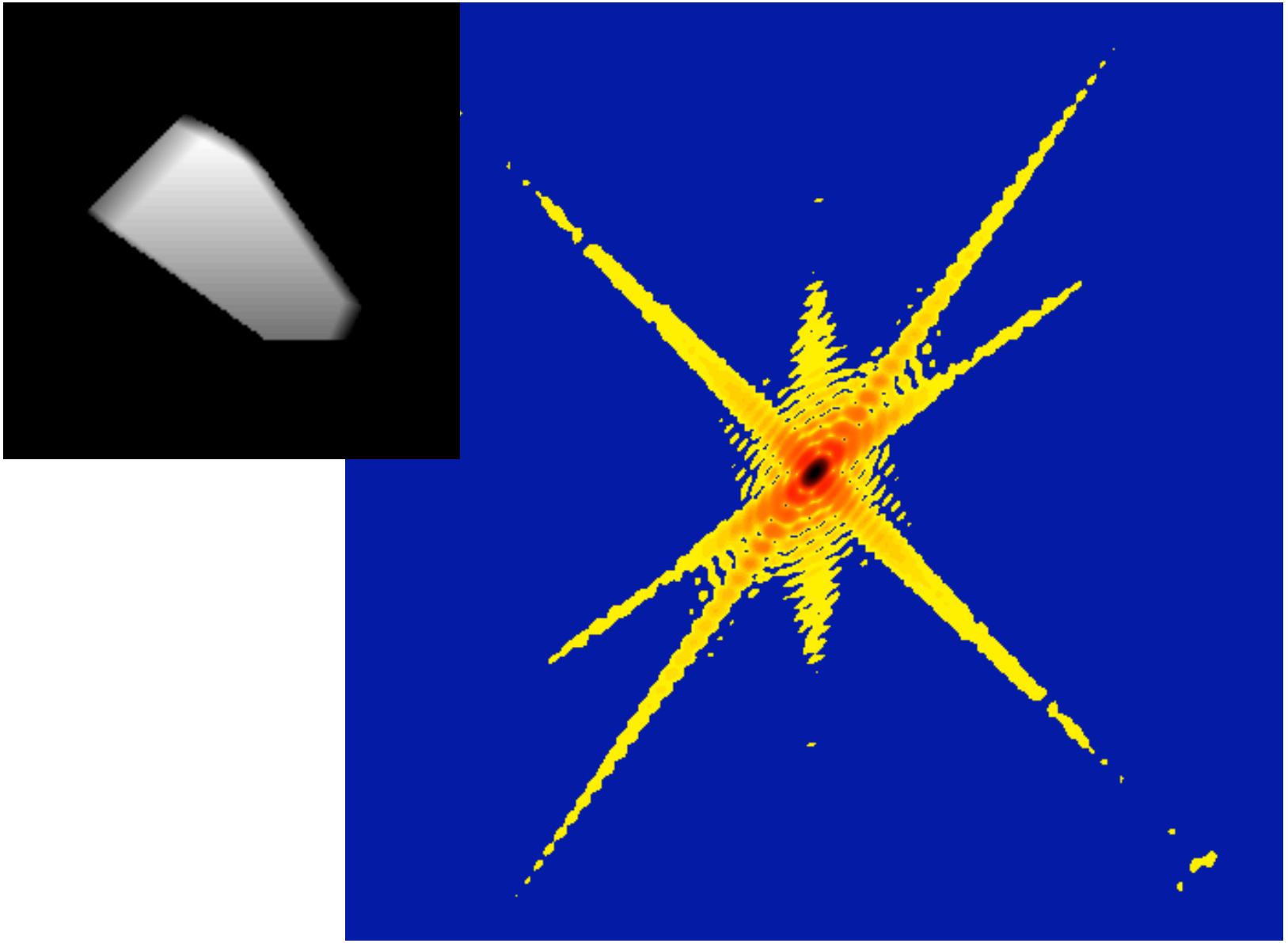
I

Coherent X-ray Diffraction Imaging

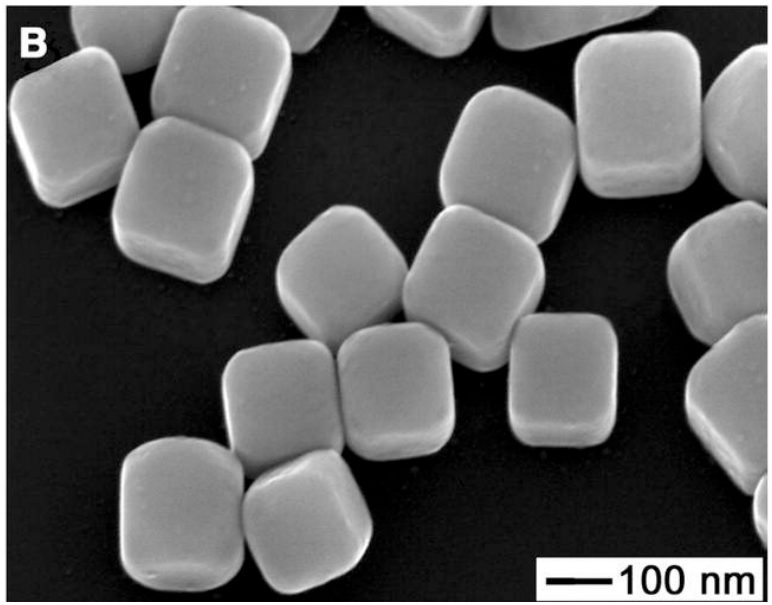
APS ξ_{HOR}= 20μm, focus to 1μm

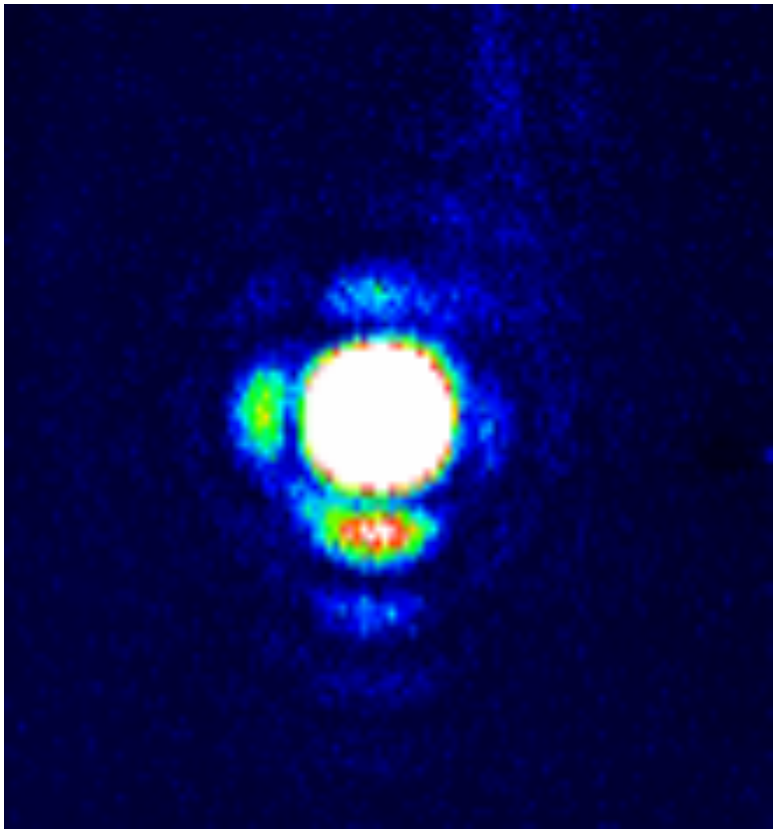
LCLS ξ_{HOR}> 500μm, focus to 0.1μm





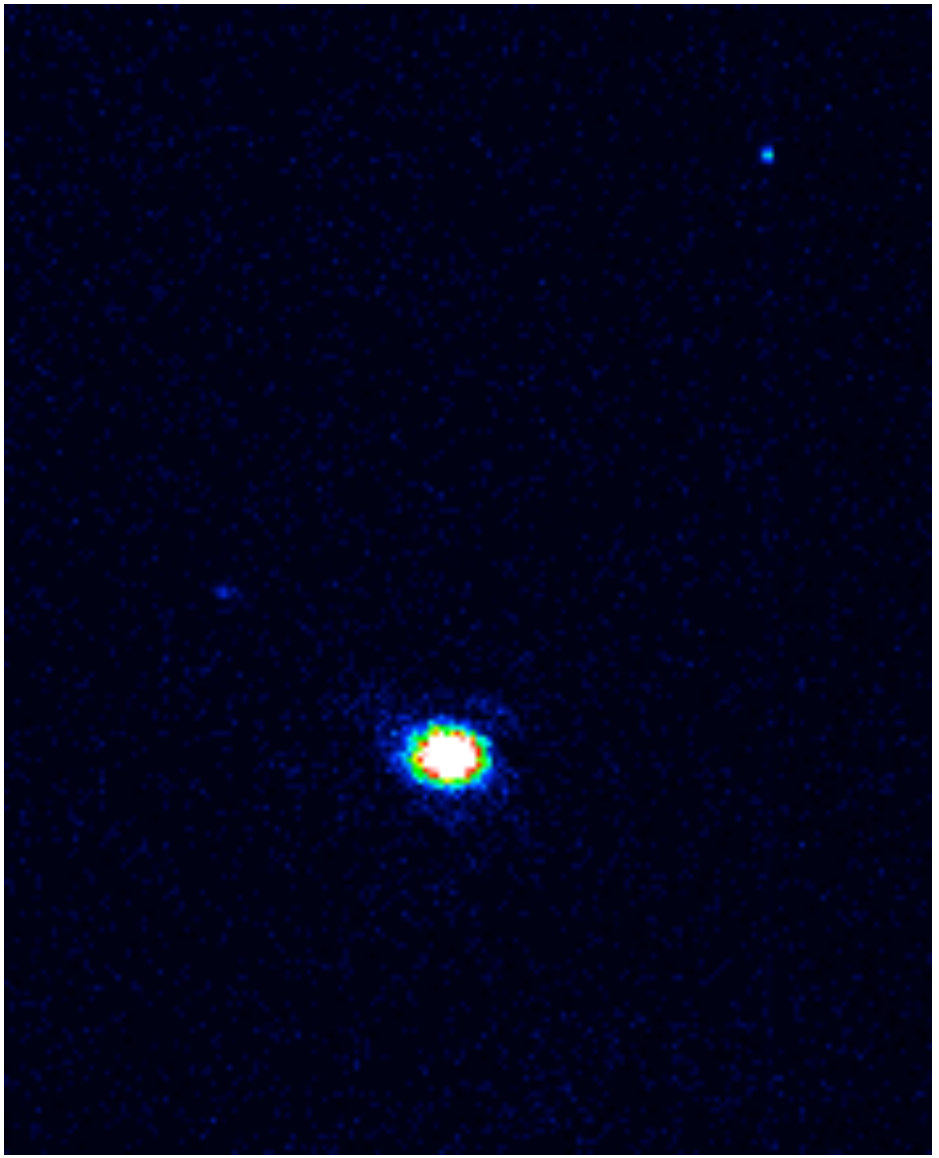
Chemically Synthesized Silver Nanocubes

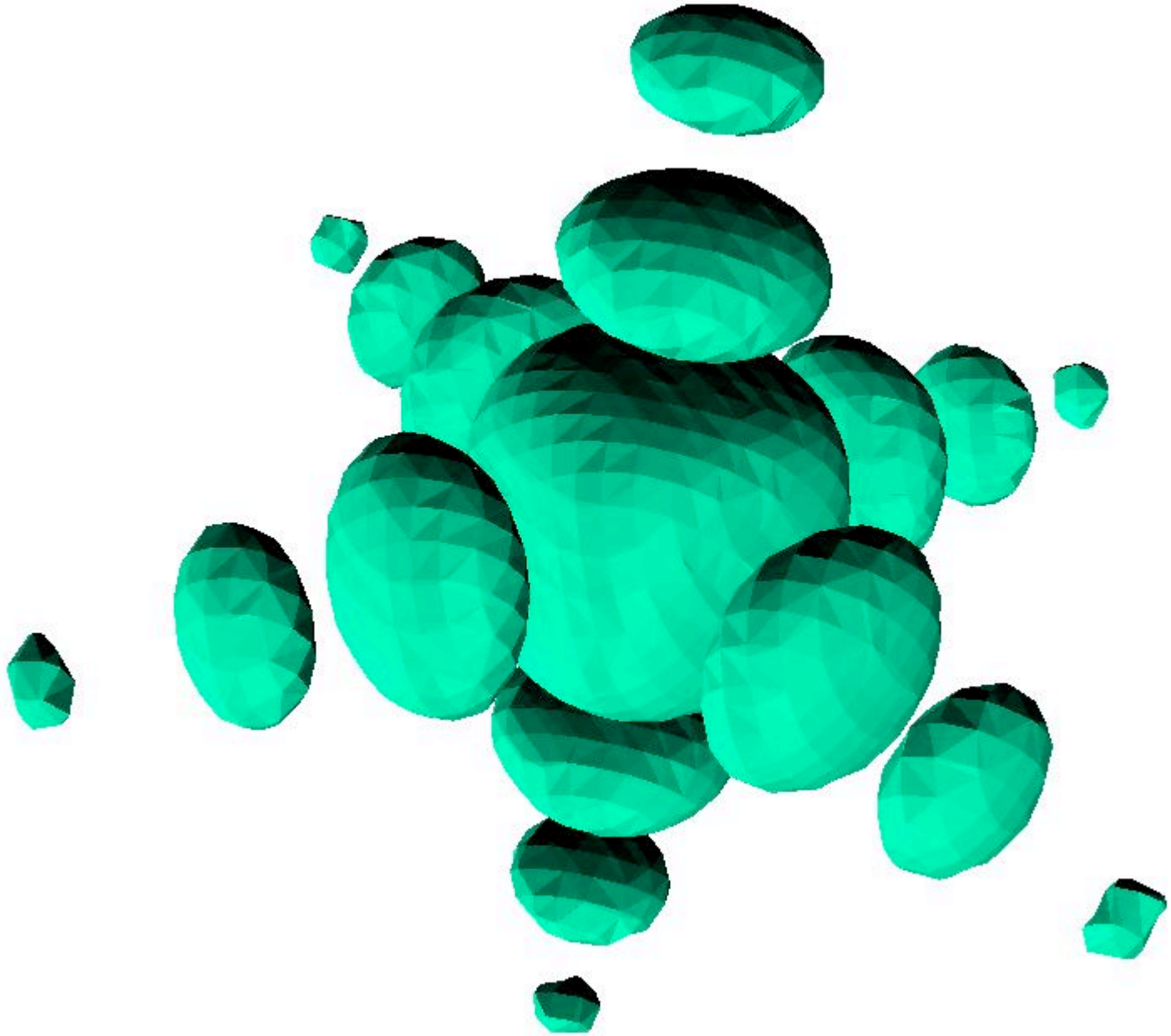


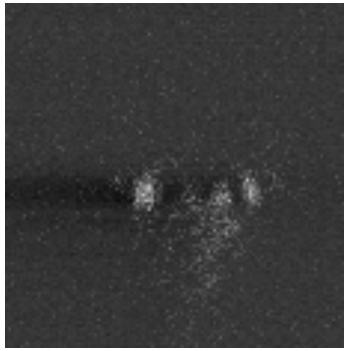


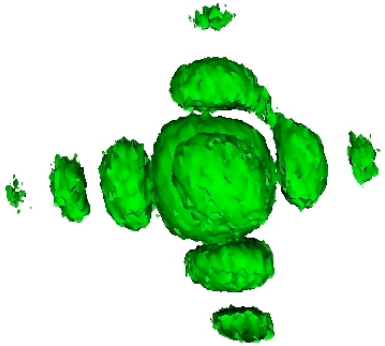
Yugang Sun and Younan Xia,
Science 298 2177 (2003)

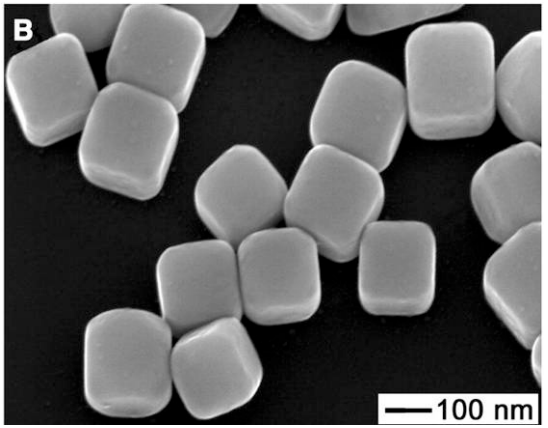
Rocking scan of Ag cubes with 0.01° steps

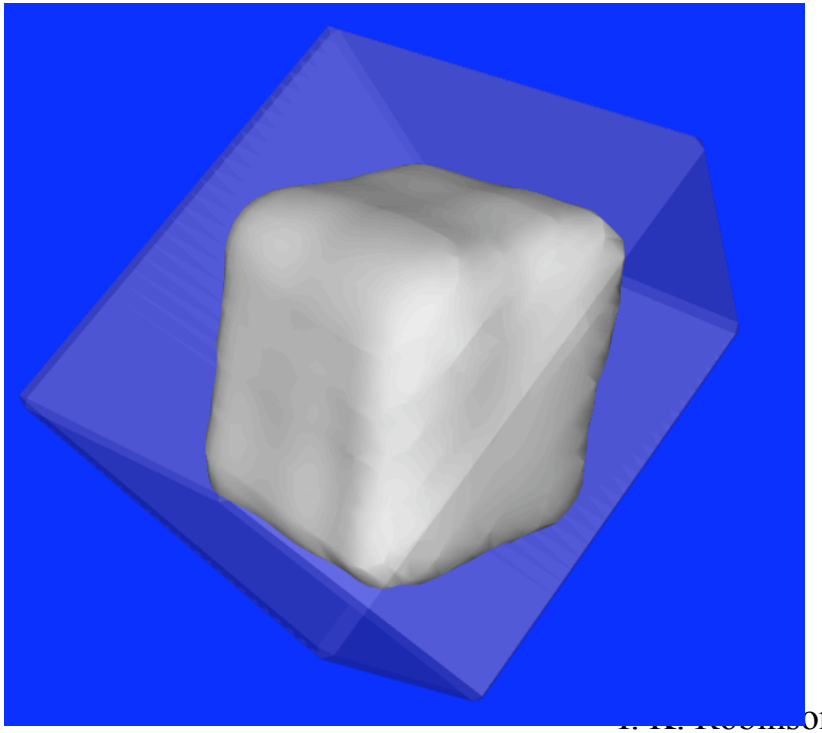


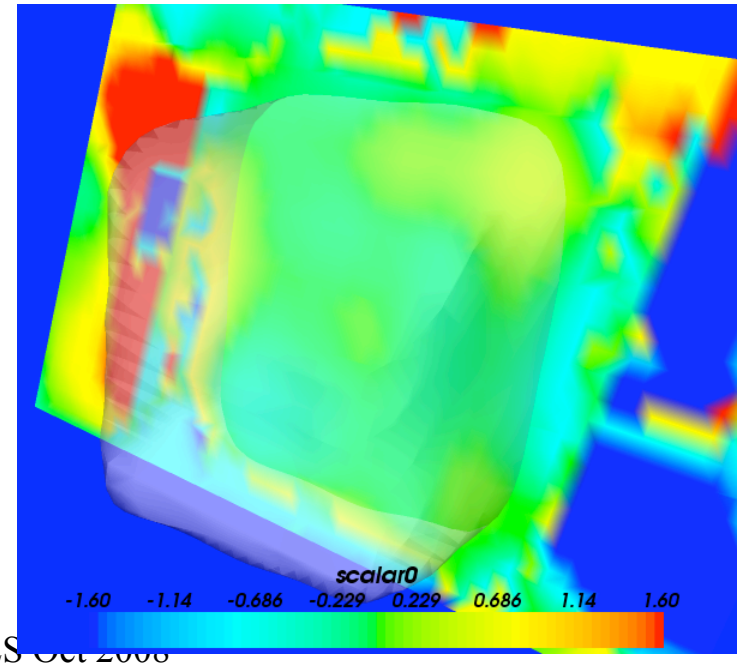






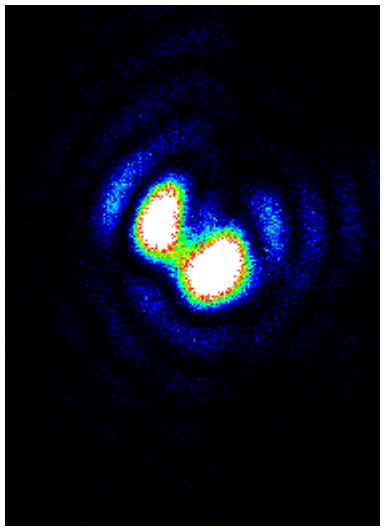

B
100 nm

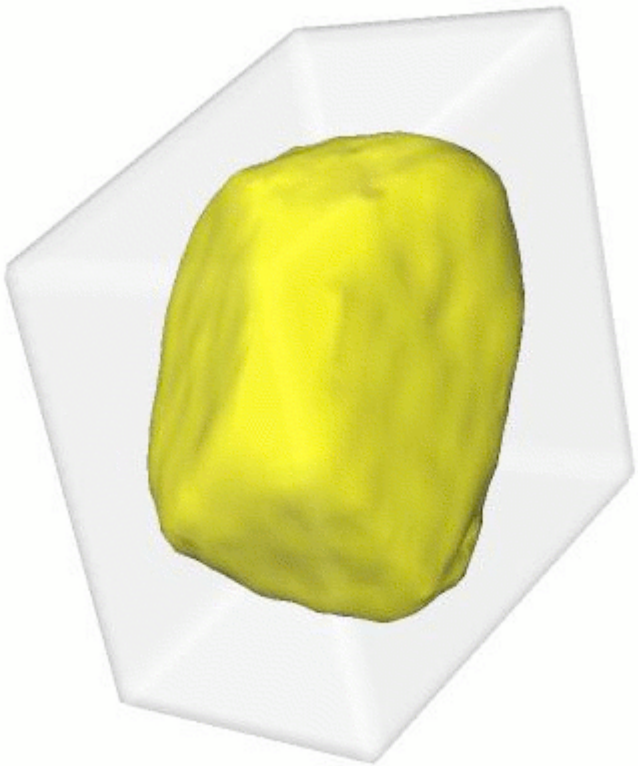



scalar0
-1.60 -1.14 -0.686 -0.229 0.229 0.686 1.14 1.60

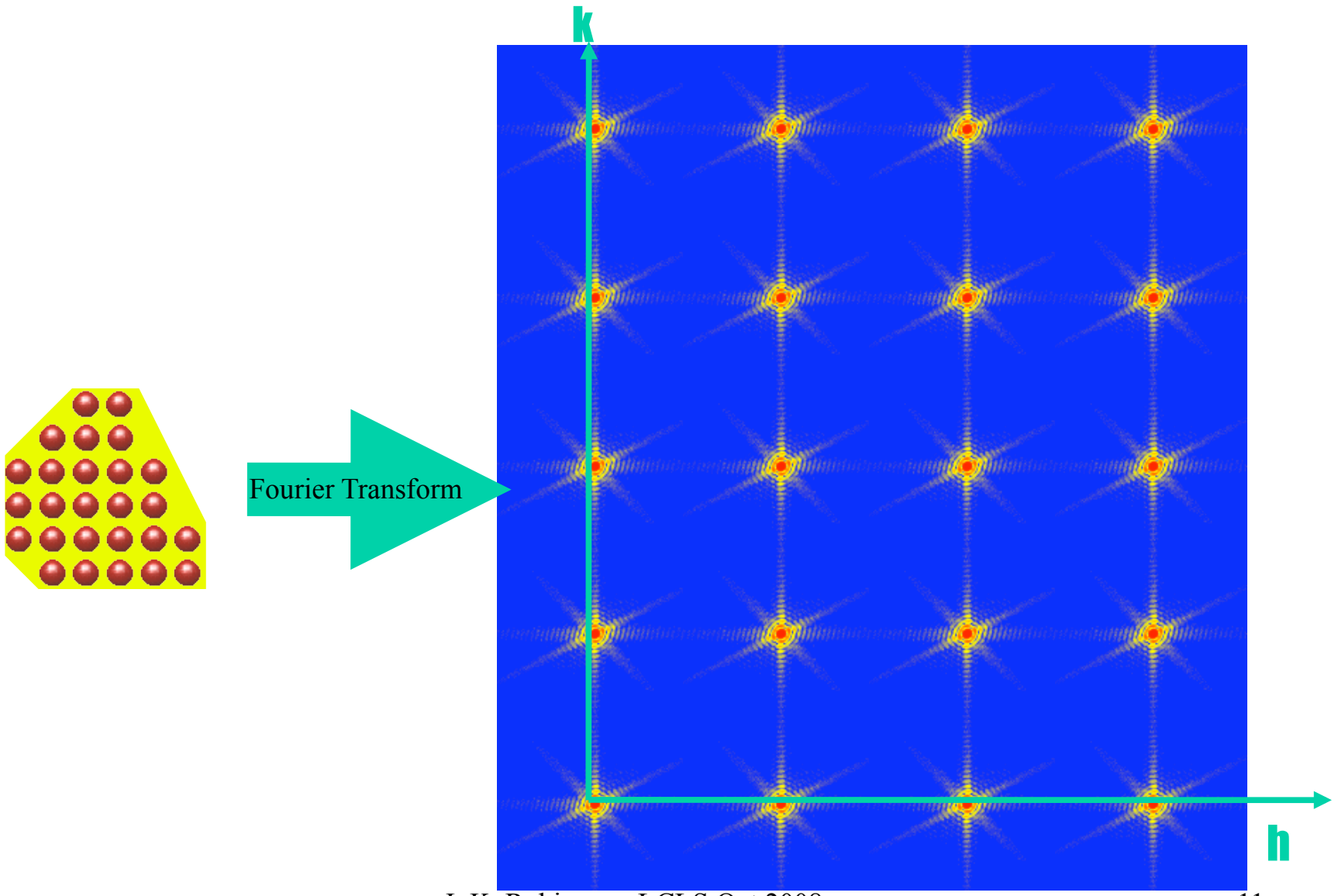
Gold nanocrystal reconstruction

showing support used for 20 HIO followed by 10 ER





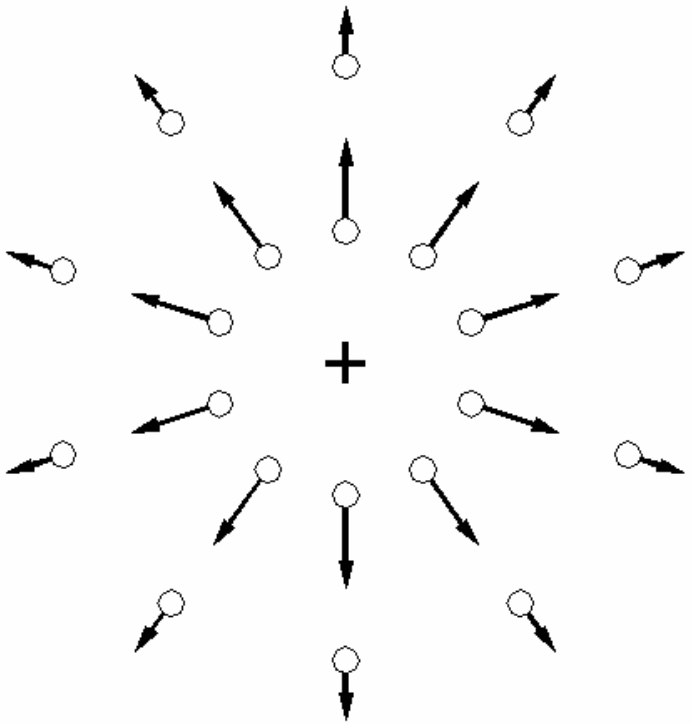
Coherent Diffraction from Crystals

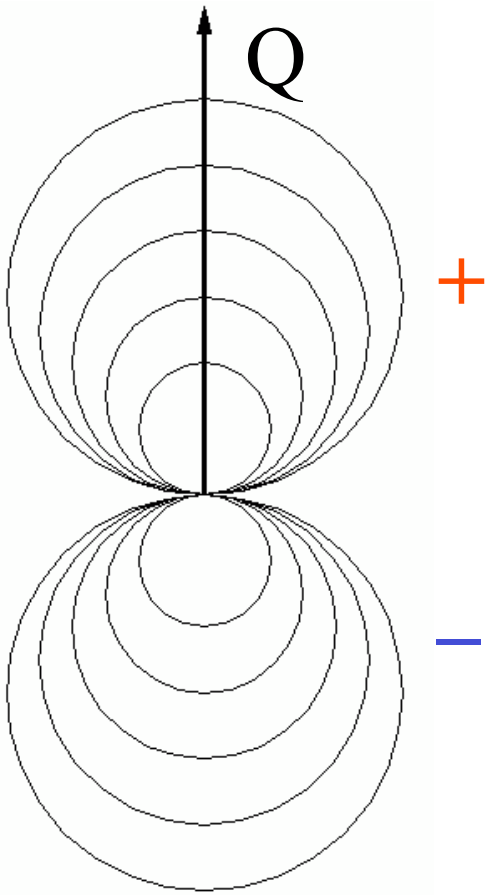


Diffraction by Strain of Point Defect

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

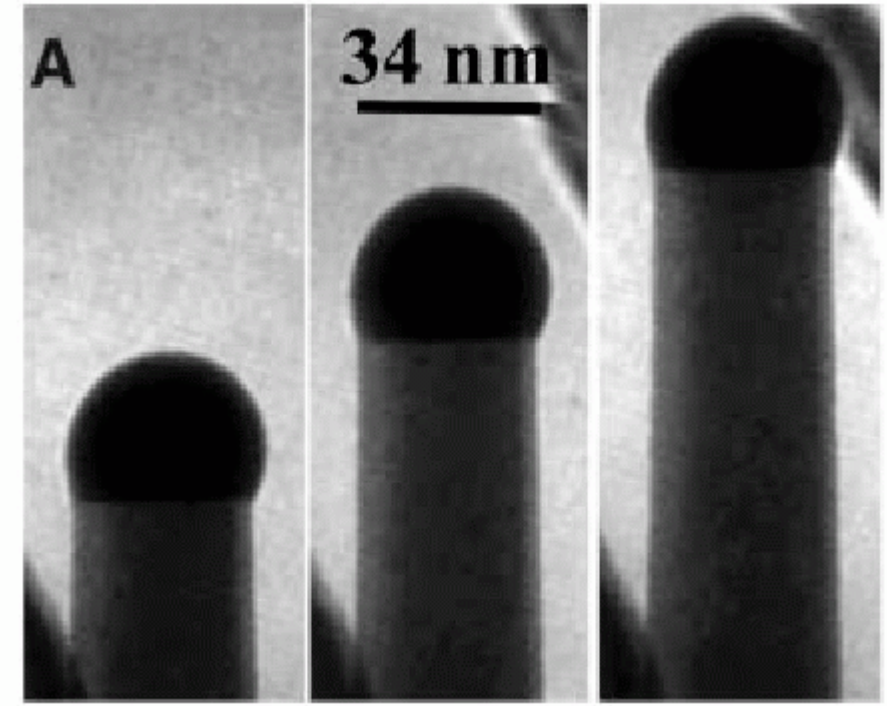
Imaginary density

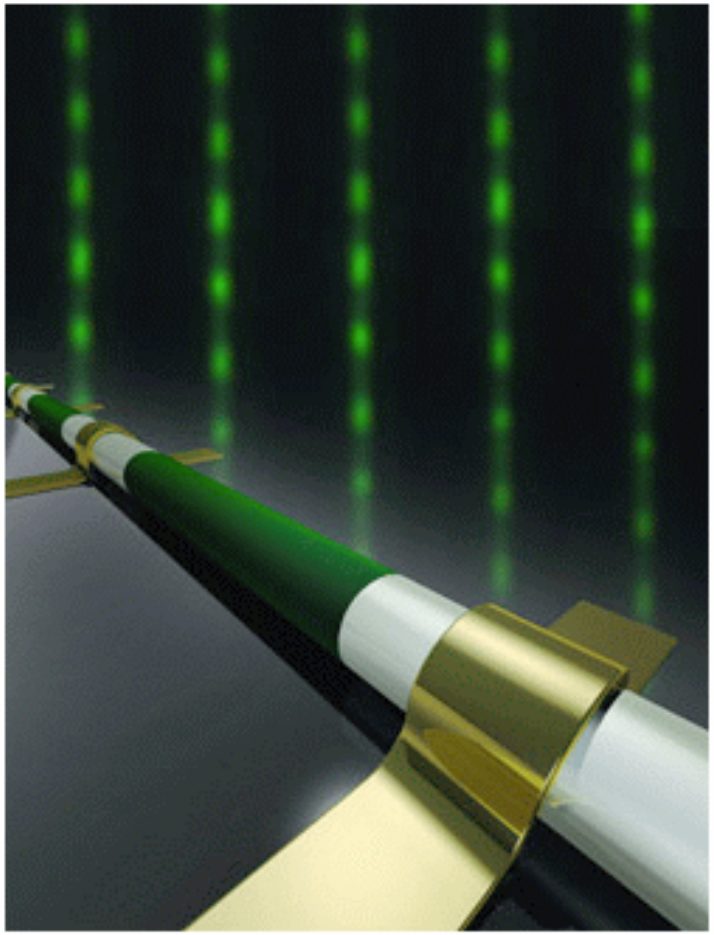




VLS growth of nanowires

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

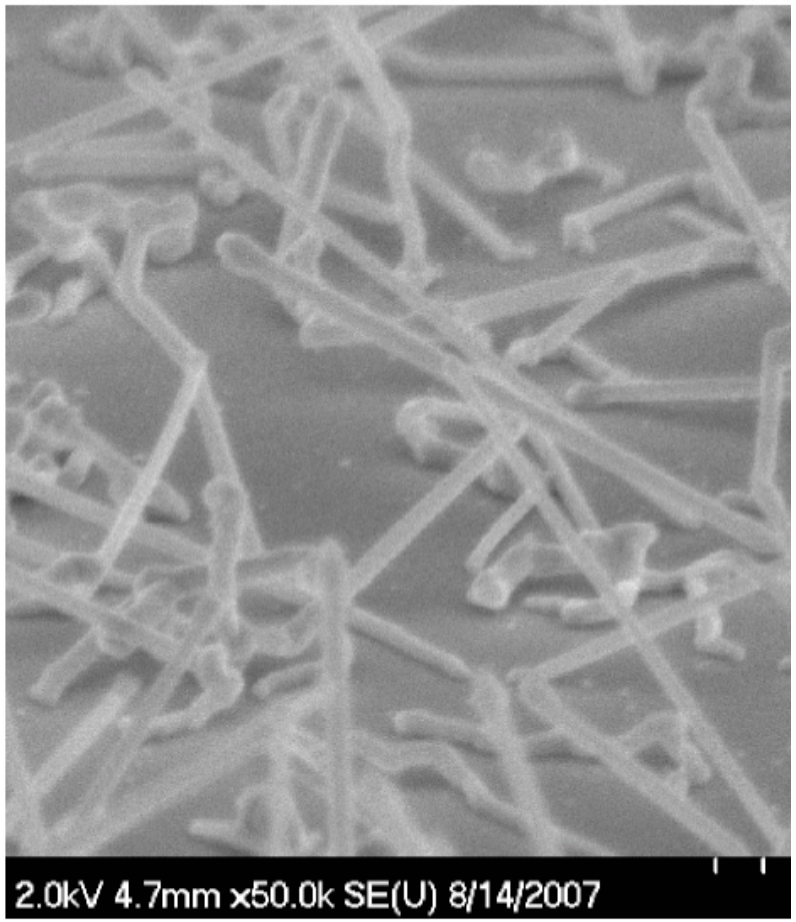




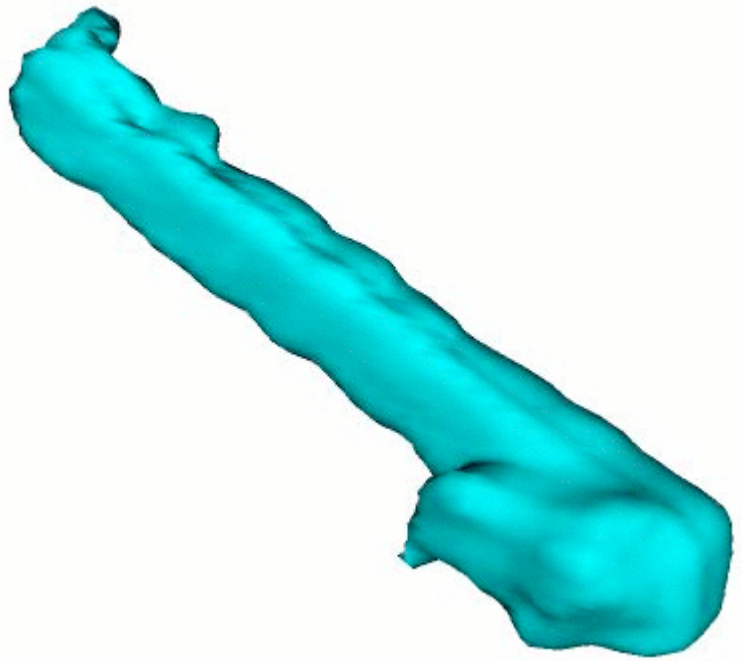
NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

Reconstruction of InP nanowire

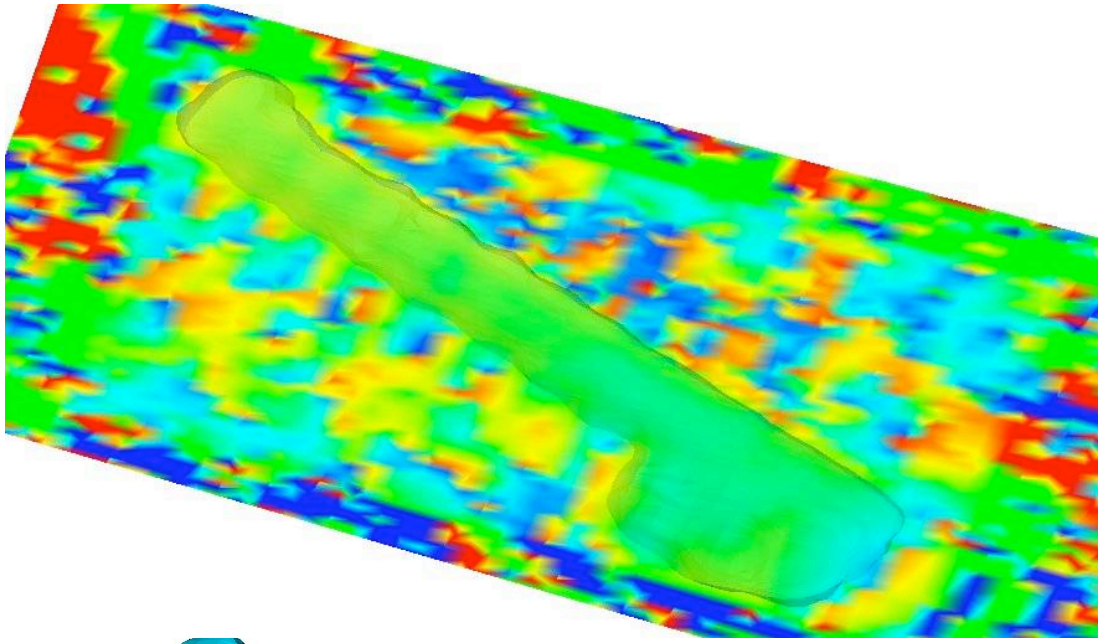
CVD on Si, Suneel Kodambaka, UCLA

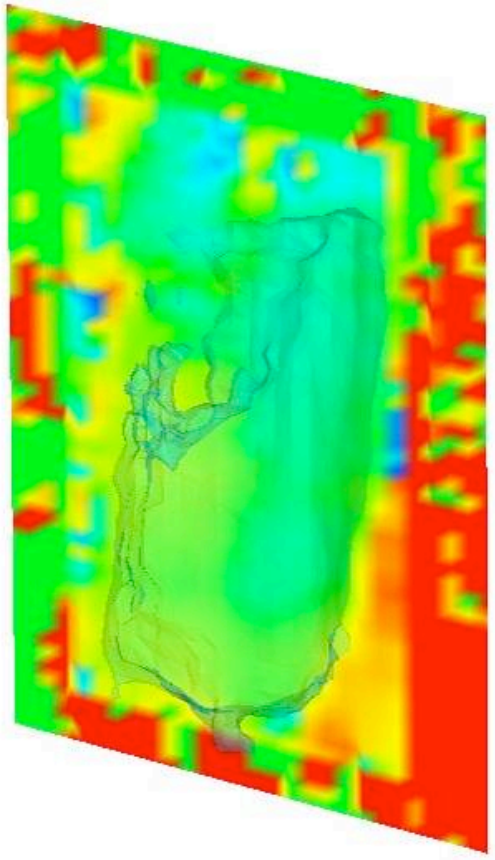


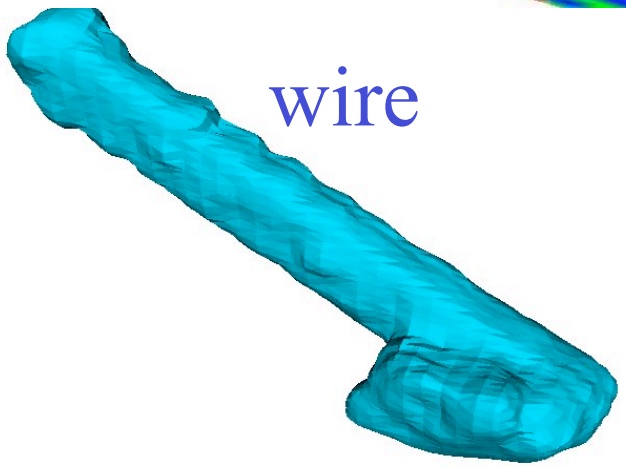
InP nanowires grown on Si (111)



Phase structure in nanowires

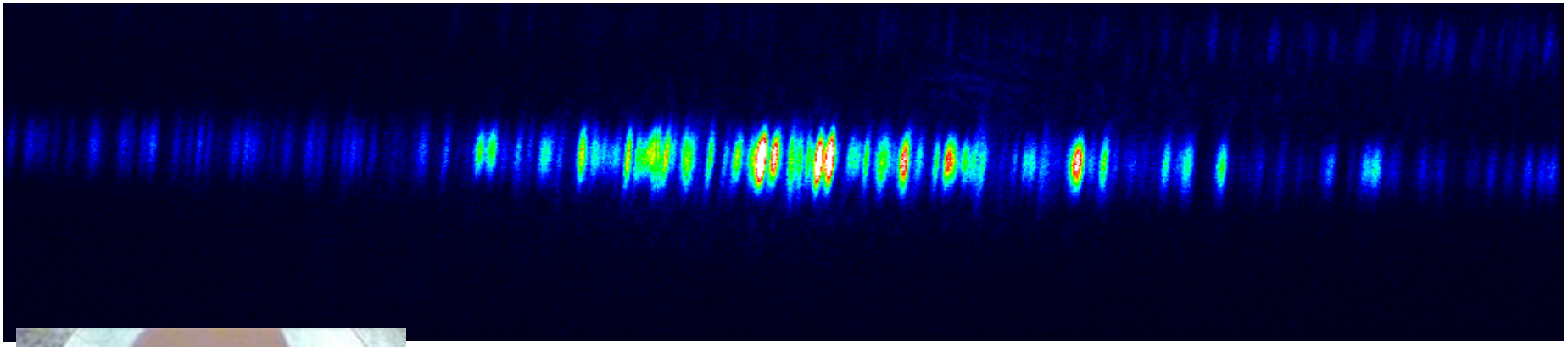


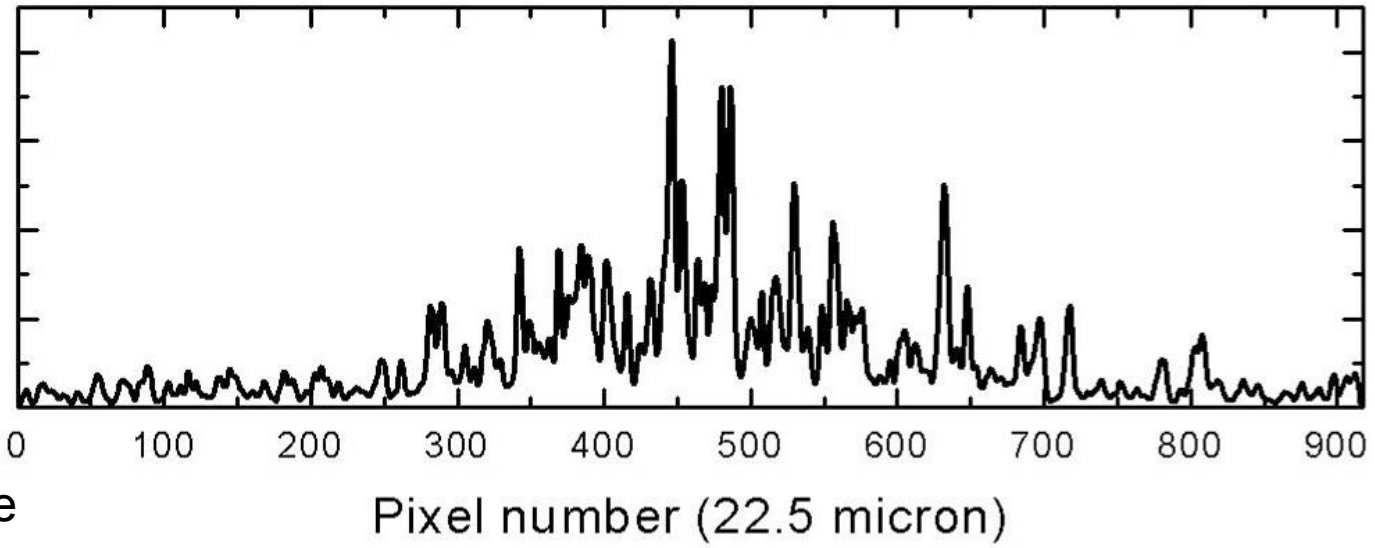




GaAs Nanowire "Barcode"

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

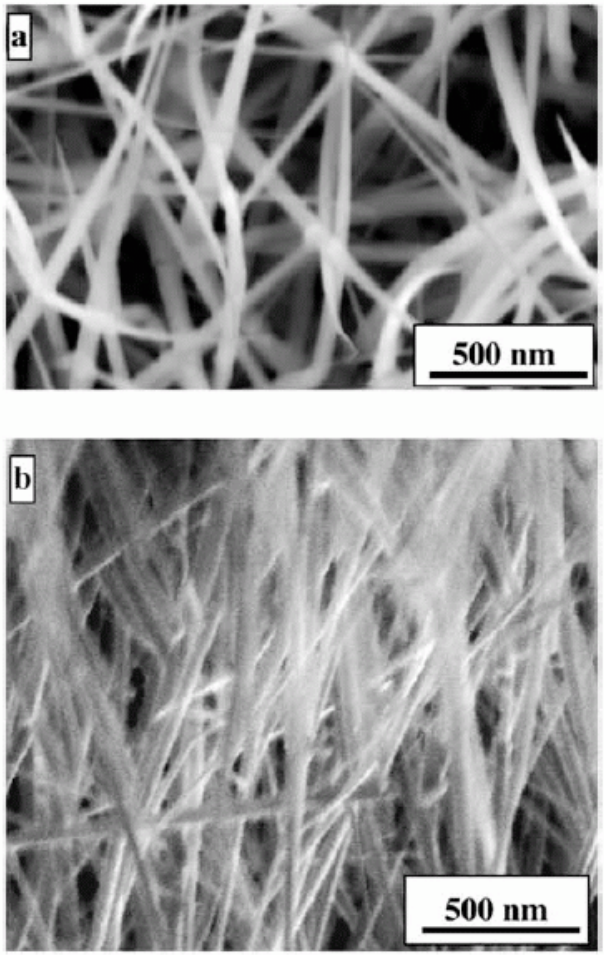


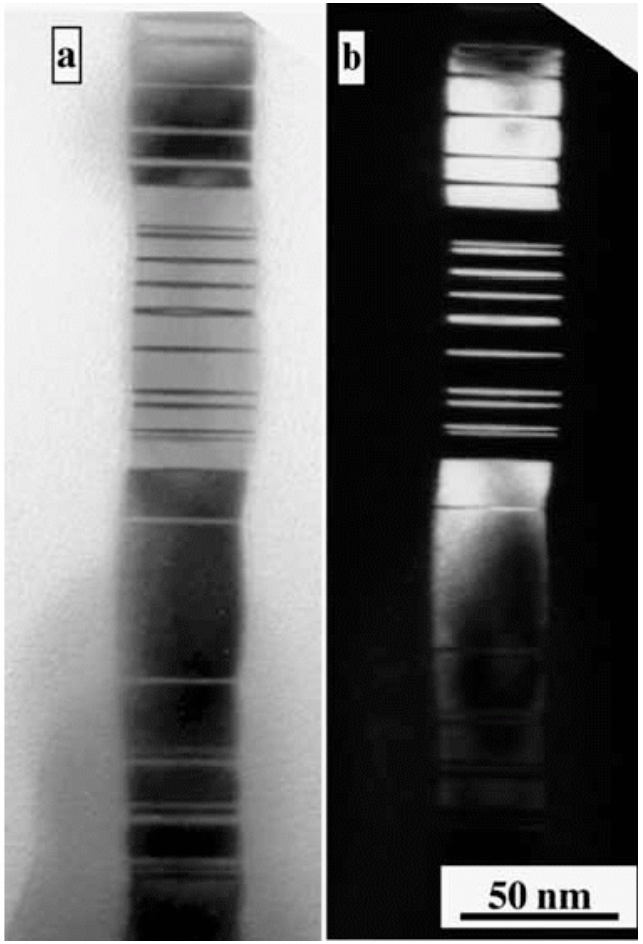


GaAsNW1106-22.spe
B9348 from Philips

Dark Field TEM of GaAs Nanowires

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

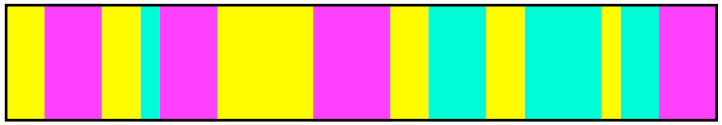




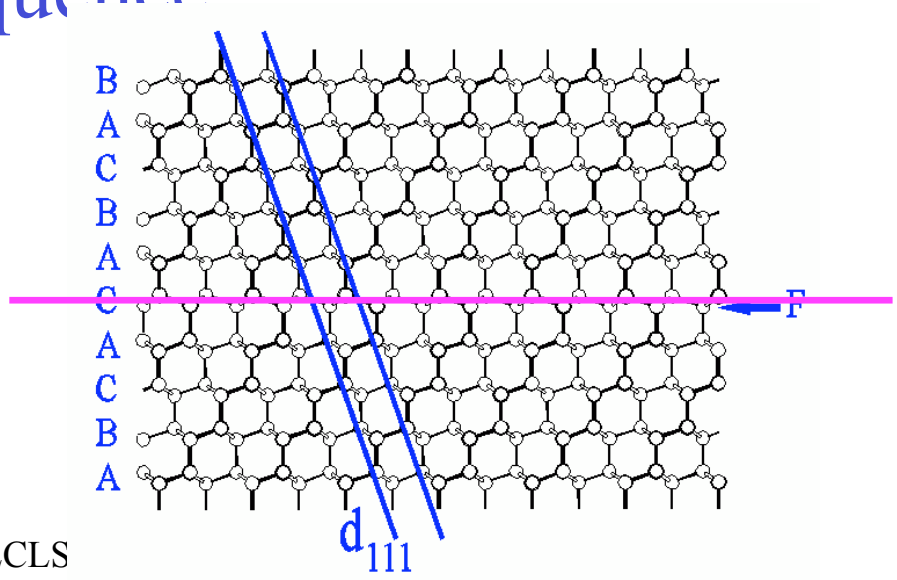
Models of Barcode Diffraction

(111) wires at (11-1) reflection

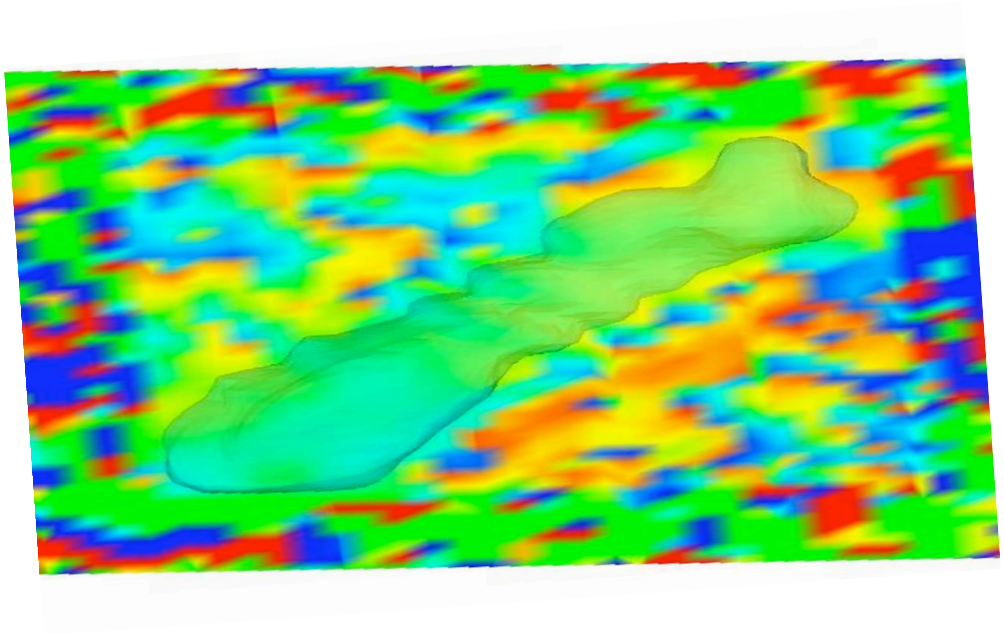
- Twinned stacking sequence

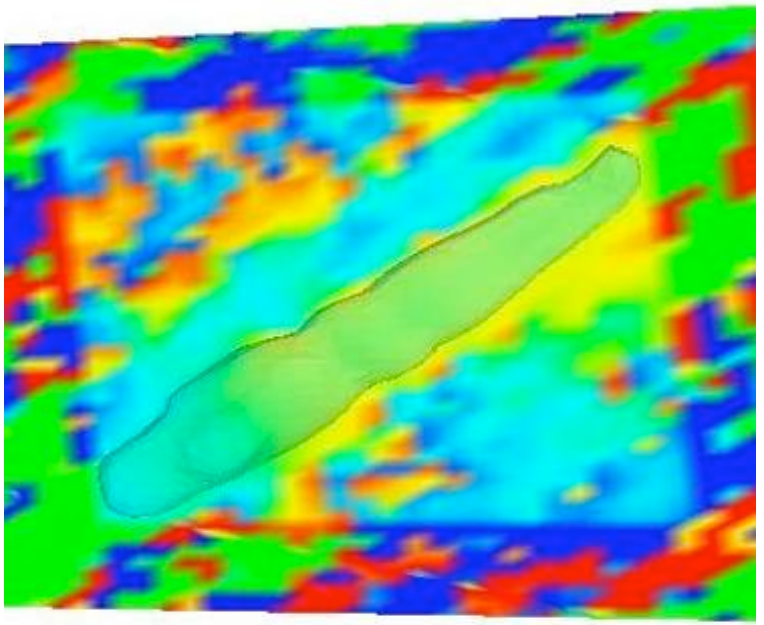


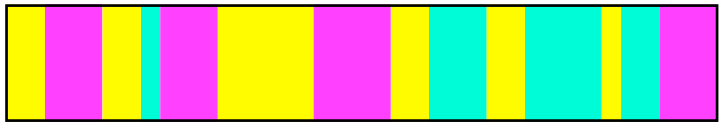
- Deformation faults



Antiphase domains in faulted wires?

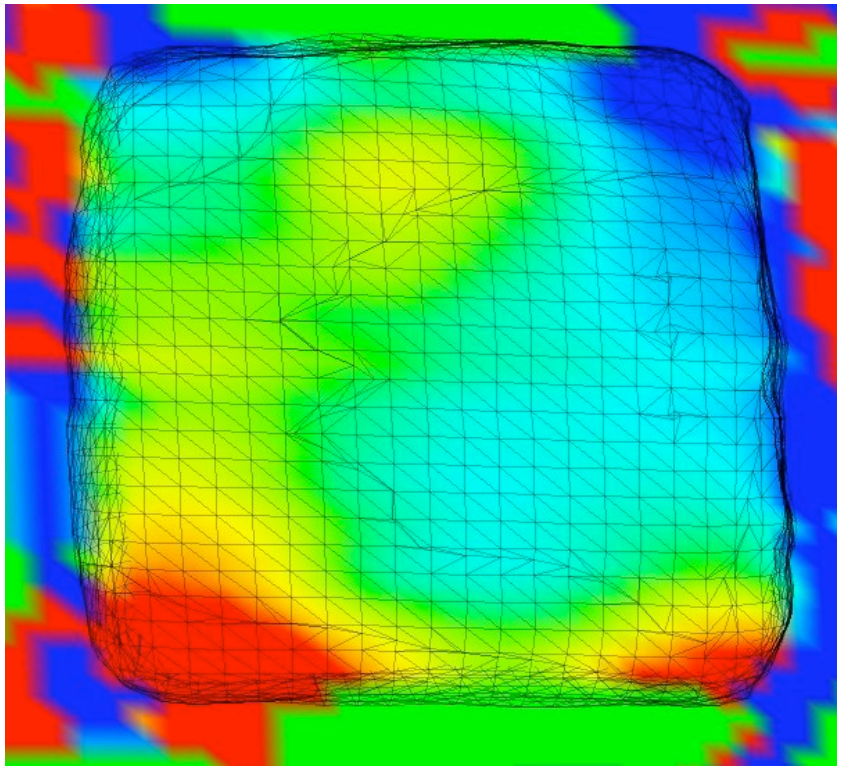


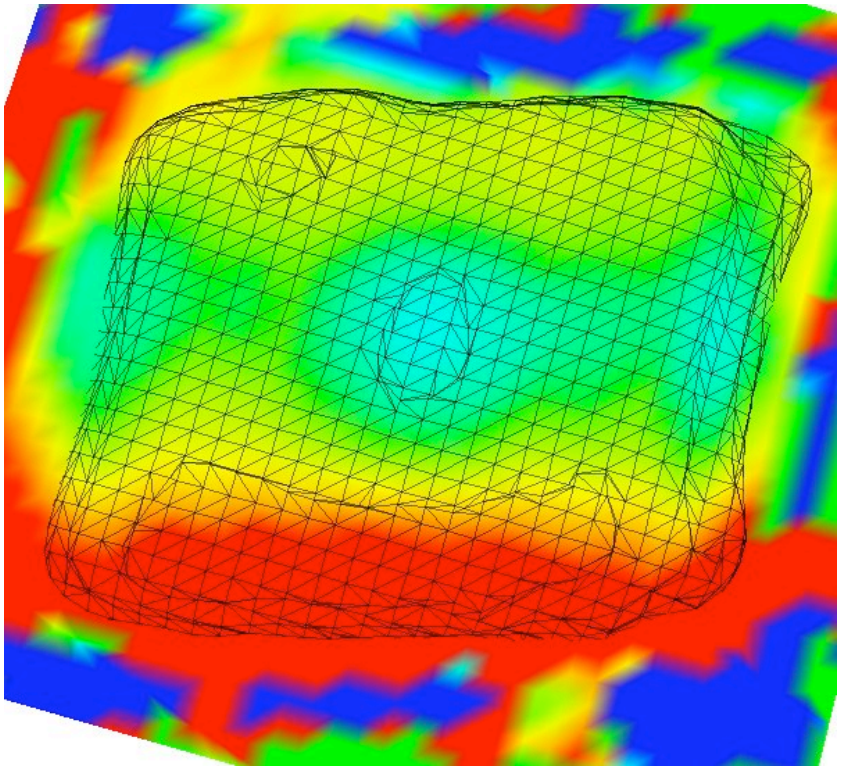




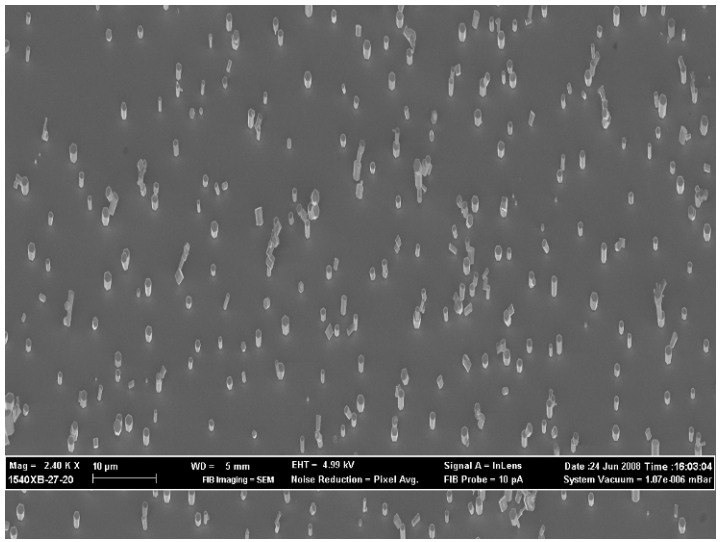
Contact strain of Zeolite ZSM-5

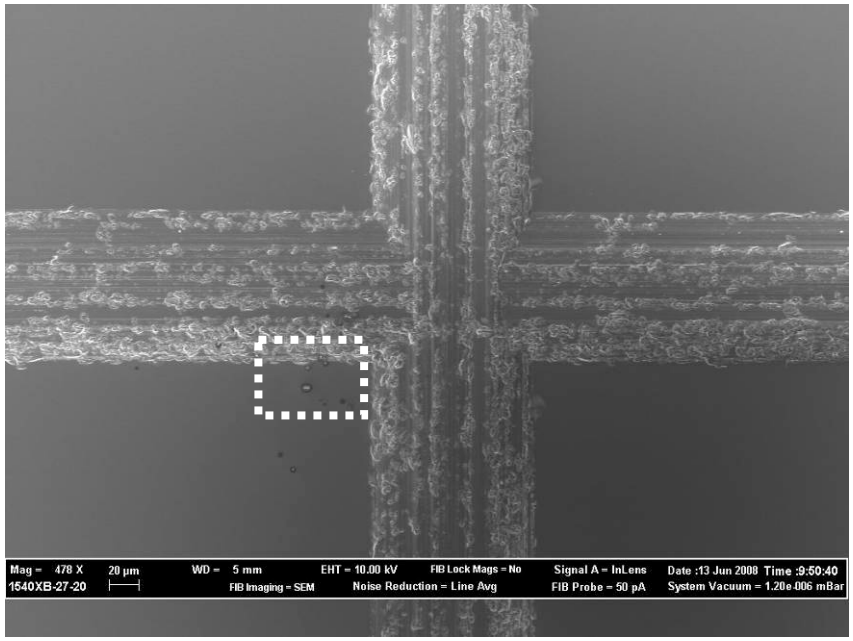
with Hyunjung Kim and K. B. Yoon at Sogang University

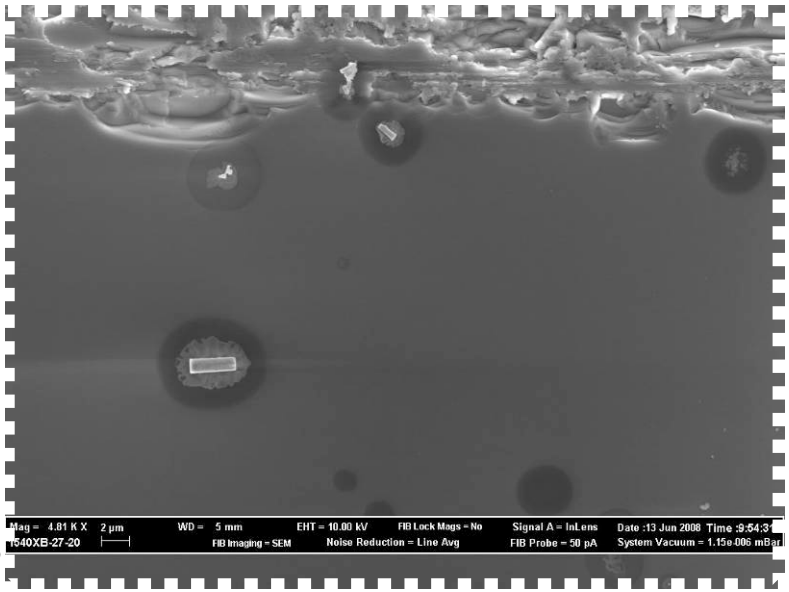




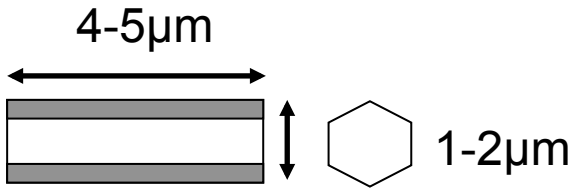
ZnO Sample Preparation







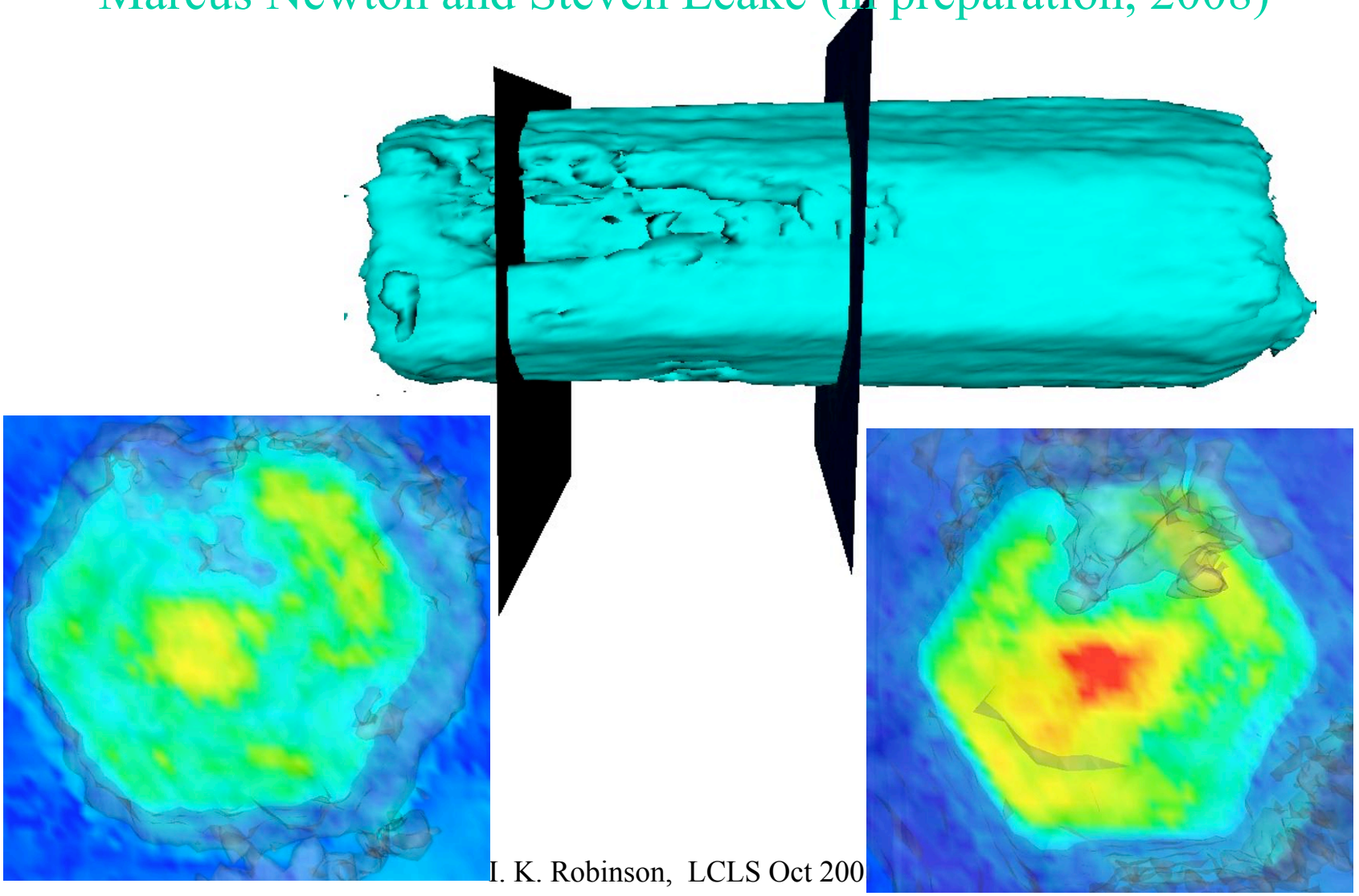
Dimensions:



I. K. Robinson, LCLS

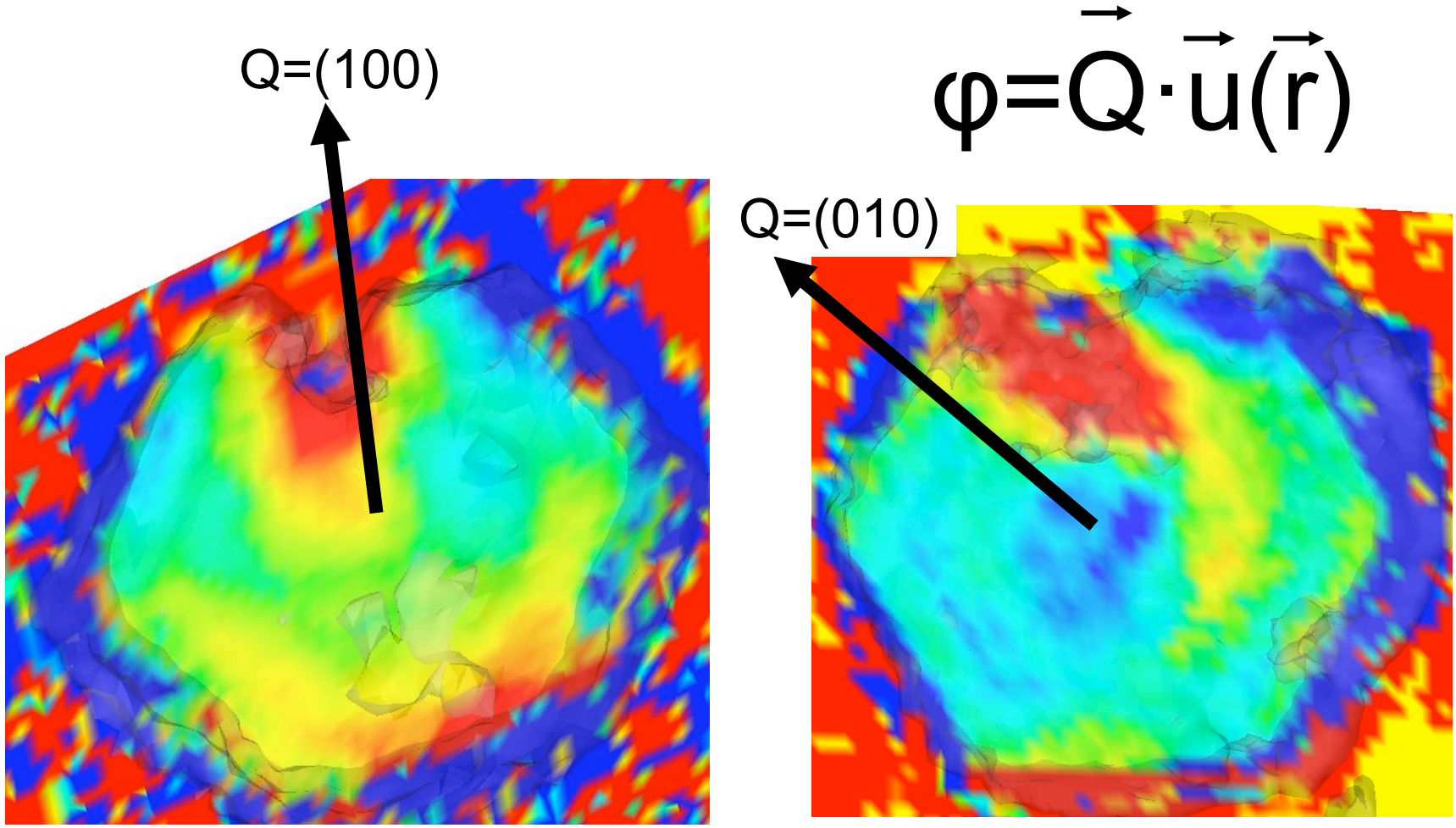
Density sections ZnO-39 (010)

Marcus Newton and Steven Leake (in preparation, 2008)

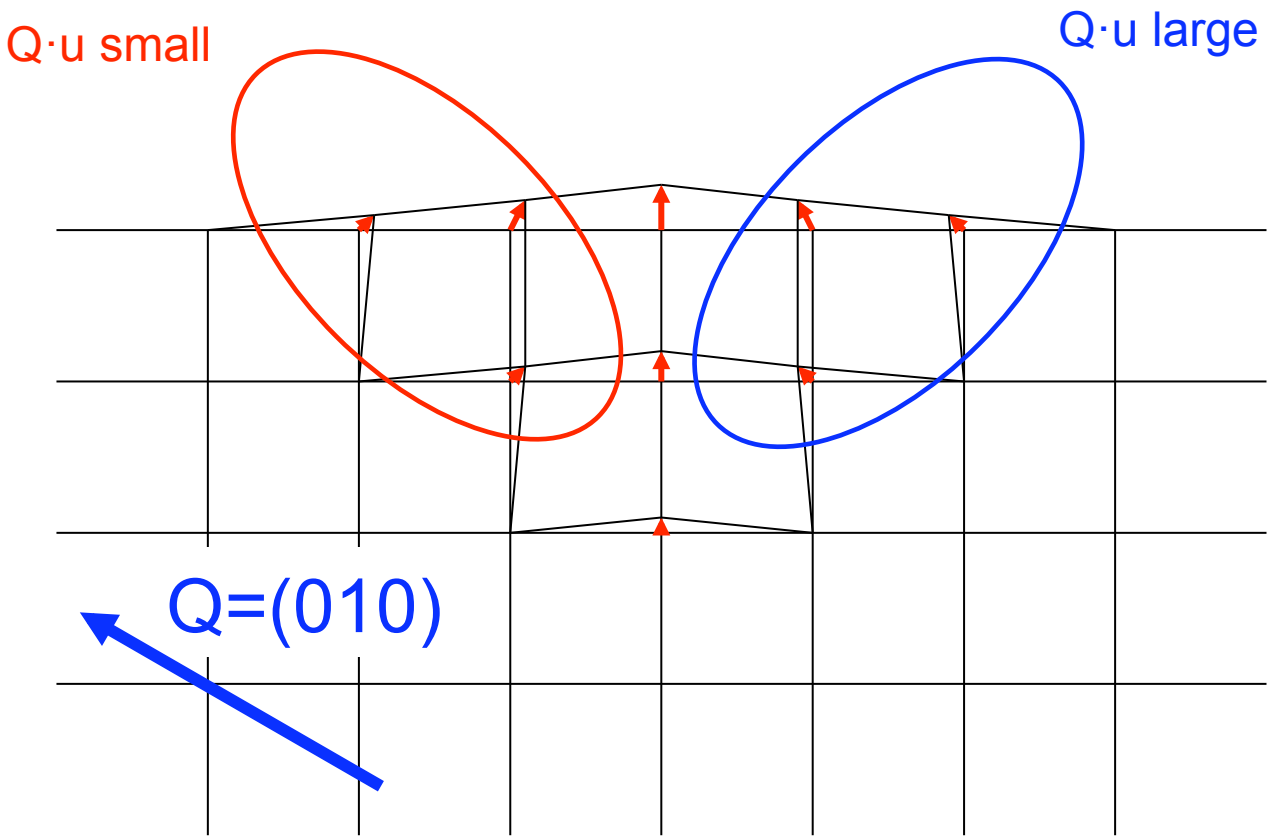


Phase maps from 2 Bragg peaks

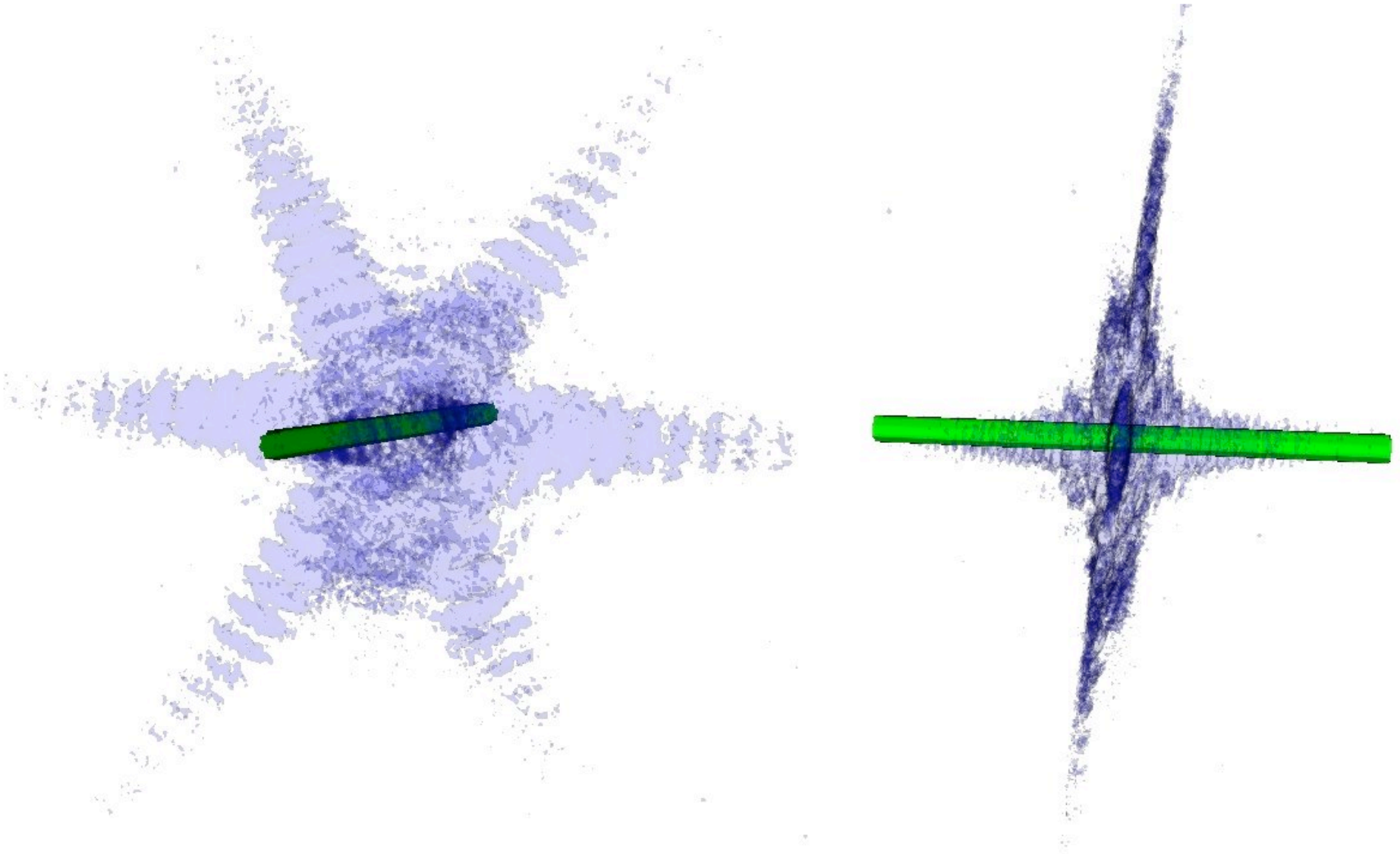
Blue-Red is +2 radians. Slice at -1500nm from centre ZnO-5 -39

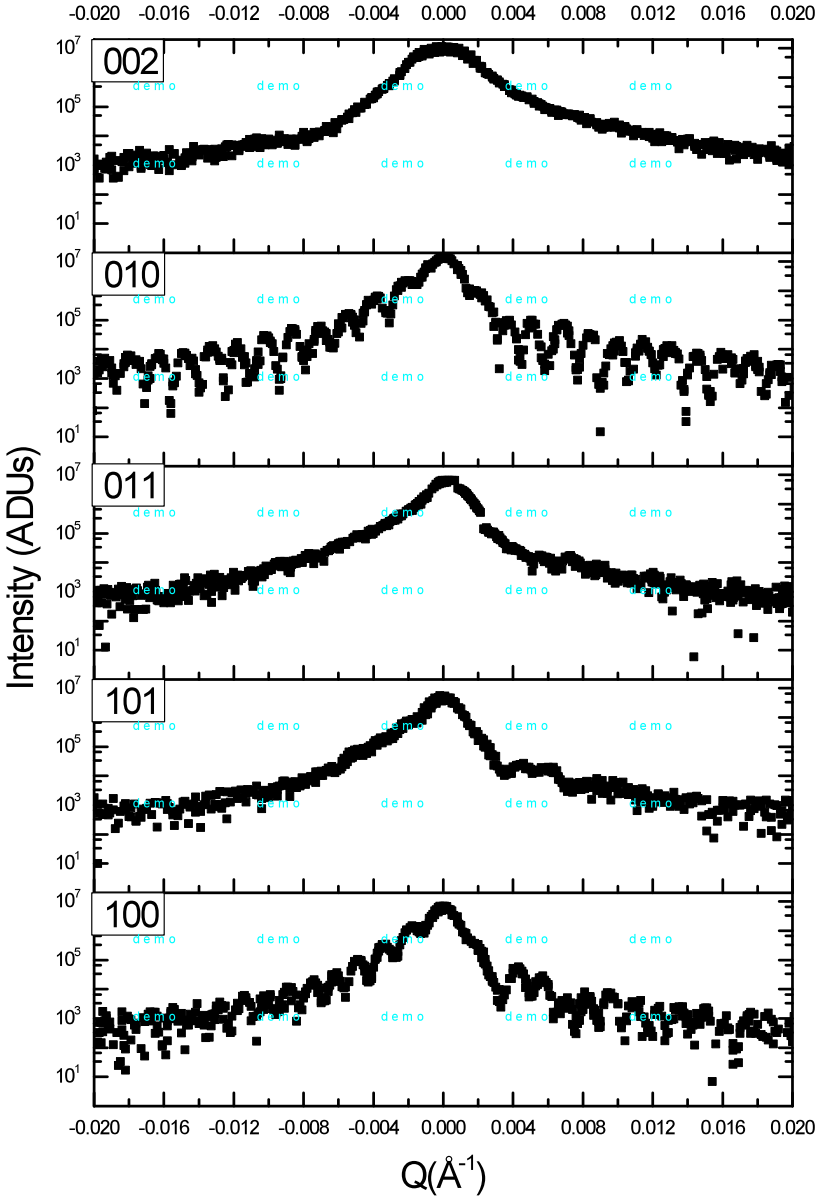


Typical displacement field



How to extract the contrast data





Five Bragg peaks

002 no fringe visibility

010 & 100 good fringe visibility

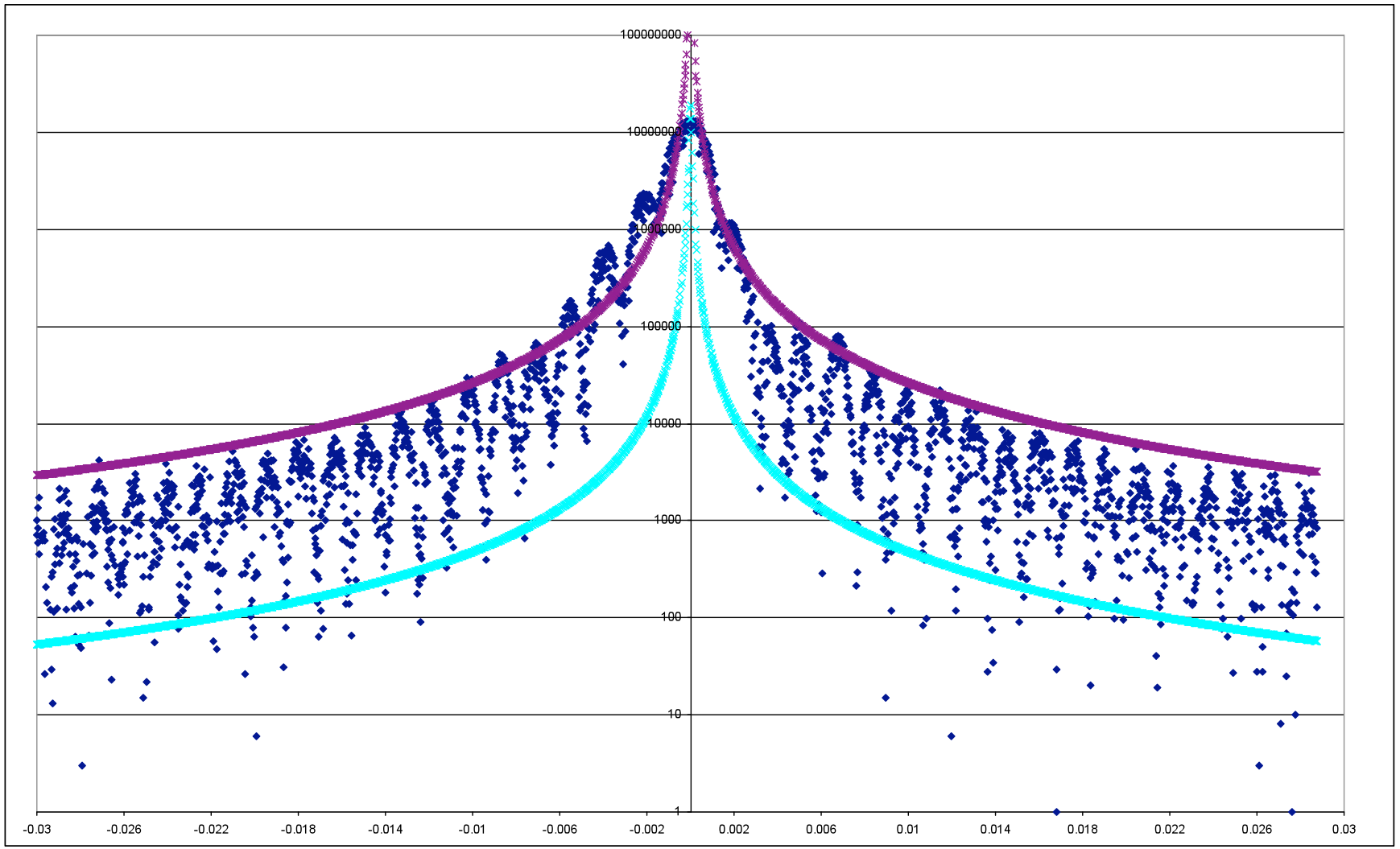
101 & 011 diminished fringe visibility
but fringes still evident

010:011 & 101:100
show complementary fringes
but not between each other

Error in coordinate transform ruled out

010 and 100 reflections fringe spacing
difference ~ 20%

Fringe Visibility 96±2% @010



How much information in a single shot?

- Phase problem can be solved beforehand:
  - Low dose rocking curve before ‘shot’
  - Ptychography scan before ‘shot’
- Phased diffraction allows full imaging during transient
- Phases are little changed during perturbation
  - localised change in real space affects all of reciprocal space
  - traditional “difference map” principle

3D solution from a single shot?

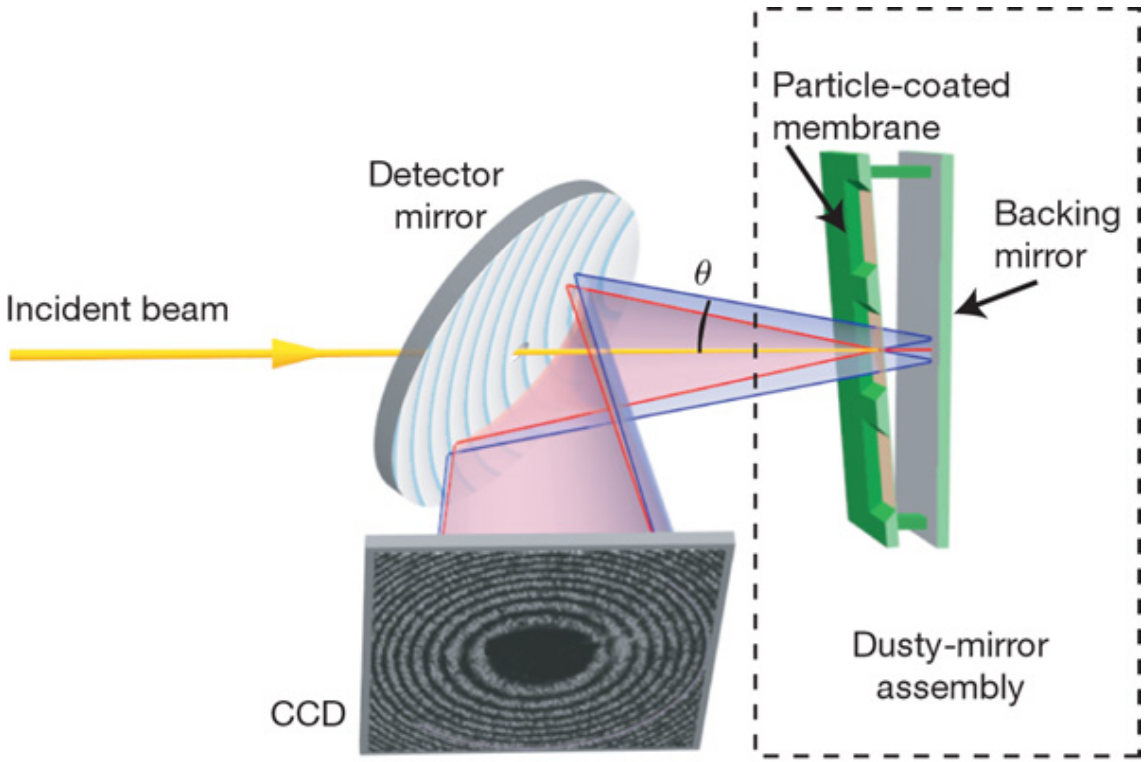
- Keyhole imaging with curved beam
  - multiple views of sample?
- Reconstruction is of exit wave field
  - can't propagate to general 3D object
- Phase problem easier to solve for real objects
  - logo physics and cowboys
- Free-space propagation of phased wave field
  - valuable for ptychography probe

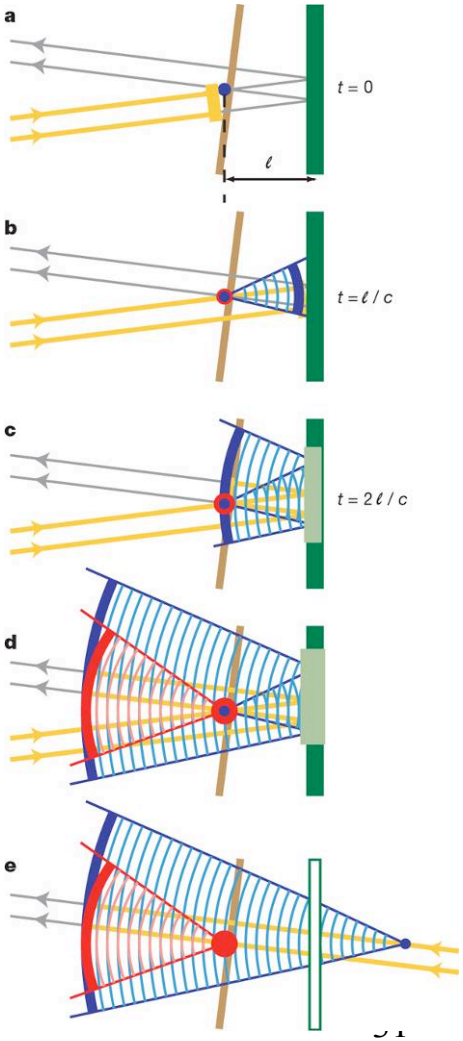
XPCS or Imaging approach?

- Fluctuation-dissipation theorem:
  - transient response "=" fluctuation due to noise
  - complex susceptibility, eg shear modulus
  - 1-point or 2-point correlations?
- Beam 'heating' anyway, use as impulse:
  - Split-and-delay technique
  - "Dusty Mirror" experiment

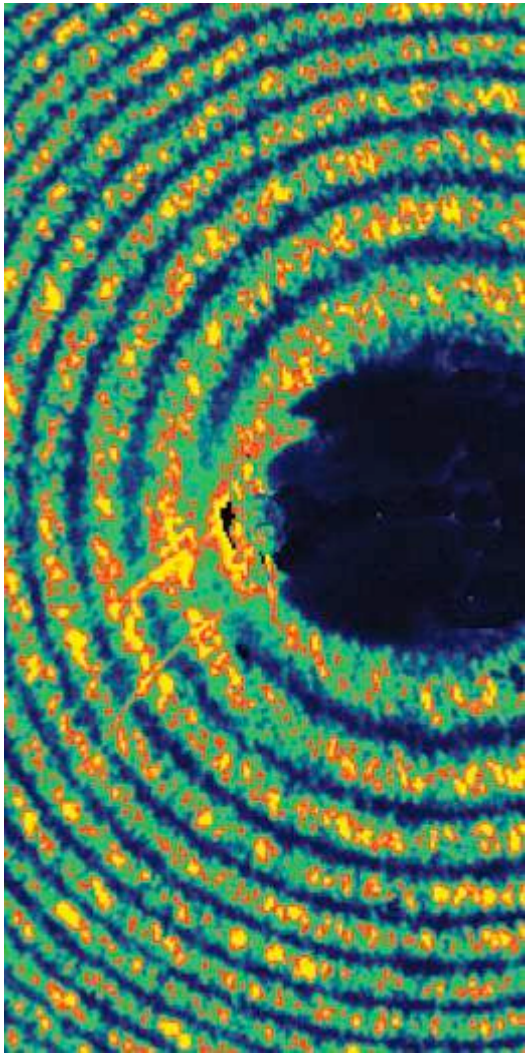
“Dusty Mirror” experiment

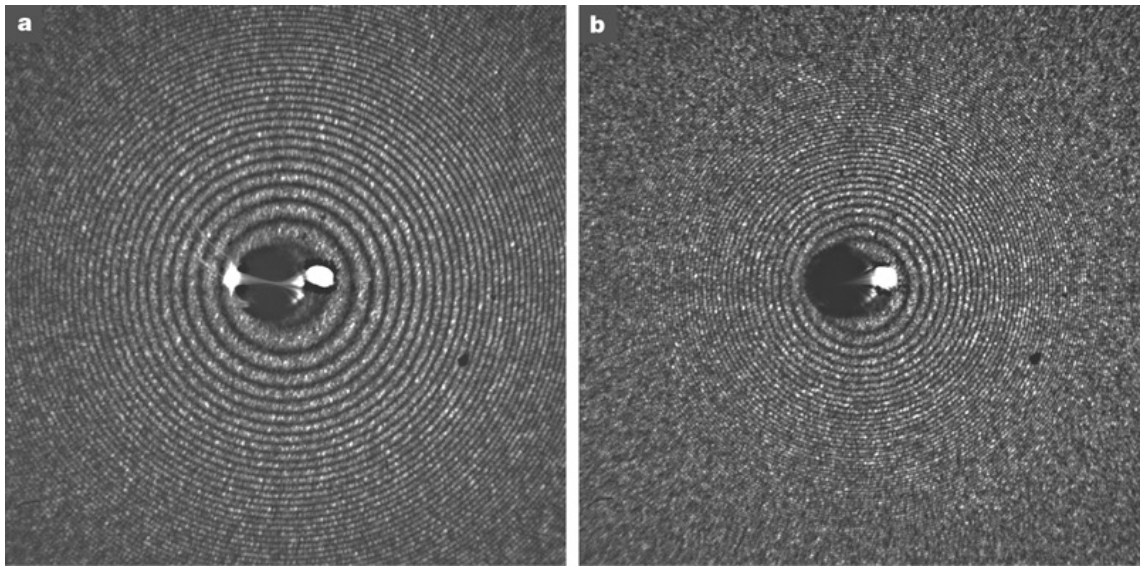
HN Chapman et al Nature 449 677 (2007)

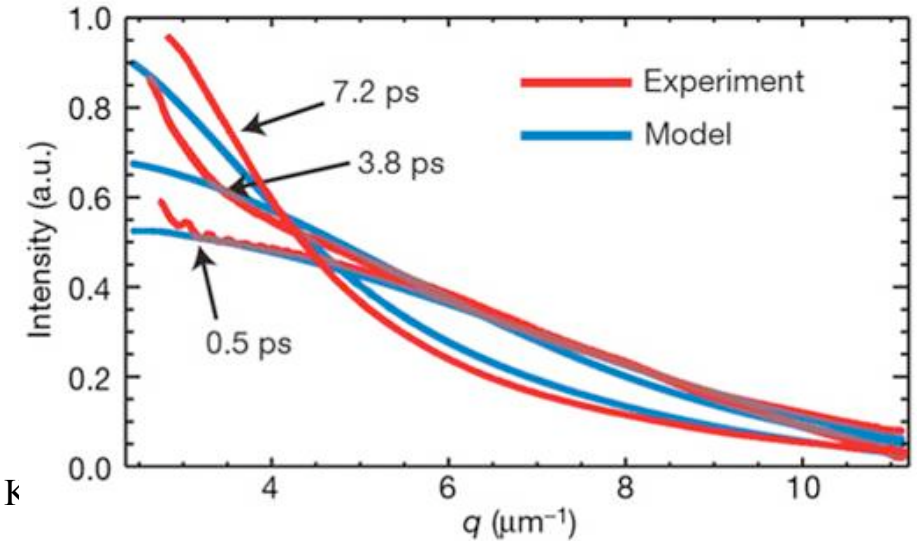




Loss of fringe visibility in (ps) time







Real or Reciprocal space view?

- Free to choose once phase problem is solved
  - Low dose rocking curve before ‘shot’
  - Ptychography scan before ‘shot’
- “Dirty mirror” was recip space information
  - OK because many similar samples in beam
- Real space avoids drifts, pulse-to-pulse variations
  - good for localised changes, rare events
- Reciprocal space better for self-similar objects
  - average over multiple copies

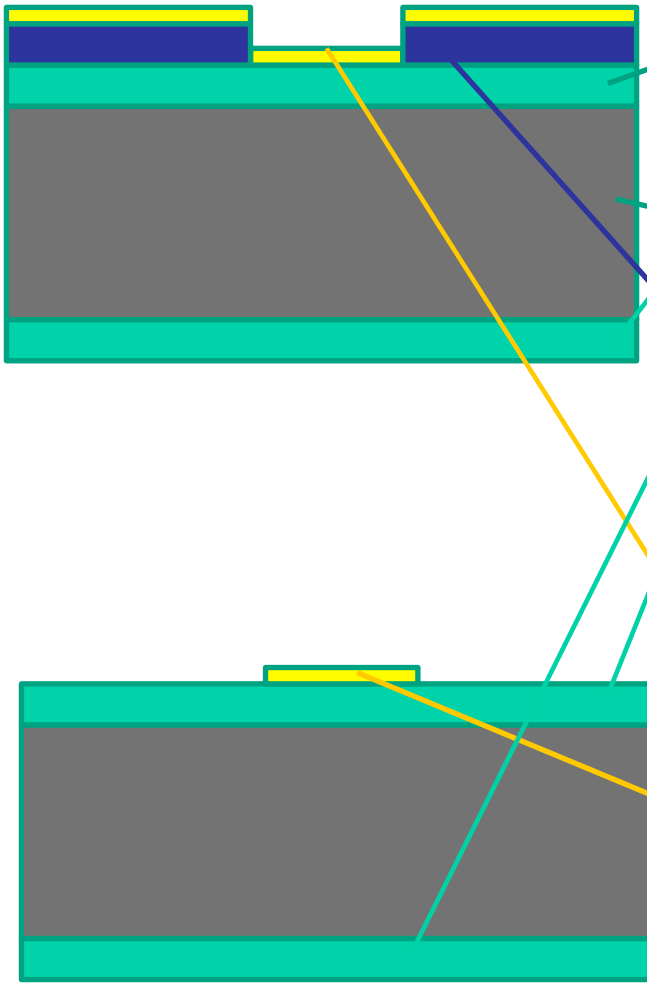
Generic aspects of speckle

- First-order change is of intensity
- Second-order change in speckle positions
  - constrast is mostly sensitive to this
- ‘Persistent’ speckle observation
  - Martin Grant & Mark Sutton
- Constrast useful to quantify degree of coherence of the beam

Planning for initial LCLS experiments

- CXI and PCS not ready in initial phase
- XPP will be first diffraction station
  - Area detector can measure CXD pattern
  - Laser pump can ‘activate’ sample
- Fabricated Gold nanocrystal arrays
  - control size, shape, orientation (est 200nm)
- Pre-align each under low dose for phasing
- Explode with full pulse: changes or not?
  - Observe melt? front after laser pump

e-beam Lithography "Lift-off" method



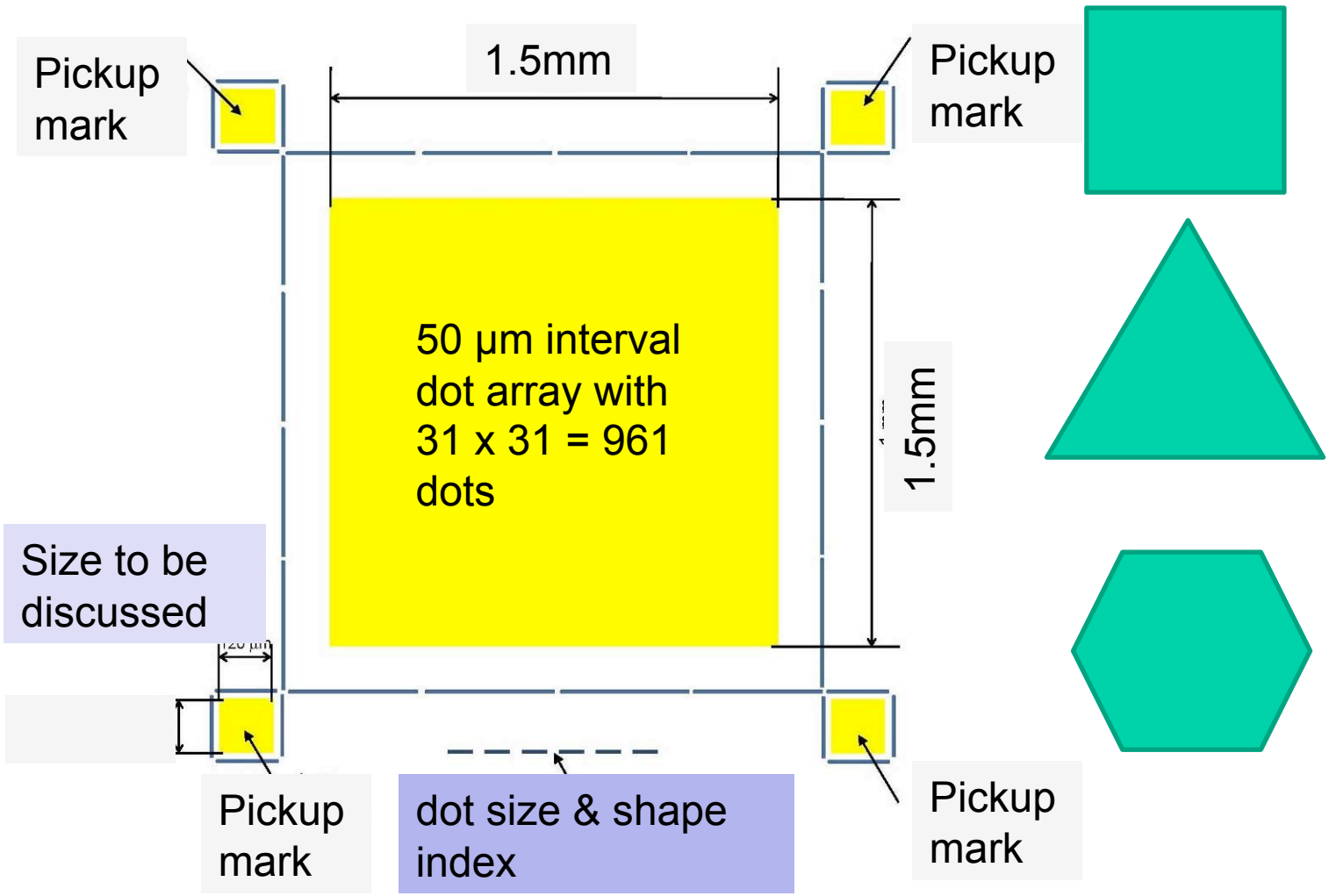
Thermally grown Si O2,
~ 100nm thick
(Back side oxide remaining)

Si (100) wafer
10(+-1) mm x 10(+-1) mm
square/rectangle

ZEP (EB) resist for lift-off

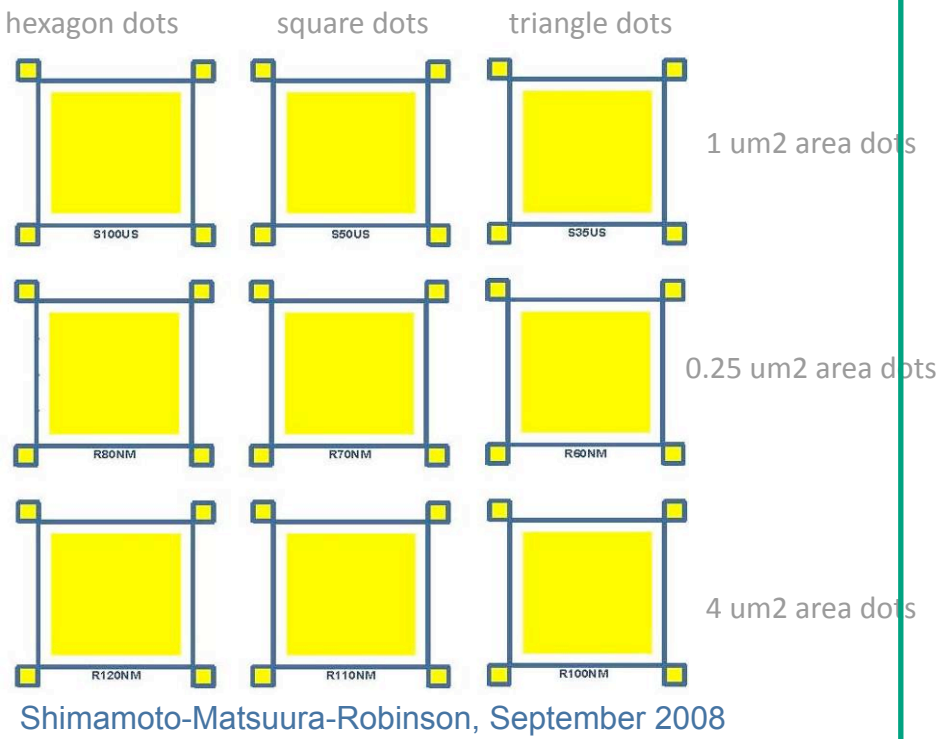
Au film 20nm thick (piece-to-piece accuracy within 10%?)
(with and without adhesion layer of Cr or Ti 2nm thick)
(EB or thermally evaporated)

Top View of basic layout plan with pickup marks



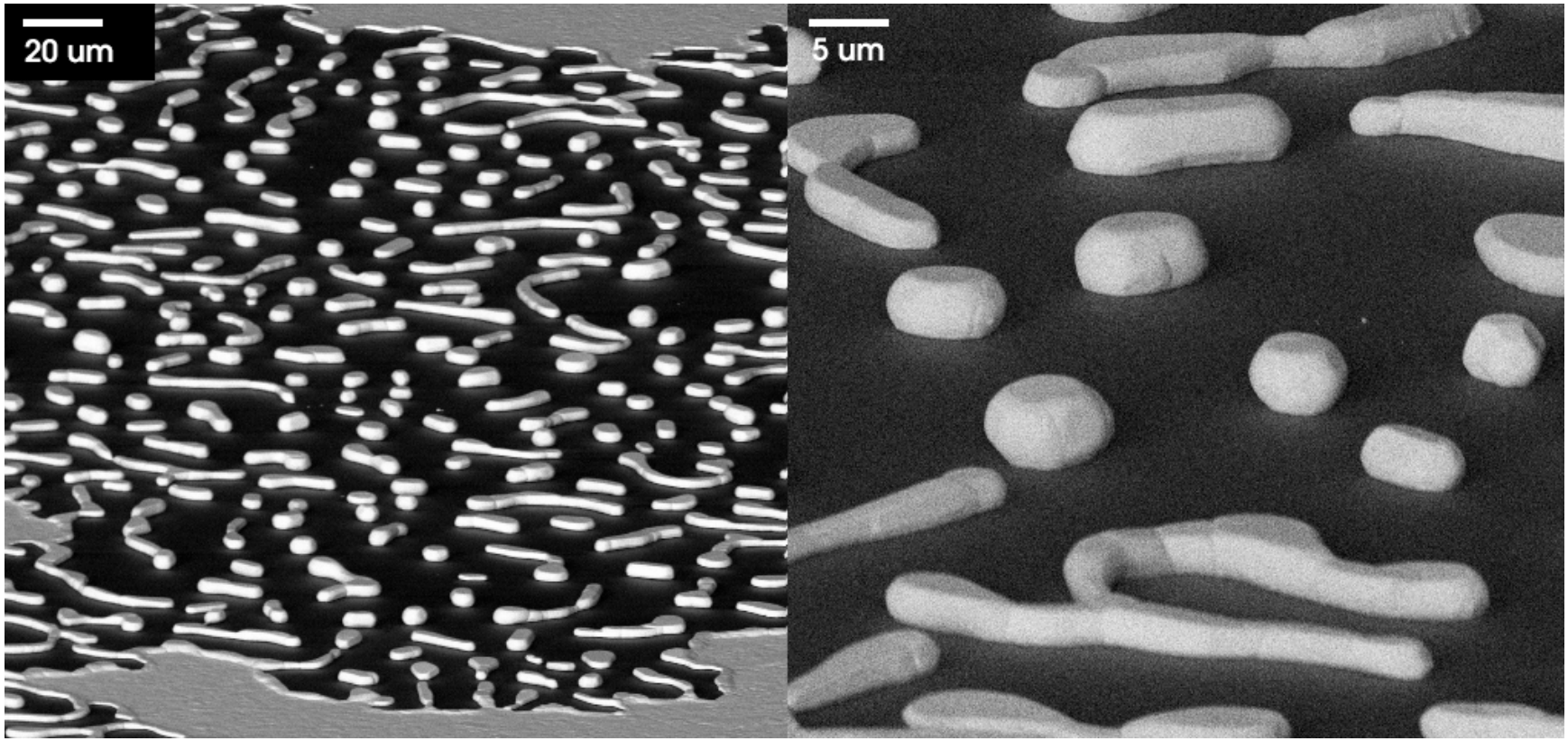
Top View of chip layout

S. Shimamoto (Waseda), T. Matsuura (UCL), Sept 2008



Dewetting to coalesce into crystals

Garth Williams thesis (2005)



Discussion Questions

- Coherent x-ray diffraction
- How much information in a single shot?
- 3D solution from a single shot?
- XPCS or Imaging approach?
- Real or Reciprocal space view?
- Planning for initial experiments