Exploiting the Coherence of Modern X-rays

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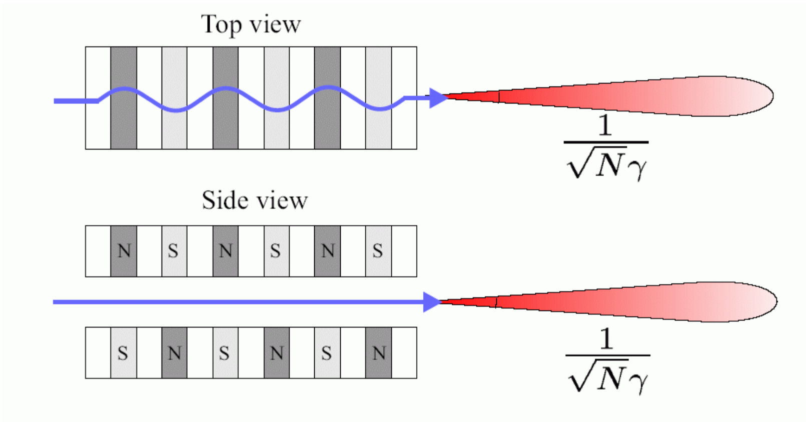
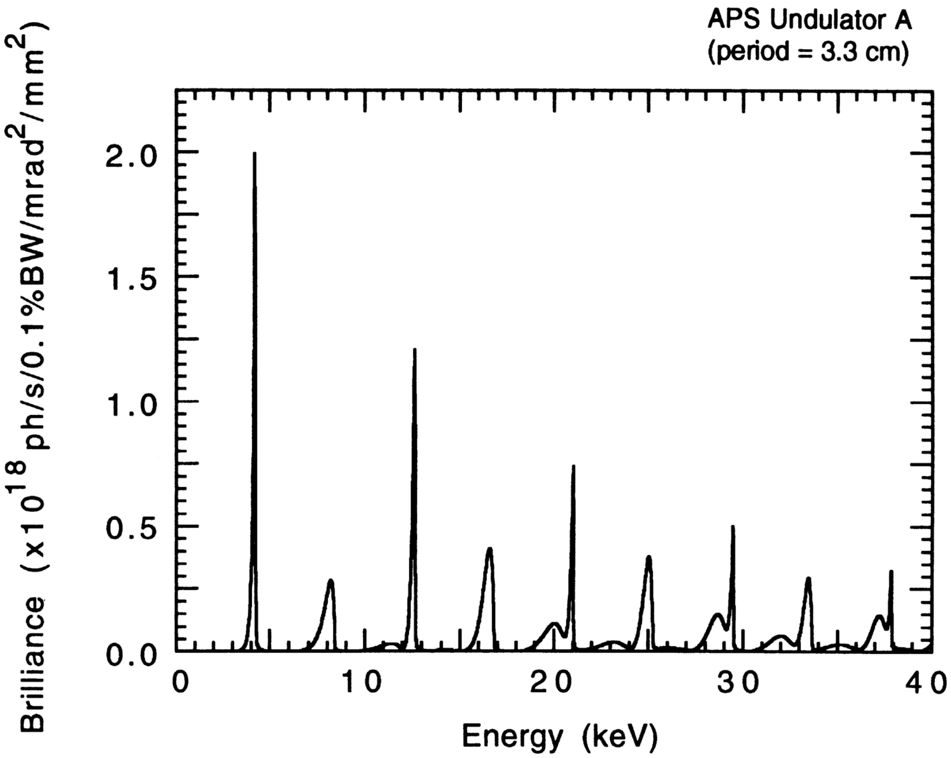
University College London
Diamond Light Source

X-ray Undulator Principle



$$\lambda_X = \frac{\lambda_U}{2\gamma^2}\left\{1 + \frac{K^2}{2} + (\gamma\theta)^2\right\}$$



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Robert Fleming
Steve Dierker
Simon Mochrie
Brian Stephenson
Steve Brauer
Mark Sutton
Eric Defresnes
Jeff Legrand
Gerhard Grubel
Doug Abernathy
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3 days at ID10
November 1993

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n of one-dimensional x-ray speckle patterns from synthetic multilayers

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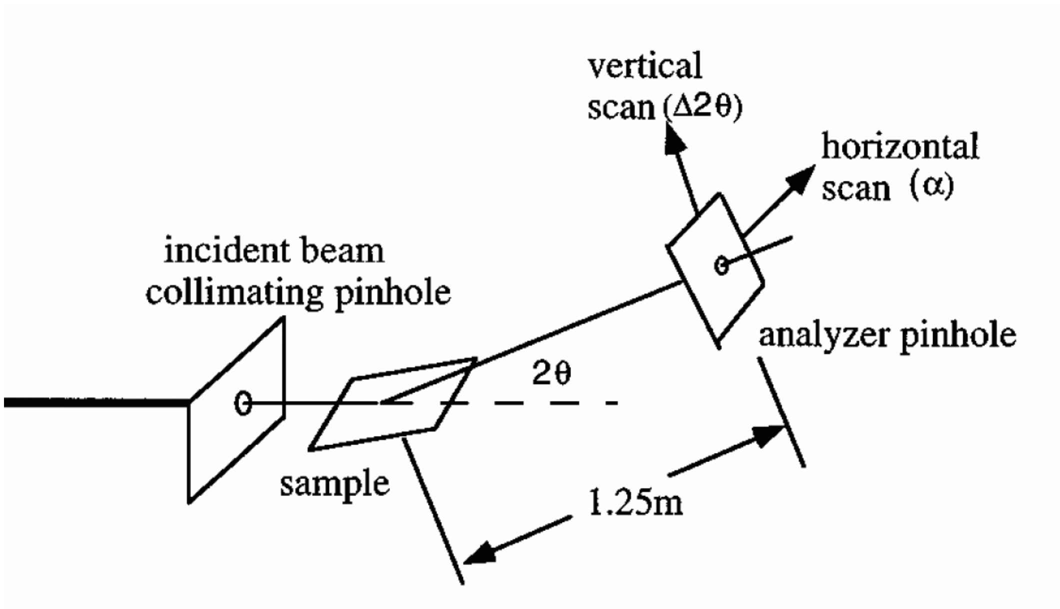
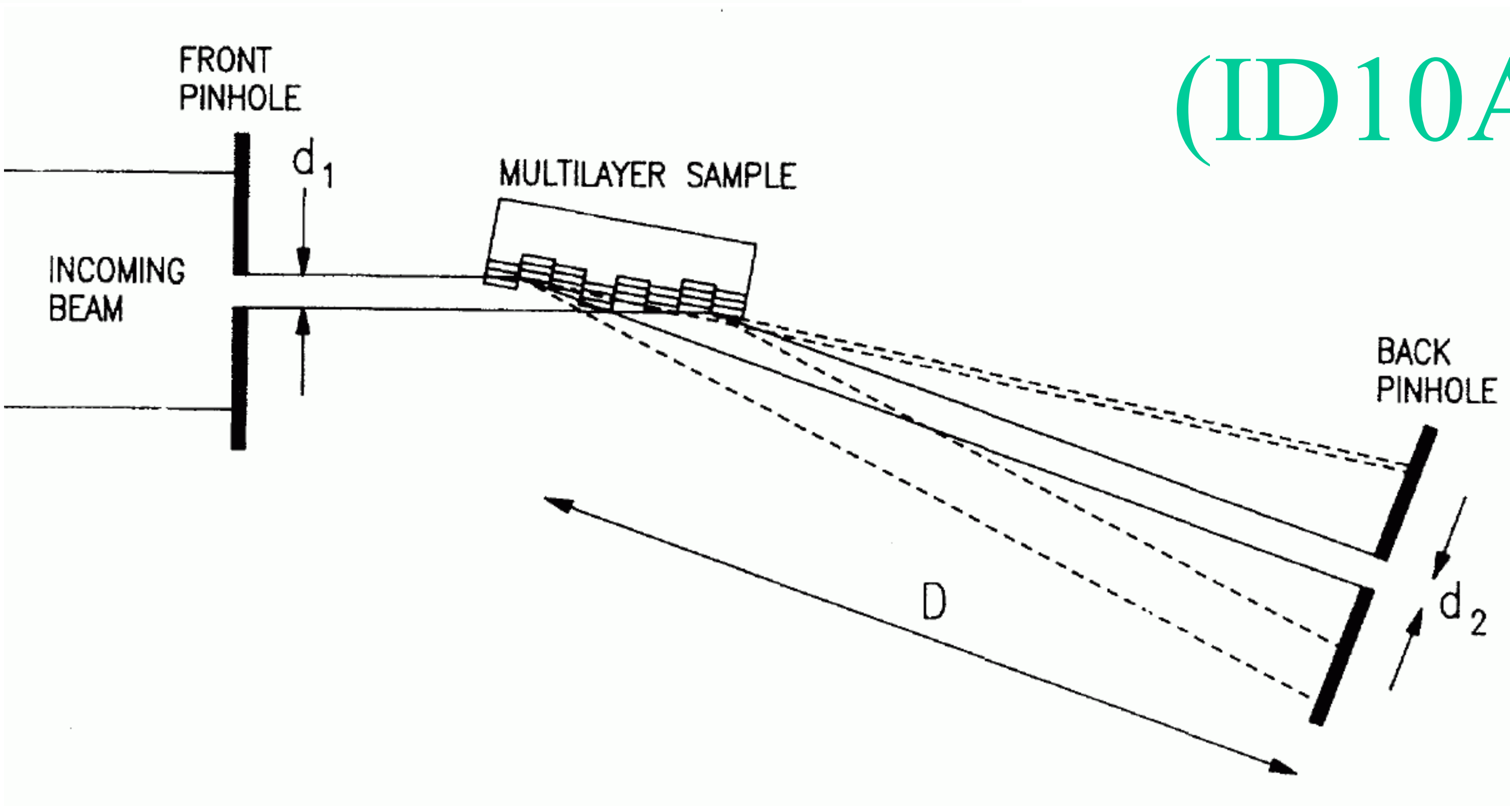
(Received 15 March 1995)

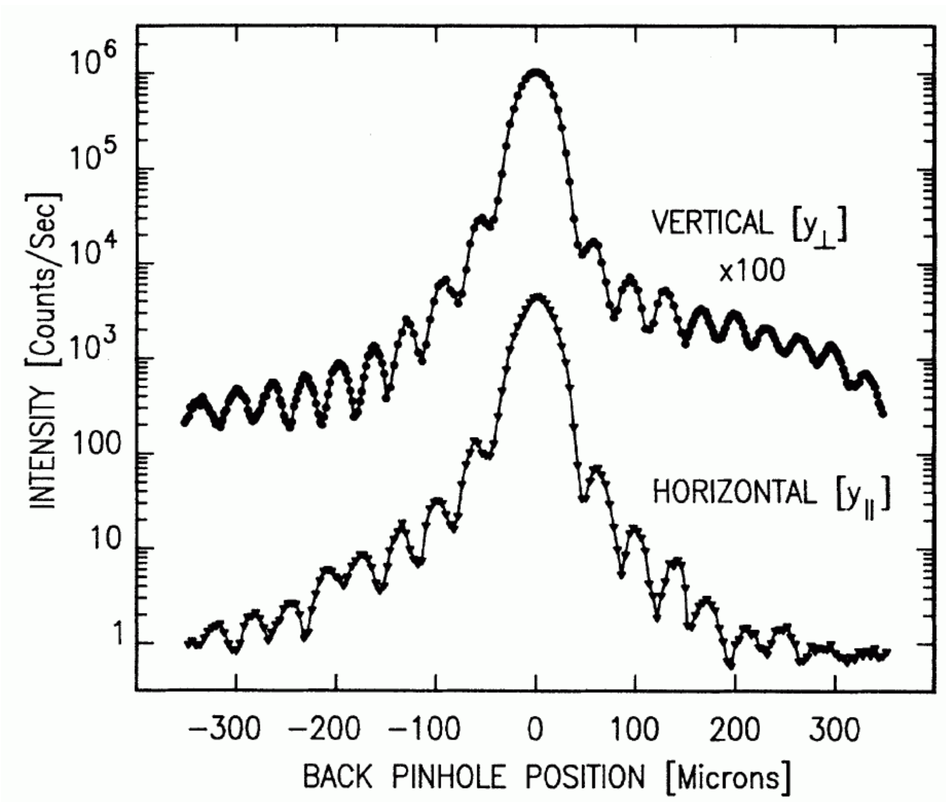
ka" x-ray undulator beamline at the European Synchrotron Radiation Facility, measuring coherent diffraction ("speckle") patterns from artificial multilayers. l in that they are unremarkable in the scan direction perpendicular to the Bragg peak of the width of the Fraunhofer maximum, but have dramatic structure in agg angle. This is shown to be consistent with the extreme asymmetry of the ore than one well-ordered domain of the sample to fall within the coherently il- patterns are sufficiently simple that we are able to model them reasonably well by rameters to a fixed number of illuminated "blocks." Two fitting procedures are some general utility.

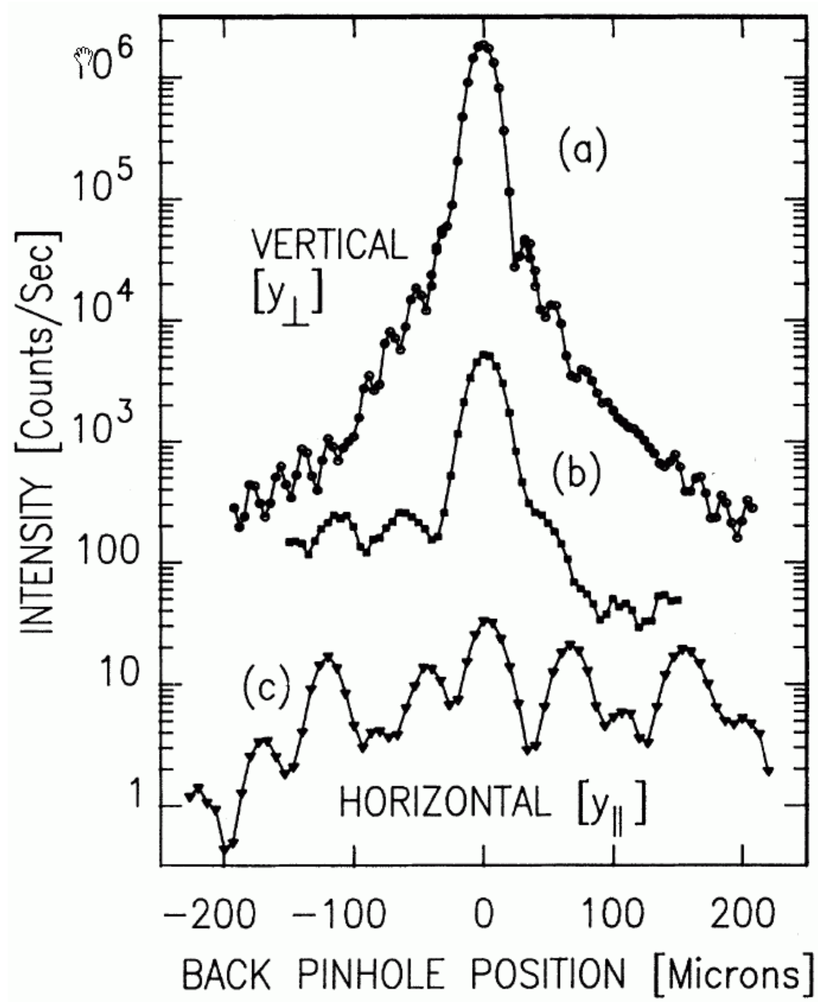
Pinhole Speckle Experiments at “Troika” (ID10A)



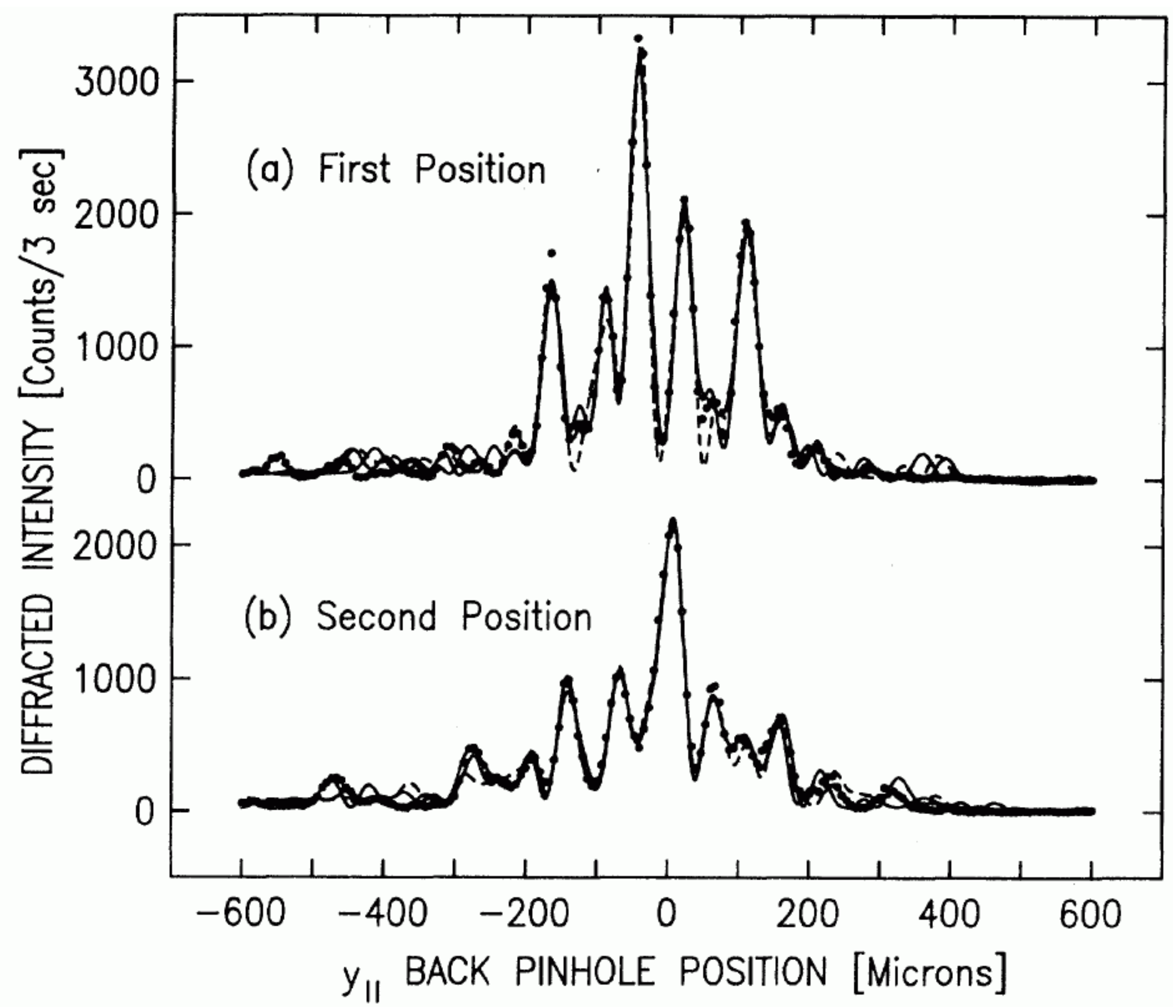


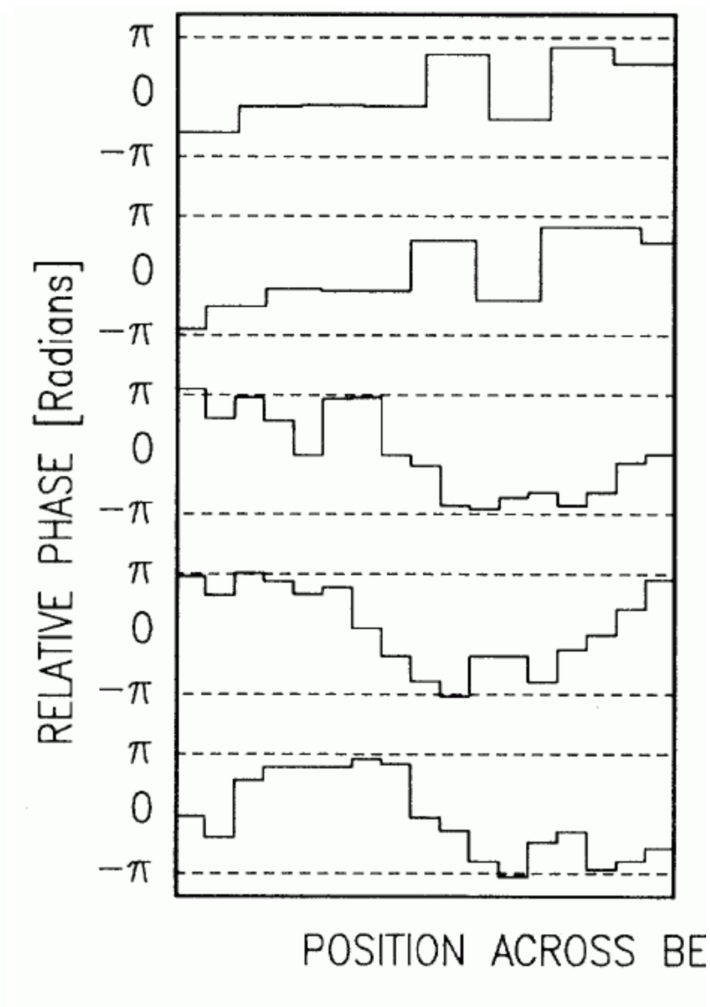
Pinhole speckle from multilayer





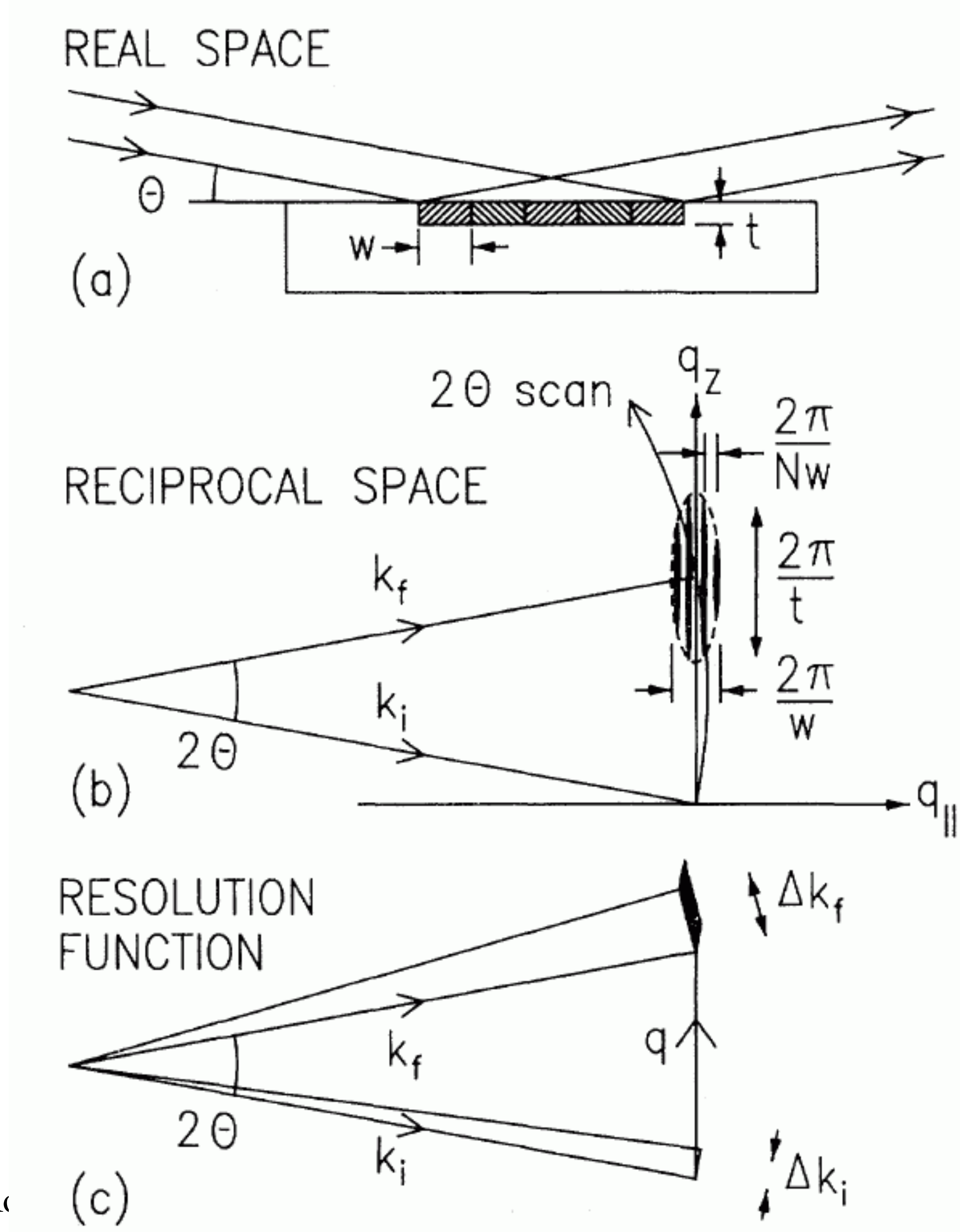
Fitting of speckle with block phase model





Jens' contribution

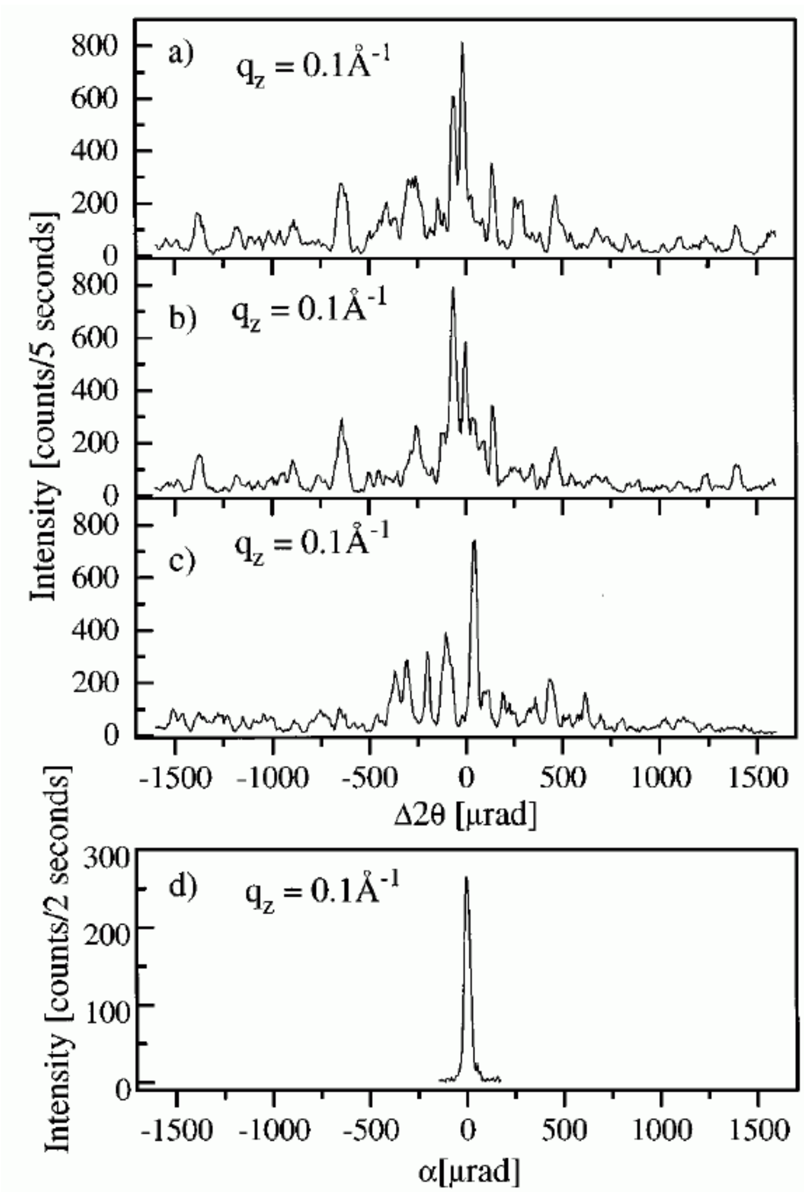
Rigorous diffraction analysis

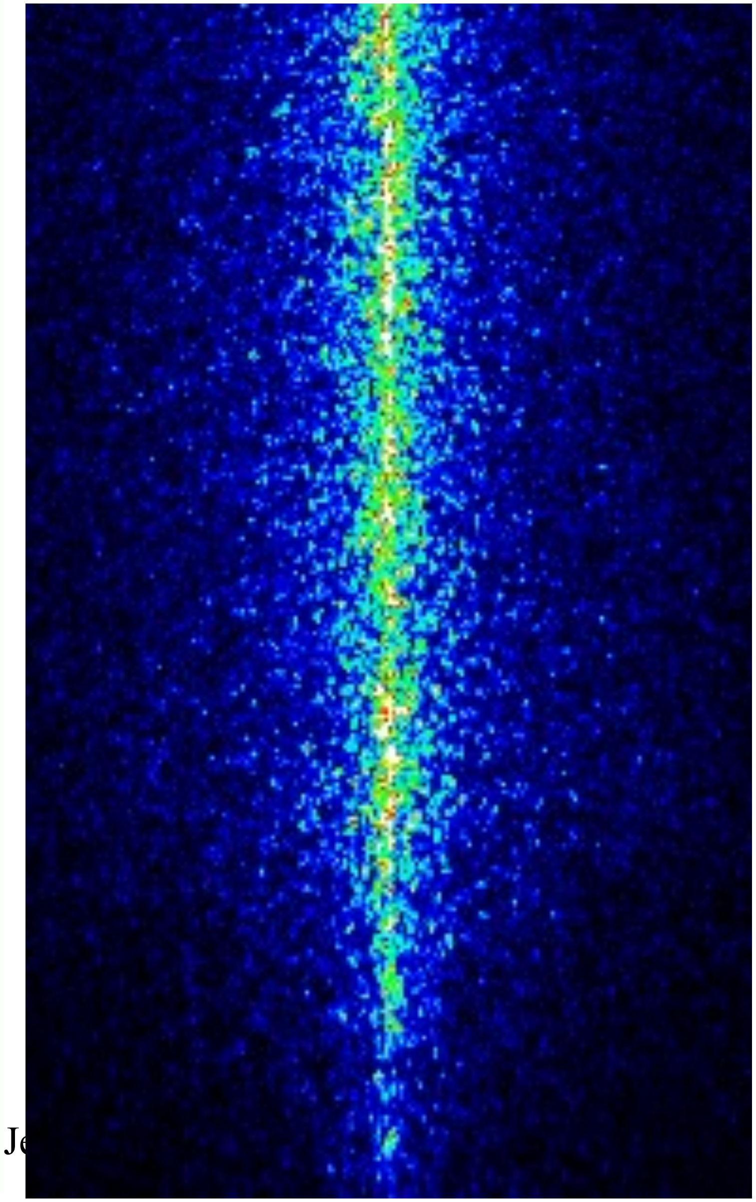


I. K. R

Speckle in Reflectivity from Si

J. L. Libbert et al Phys. Rev. B <u>56</u> 6454 (1997)

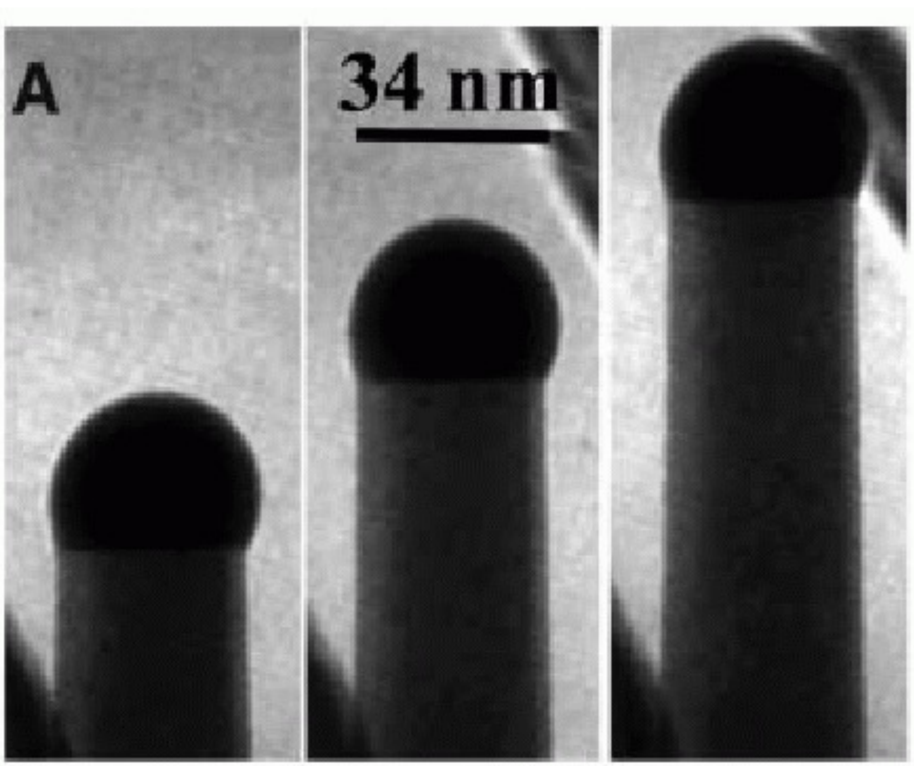


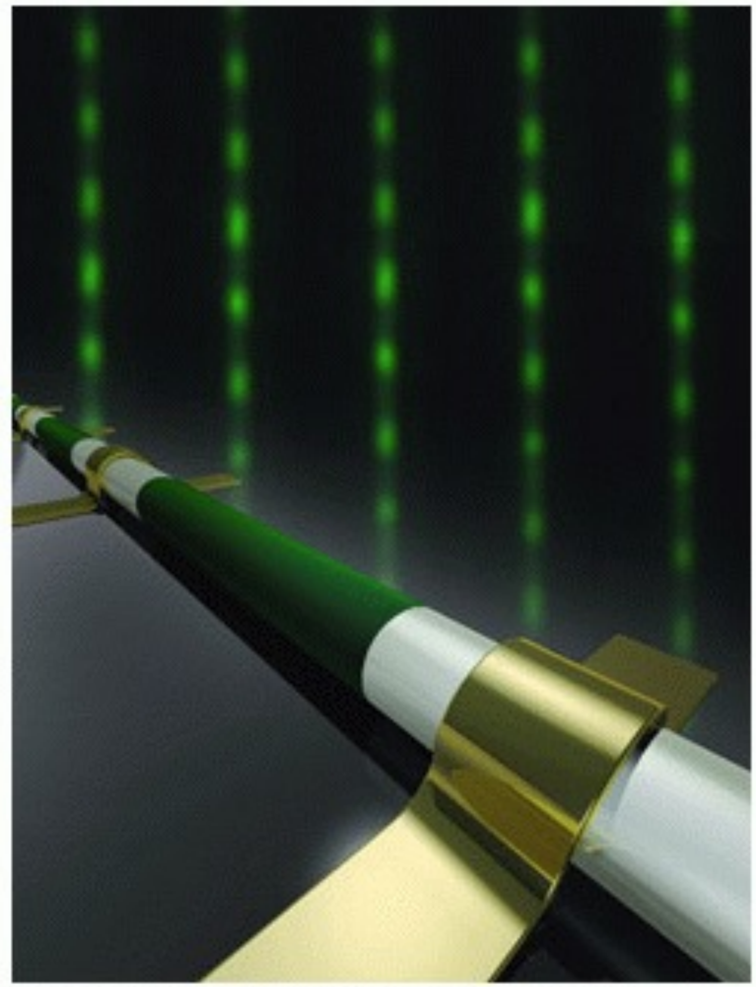


fe1103-24.spe 1x1 20 micron 20s x 31acc

VLS growth of nanowires

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



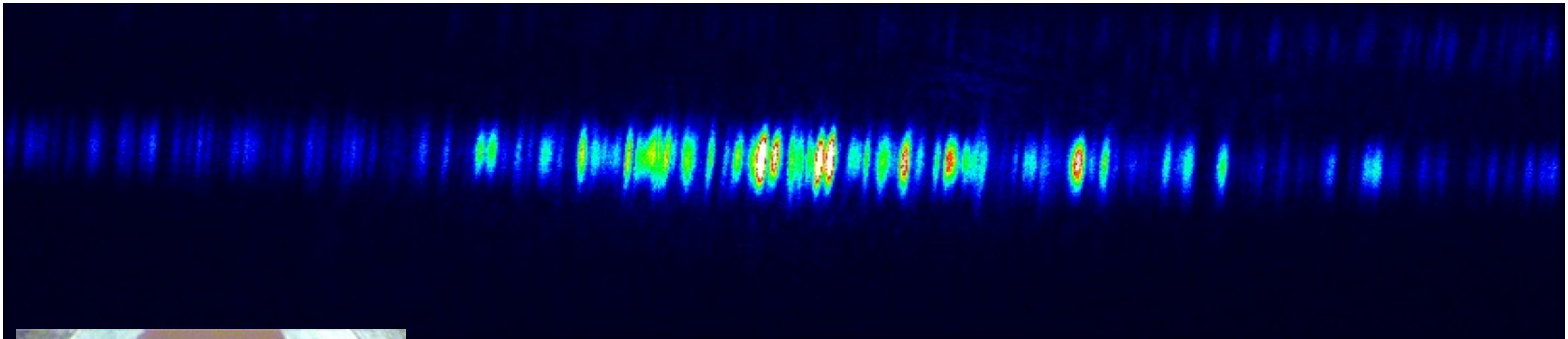


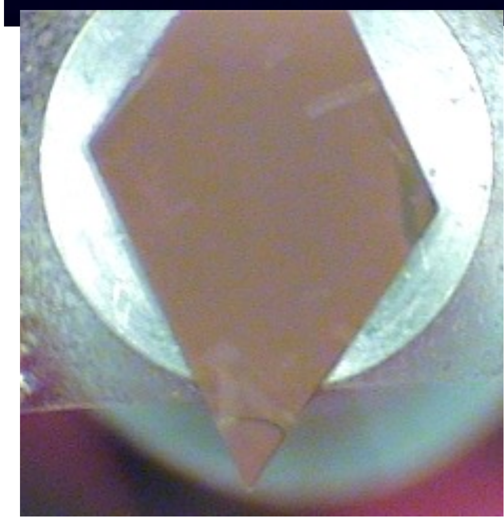
NiSi/Si nanowire heterostructure devices. *Nature* **430**, 61 (2004).

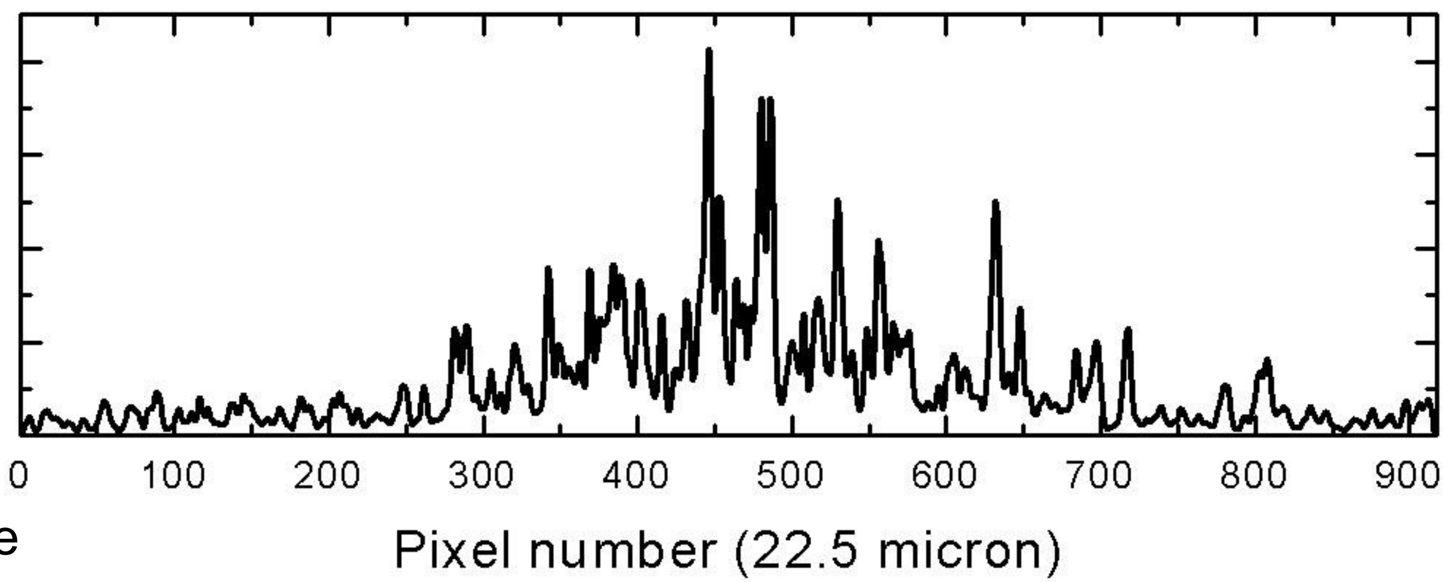
I. K. Robinson, Jens-Day

GaAs Nanowire "Barcode"

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



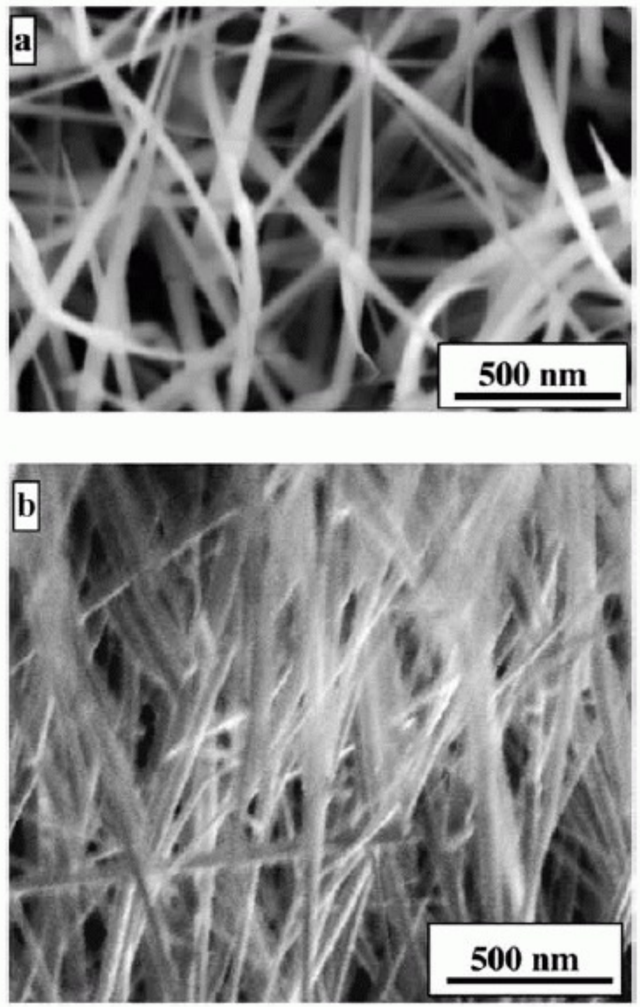


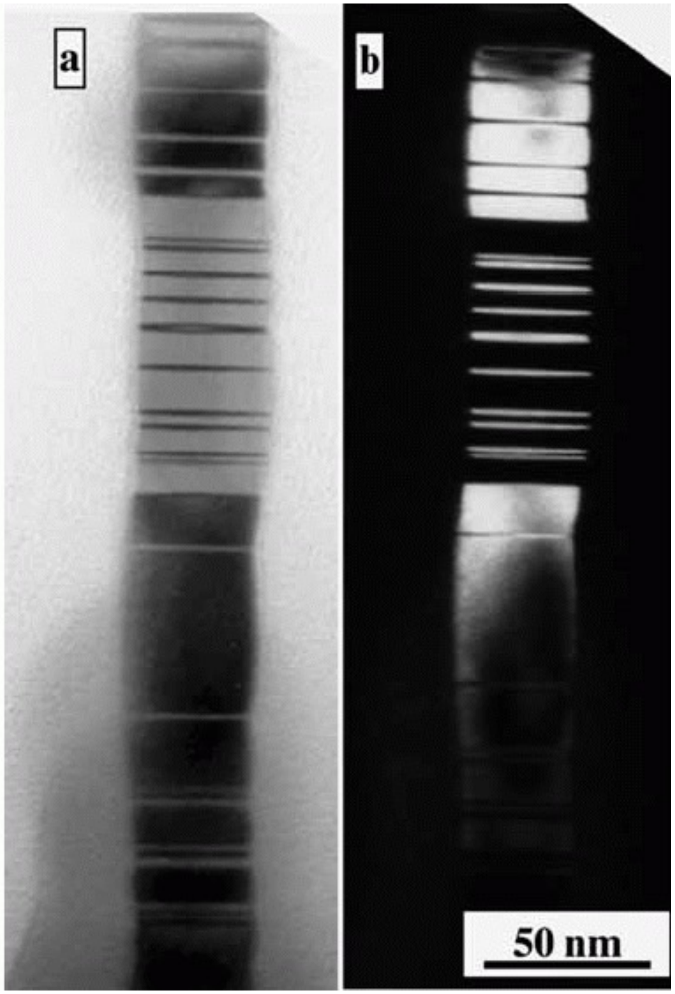


GaAsNW1106-22.spe
B9348 from Philips

Dark Field TEM of GaAs Nanowires

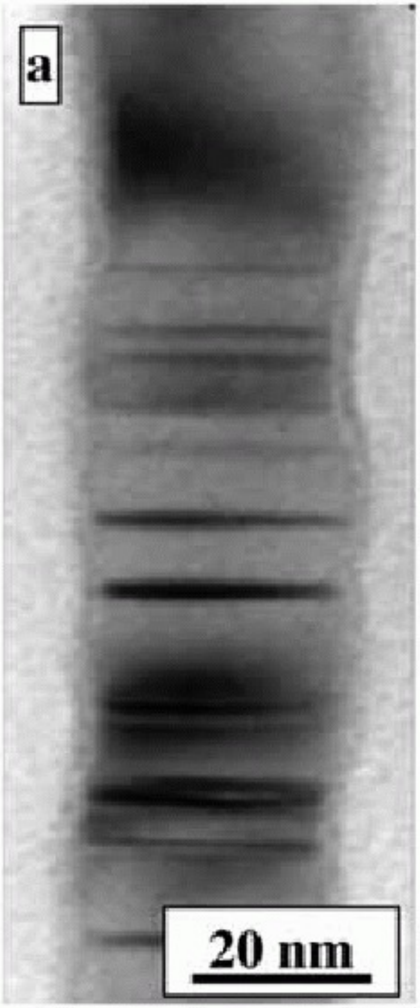
R. Banerjee et al, Phil. Mag. Lett. <u>86</u> 807 (2006)

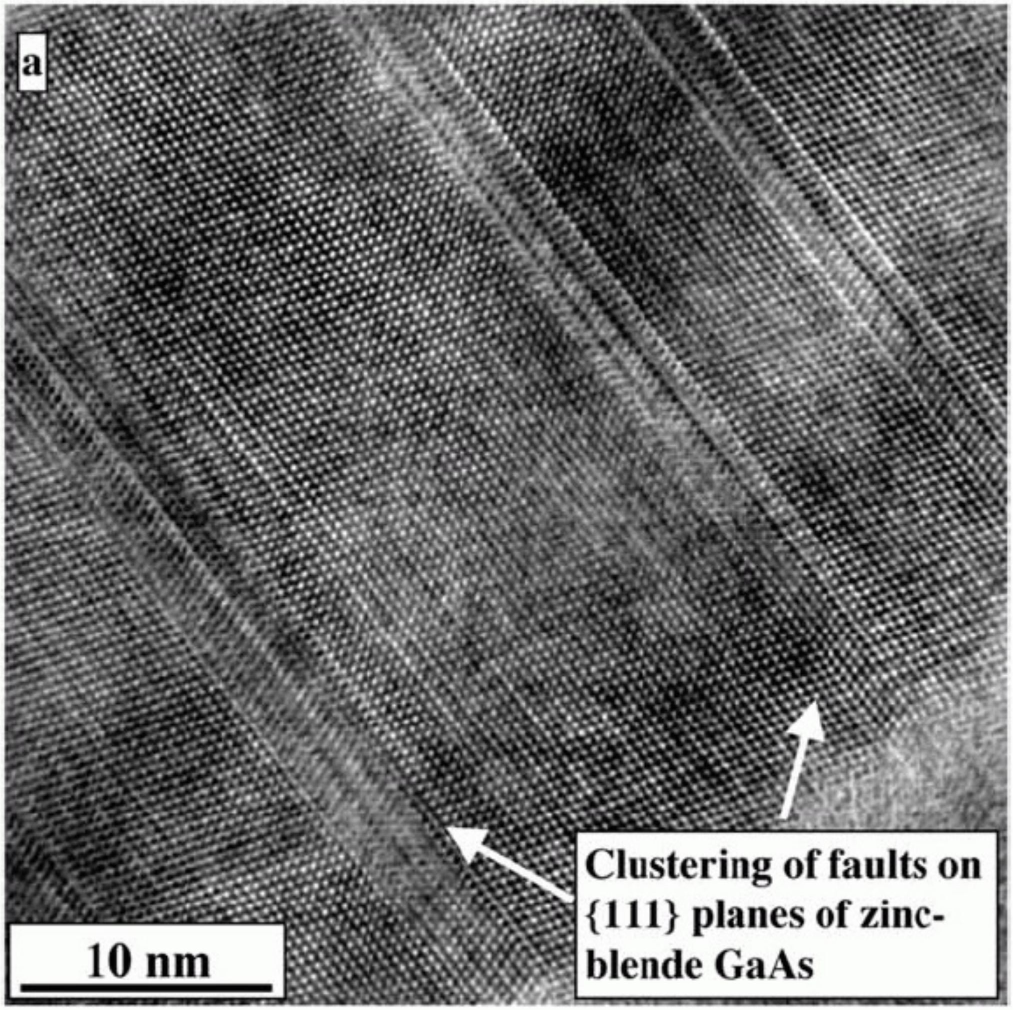




Dark Field TEM of GaAs Nanowires

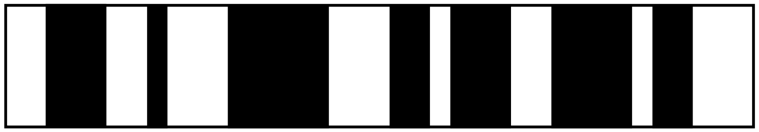
R. Banerjee et al, Phil. Mag. Lett. 86 807 (2006)



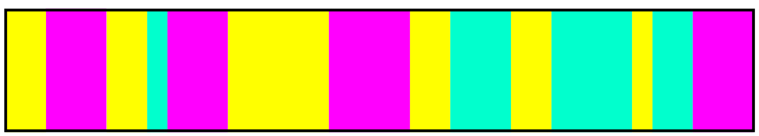


Models of Barcode Diffraction

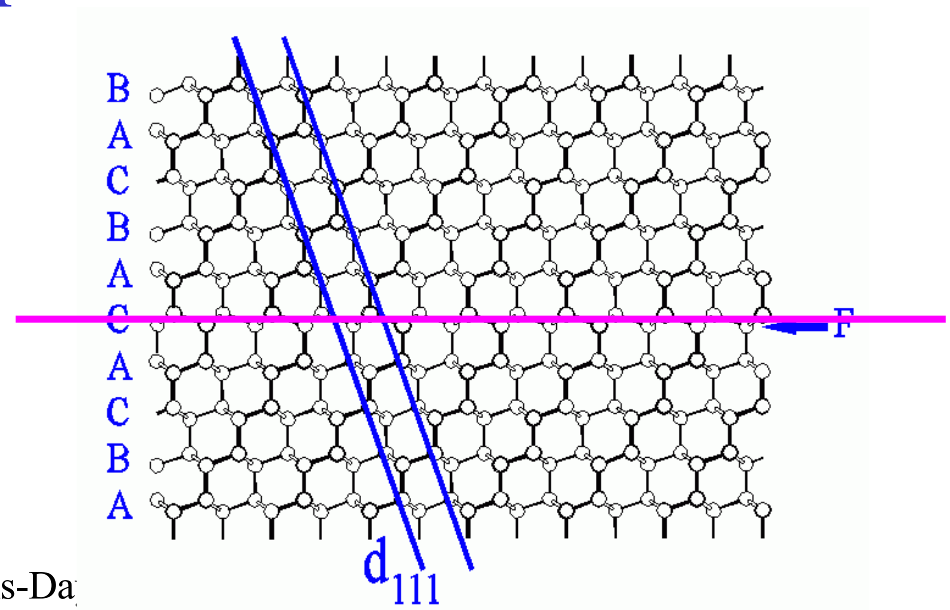
(111) wires at (11-1) reflection



- Twinned stacking sequence



- Deformation faults



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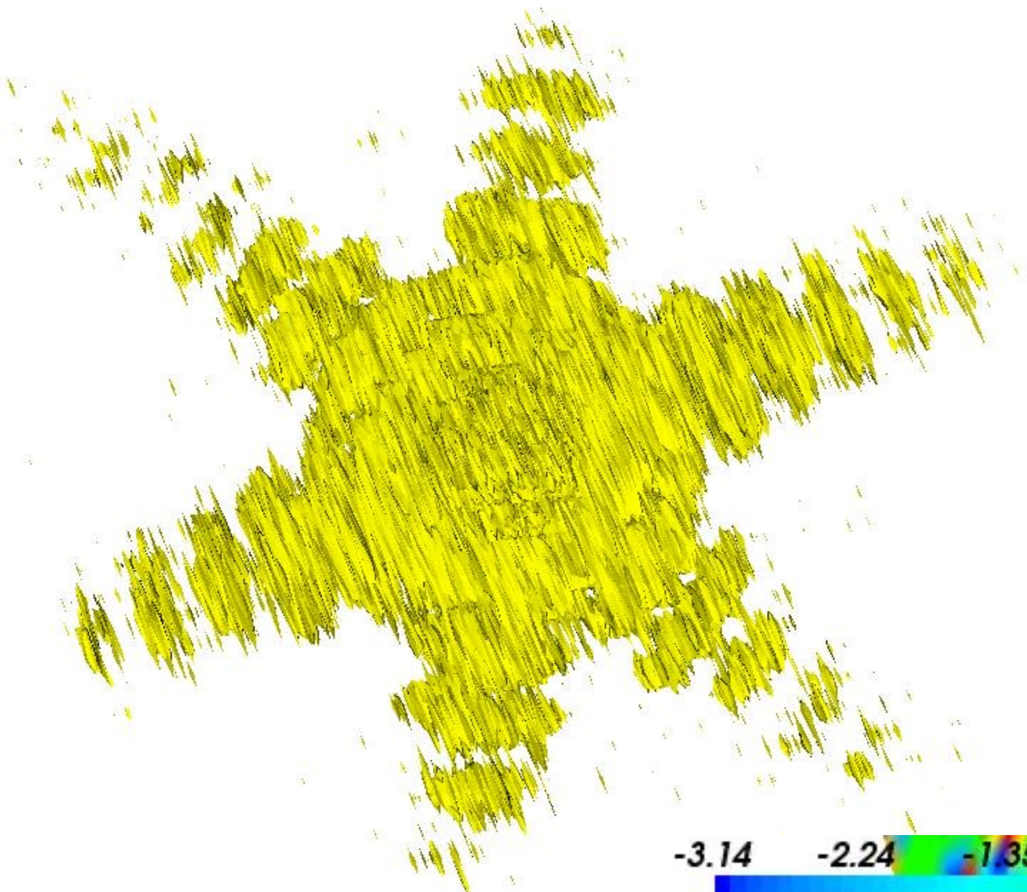
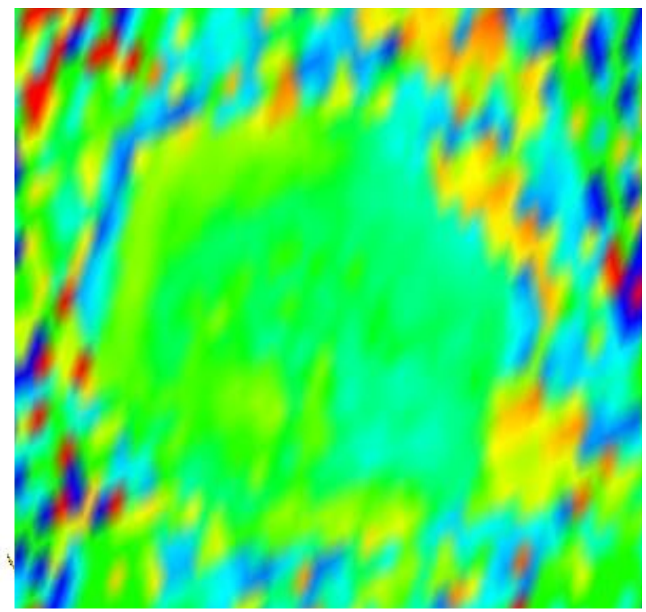
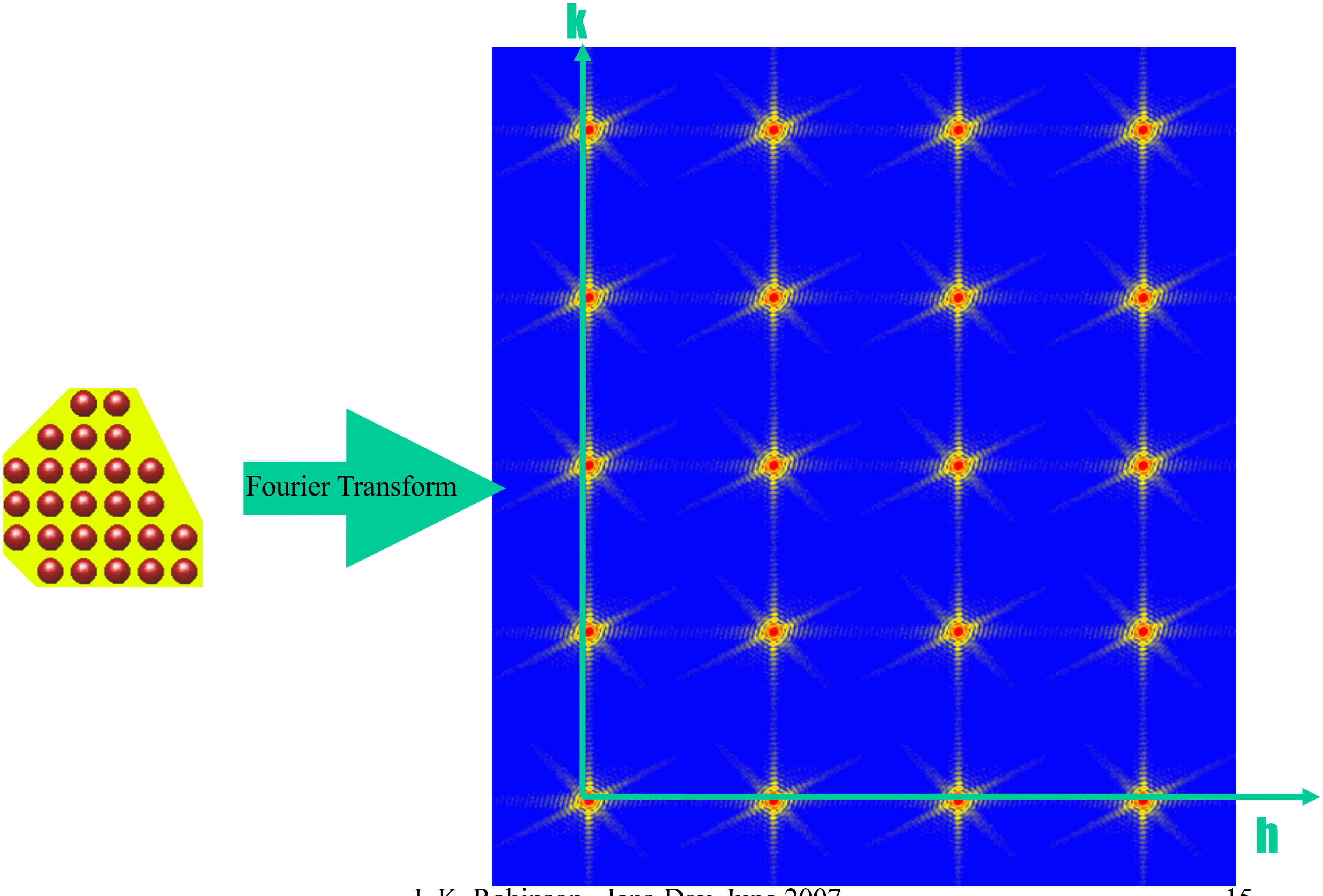
ZnO Nanowire Reconstruction

Ross Harder, Steven Leake, PhD project at UCL

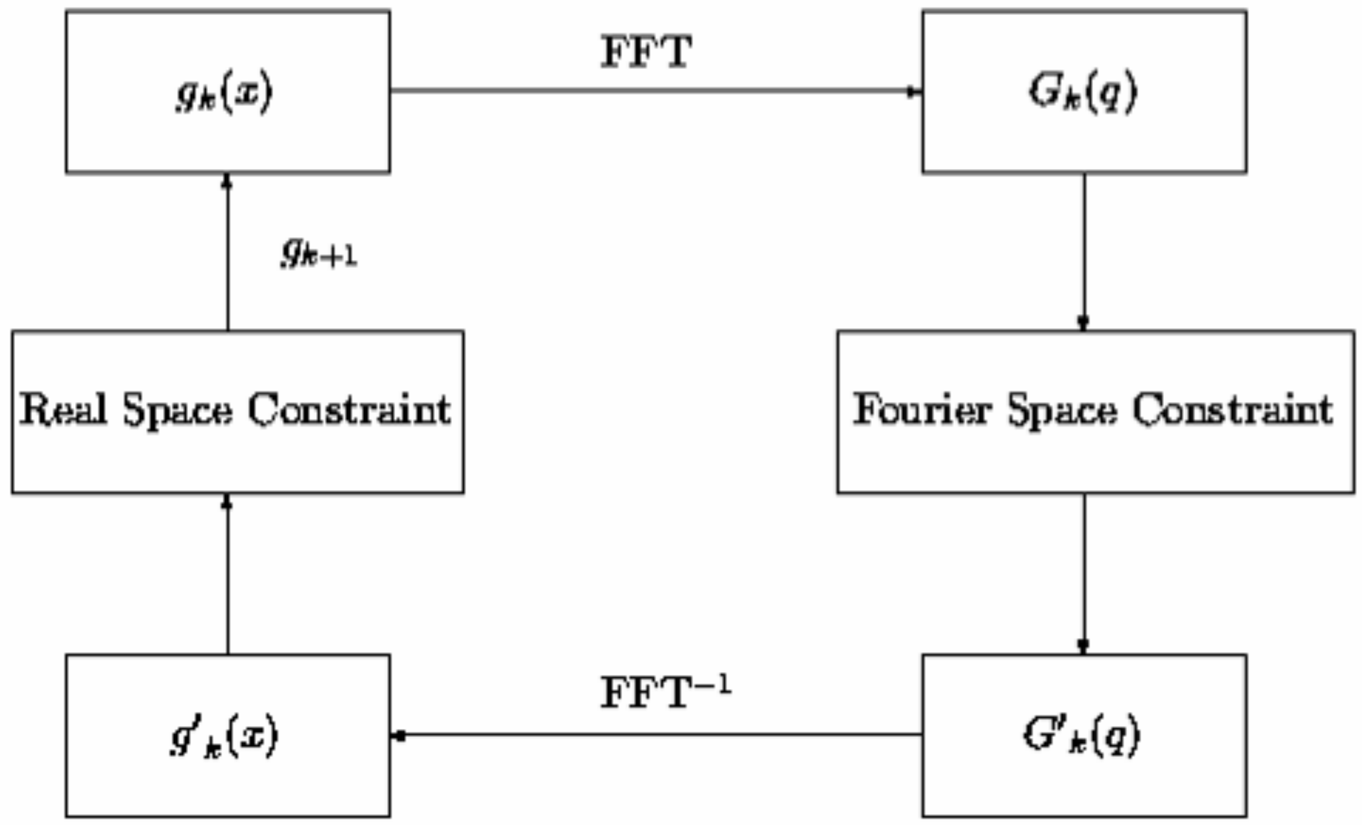




Coherent Diffraction from Crystals



Generic "Error Reduction" method



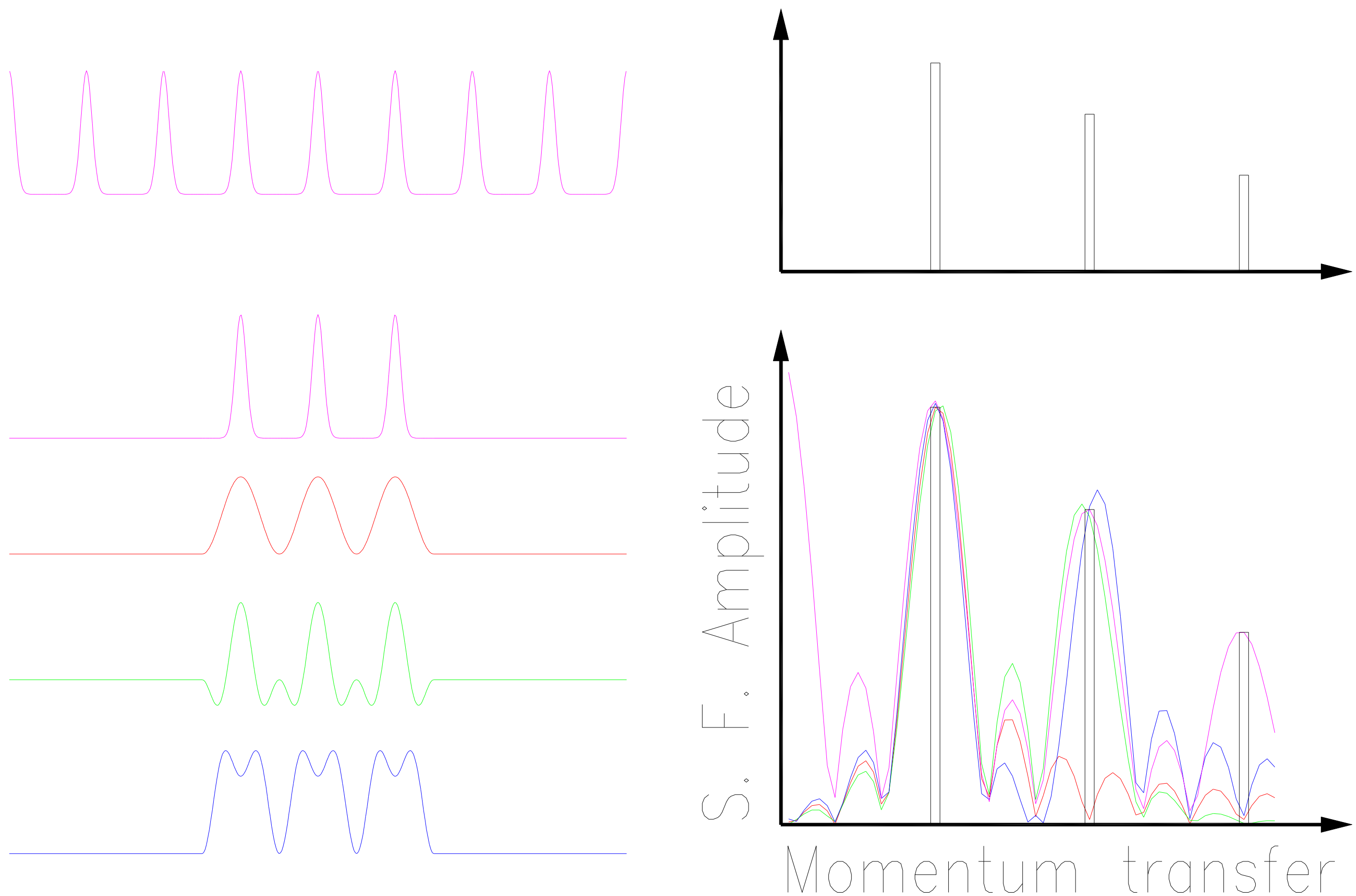
J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

Real-space Constraints in Crystallograhy

R. P. Millane, J. Opt. Soc Am. A **13** 725 (1996)

- 'Positivity' and 'Atomicity' constraints (Sayre)
- Finite support, molecular envelope
- Solvent flattening/Molecular replacement
- Non-crystallographic symmetry
- Non-uniqueness is 'pathologically rare' (d>1)
- Uses memory to avoid stagnation (Fienup HIO)

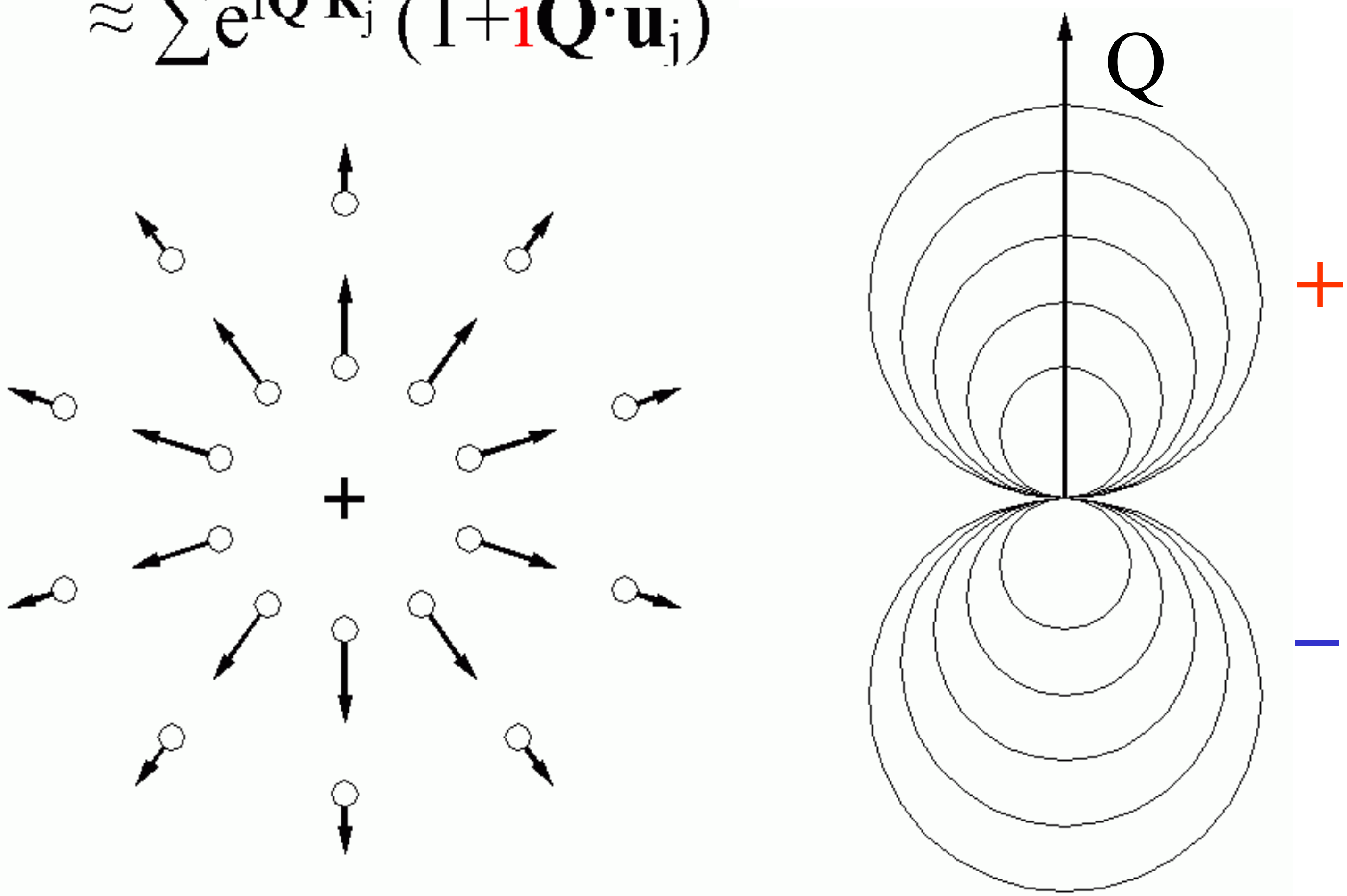
Oversampling solves Phase Problem



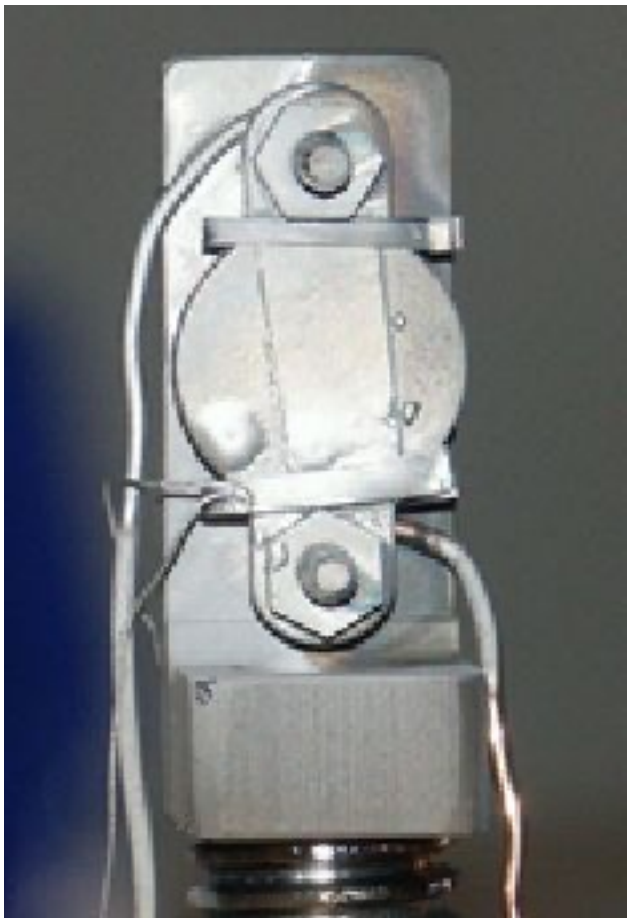
Diffraction by Strain of Point Defect

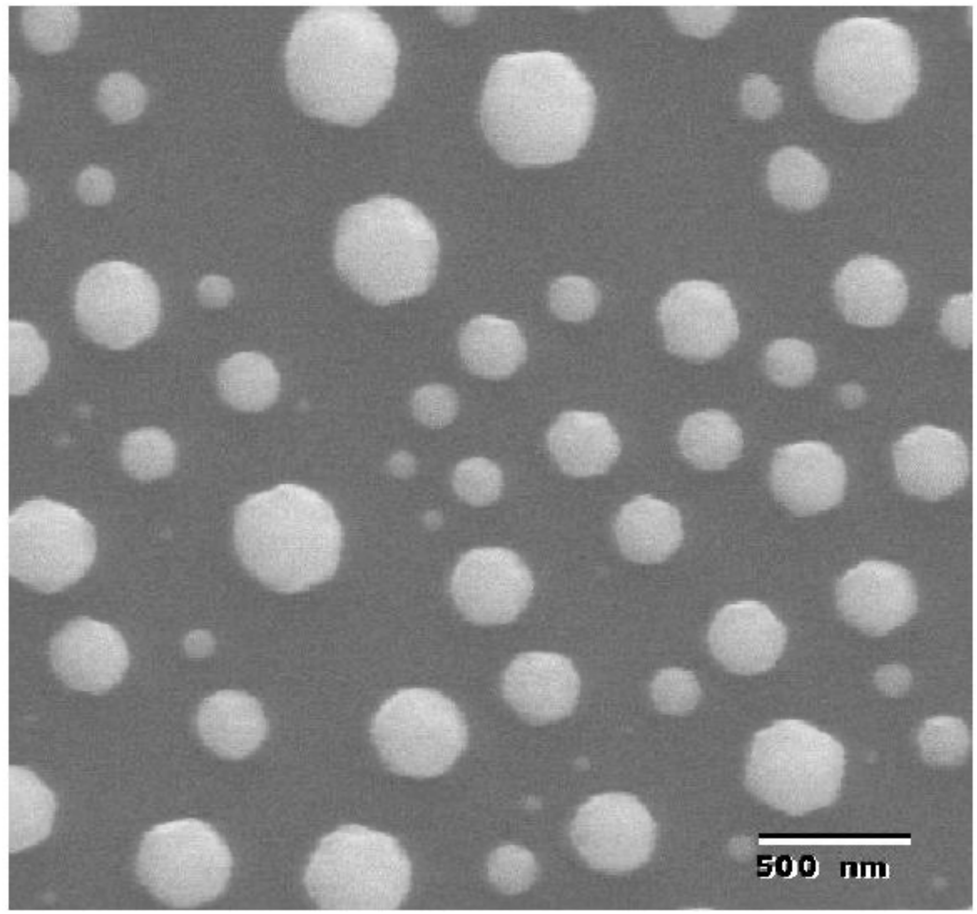
$$A \sim \sum e^{i\mathbf{Q}\cdot(\mathbf{R}_j+\mathbf{u}_j)}$$
$$\approx \sum e^{i\mathbf{Q}\cdot\mathbf{R}_j}\,(1+i\mathbf{Q}\cdot\mathbf{u}_j)$$

Imaginary density



In situ growth of Pb crystals





Good statistics, 3D diffraction data

Mark Pfeifer, Garth Williams, Ivan Vartaniants, Ross Harder

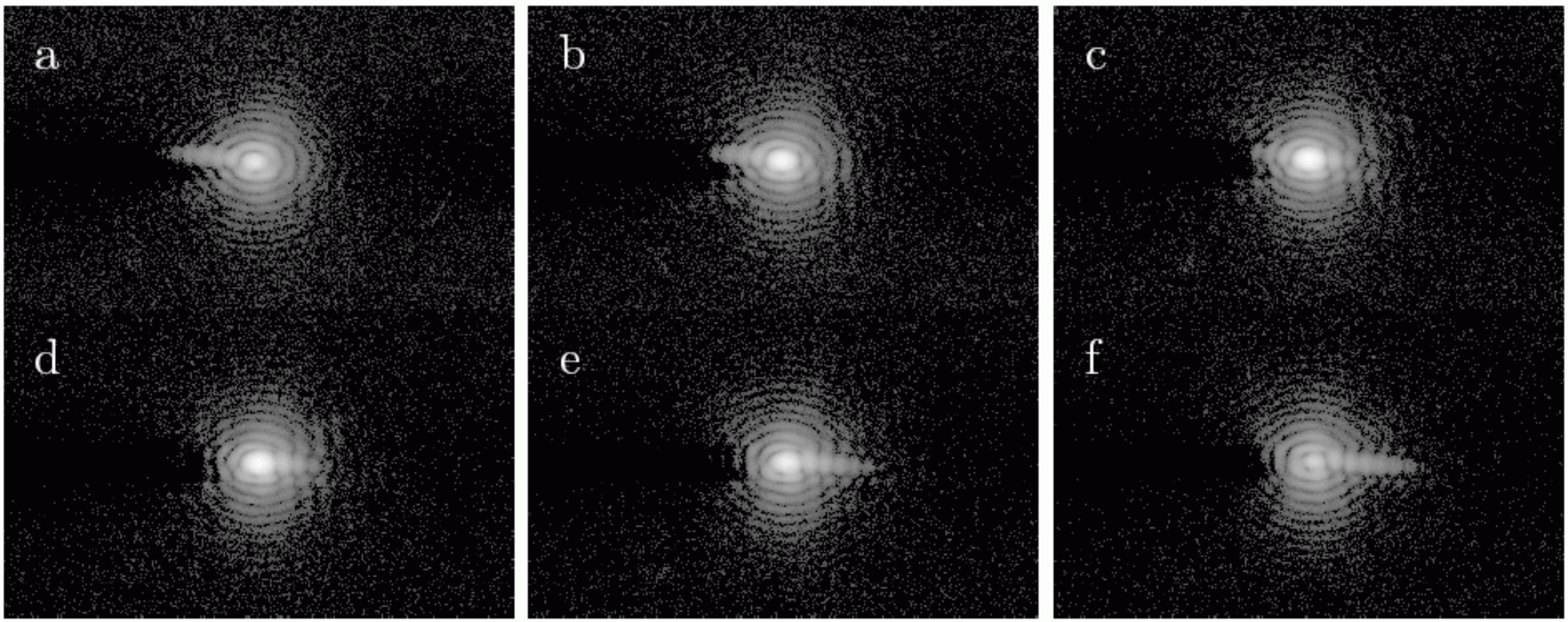
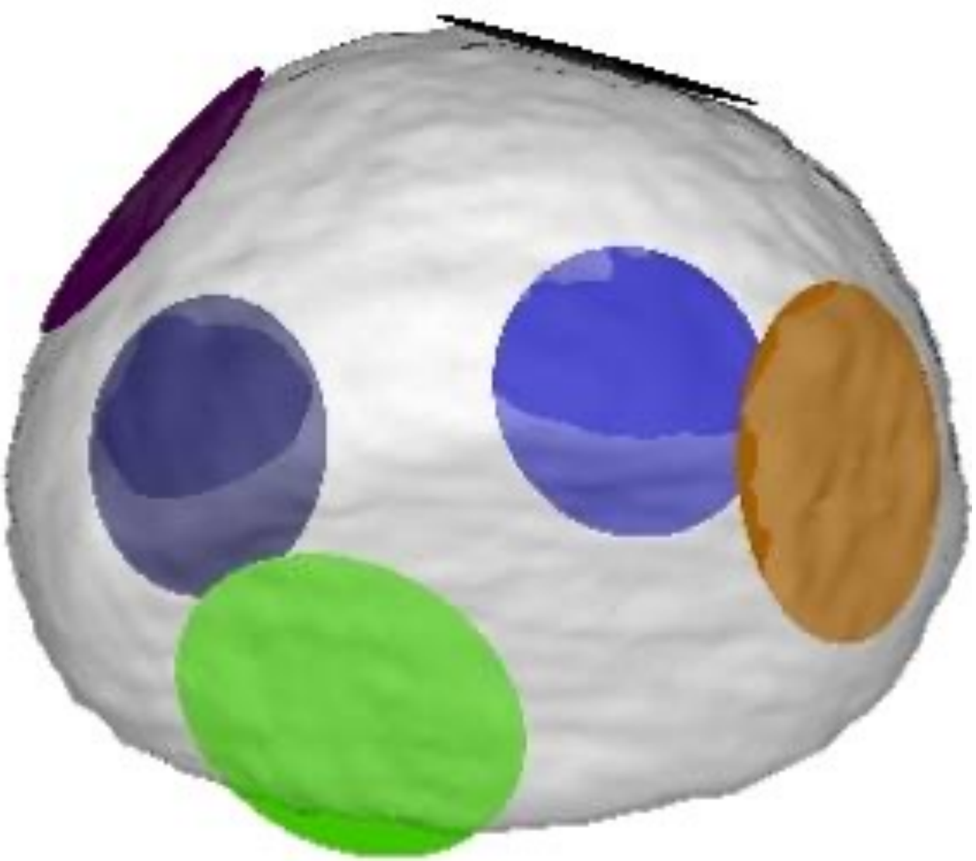
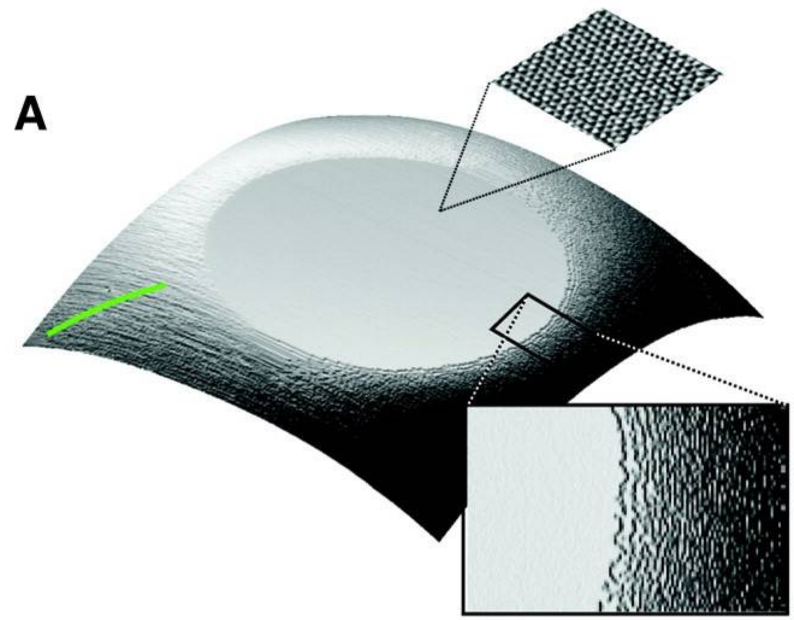


Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

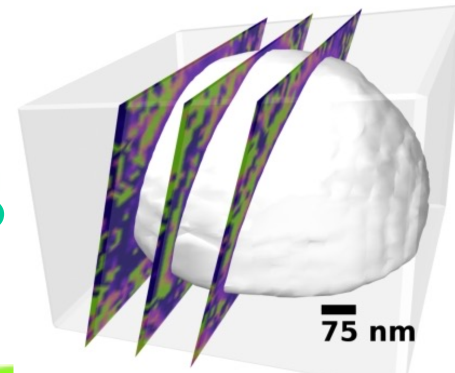
Facets of Equilibrium Crystal Shape

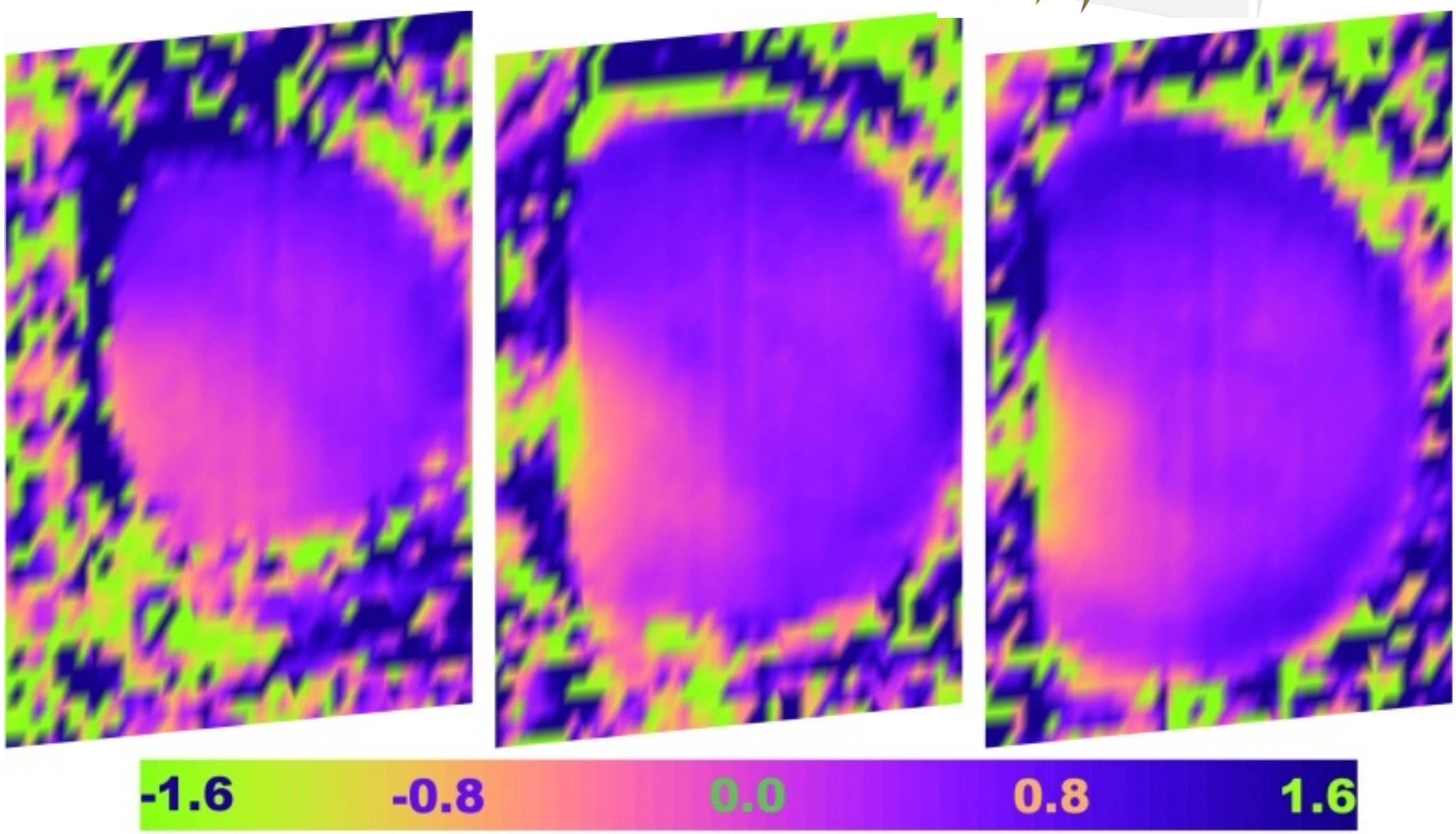


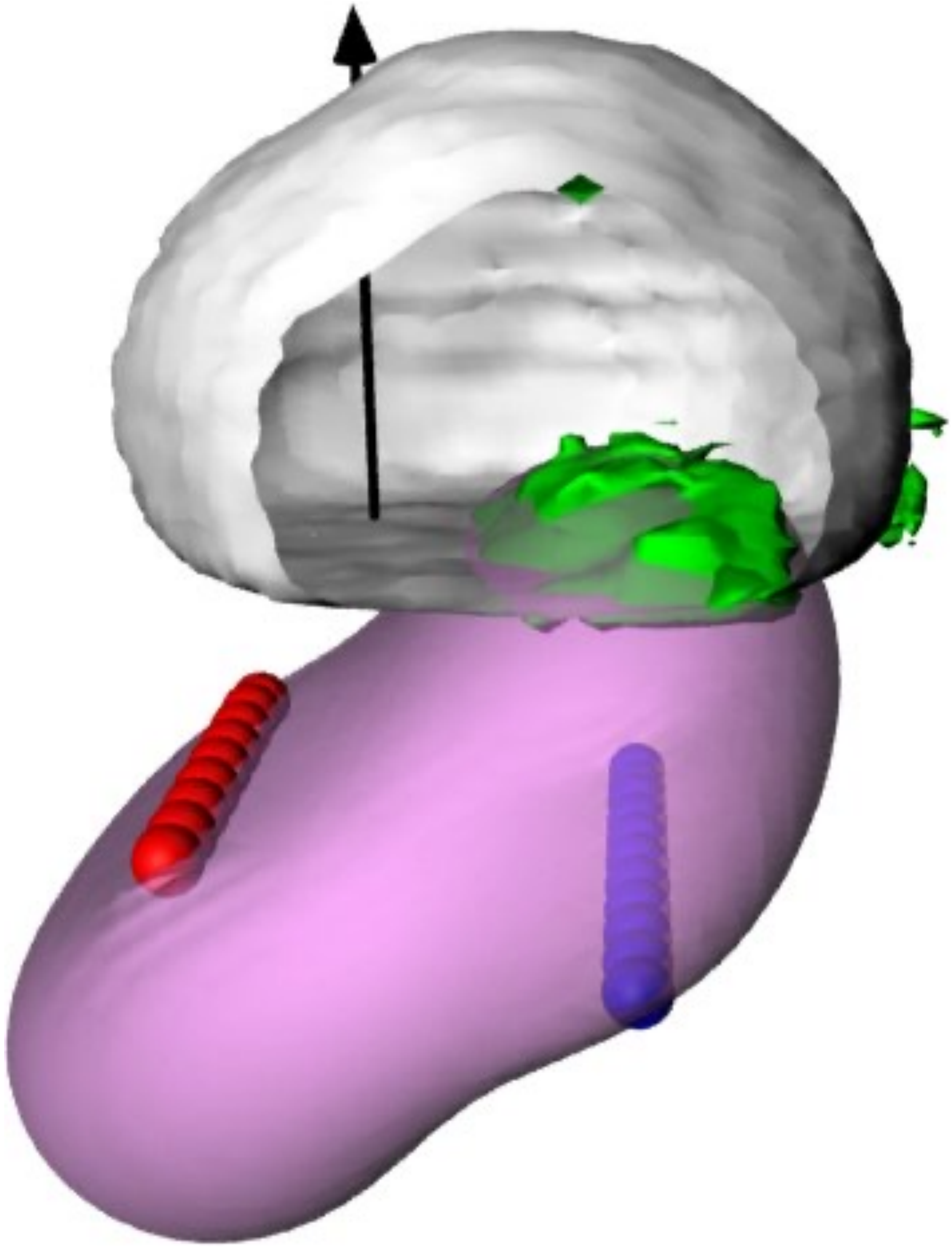


Thurmer K, Williams E, Reutt-Robey J
Science **297** 2033 (2002)

3D phase map sections

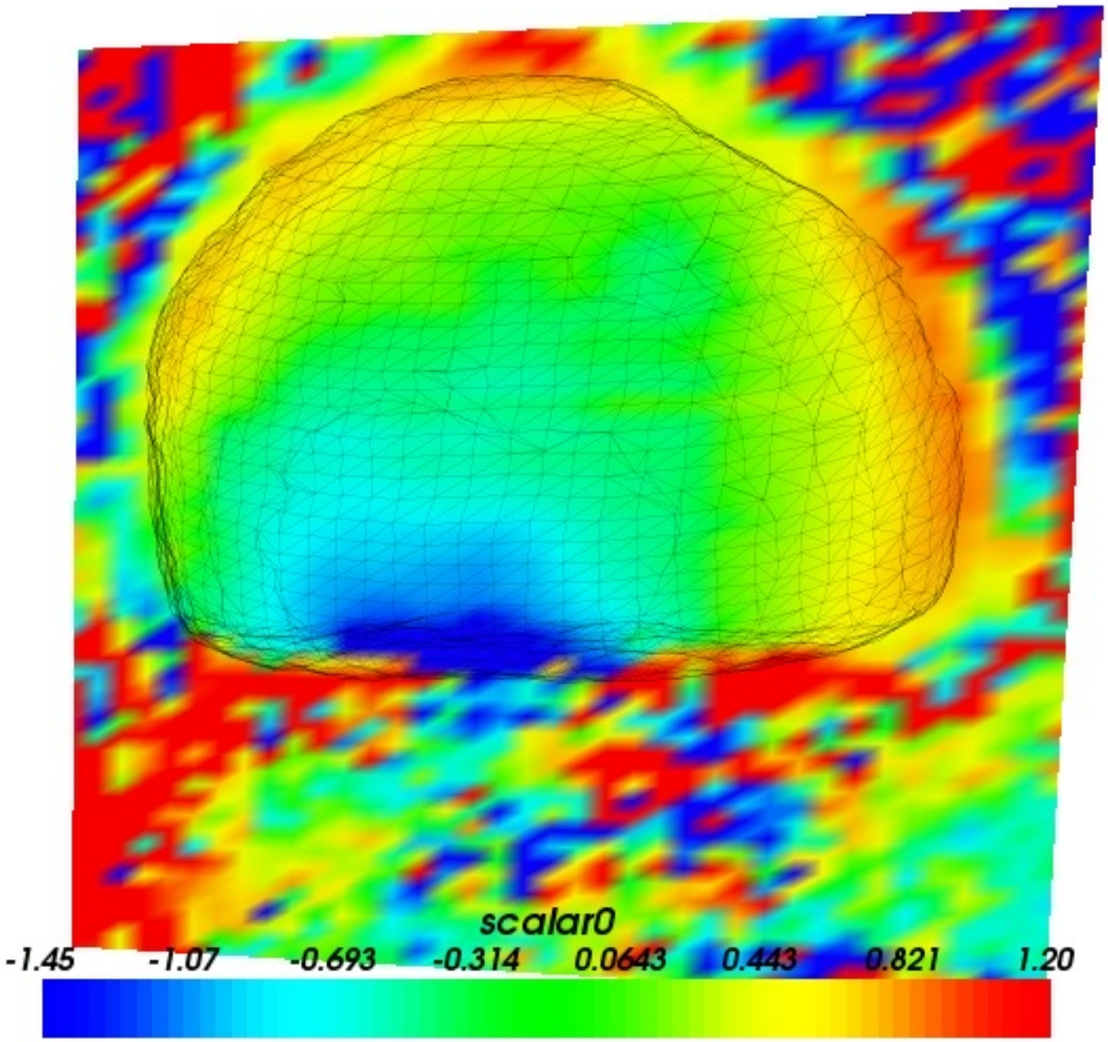






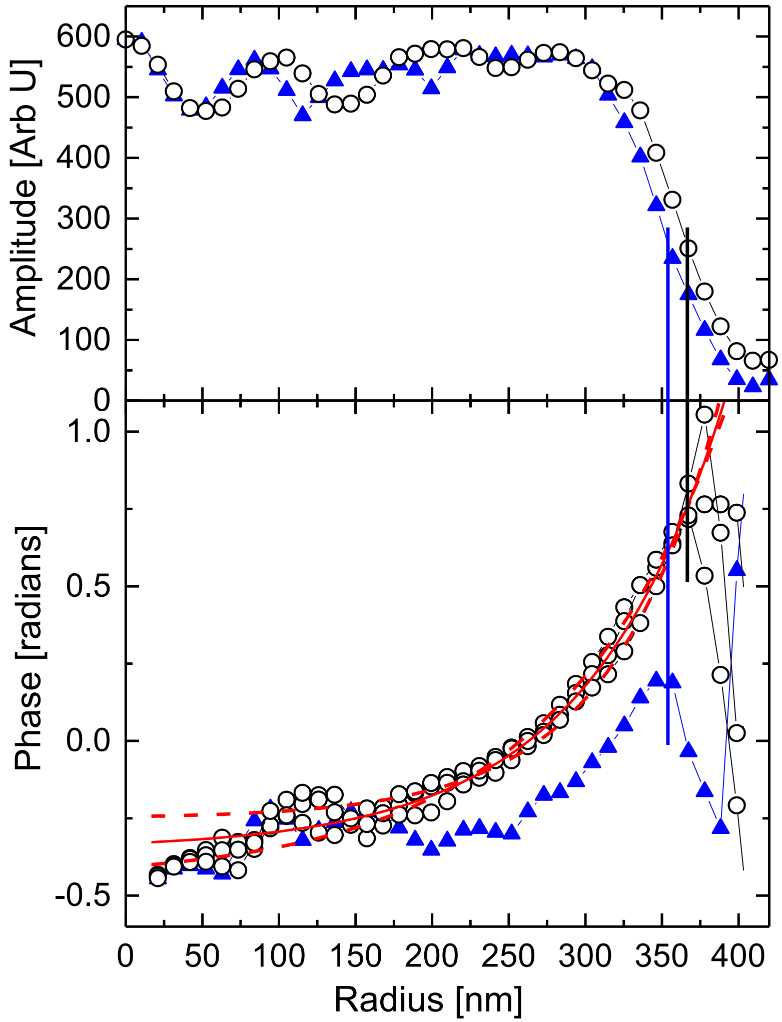
Contours showing Positive Phase

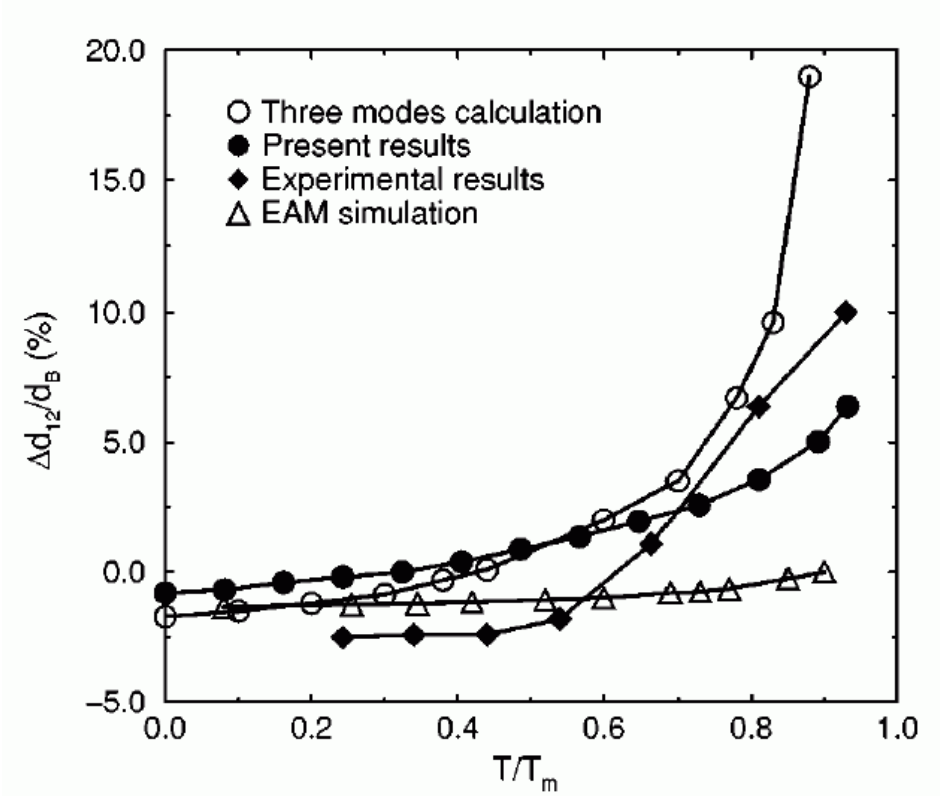
including correction for refraction by crystal



Surface Thermal Expansion

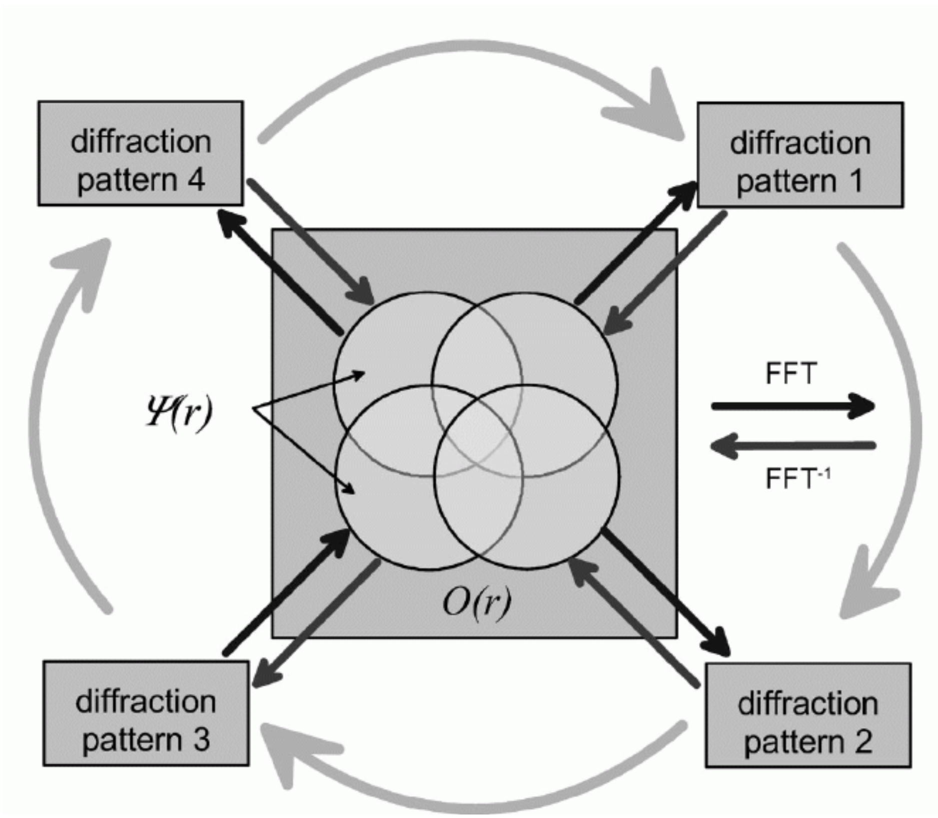
Ag(111): Scheffler et al PRB 59 970 (1999)

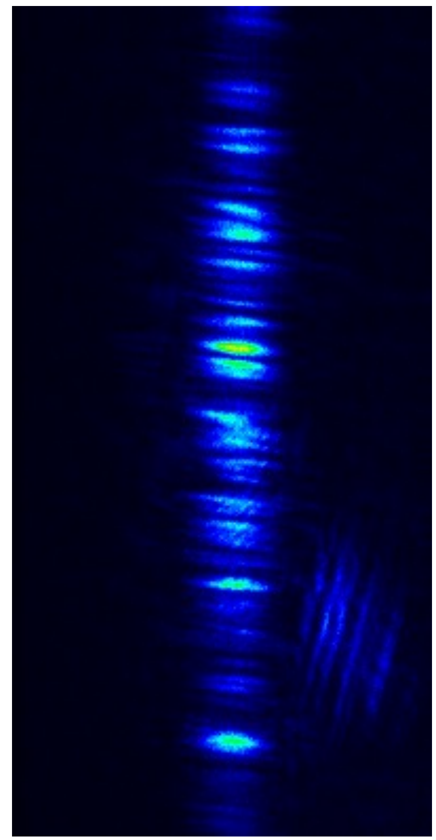




Future of CXD: Ptychography

Rodenburg & Pfeiffer, PRL (2007)





Conclusions

- Coherent diffraction from rough surfaces
- Nanowire “barcode” from stacking faults
- Wire cross sections show strain
- Strain fields imaged from asymmetric patterns
- Contact forces cause strain inside crystal
- Surface strain has orientation dependence