

Coherent diffraction analysis of dislocation arrays in GeSi thin films

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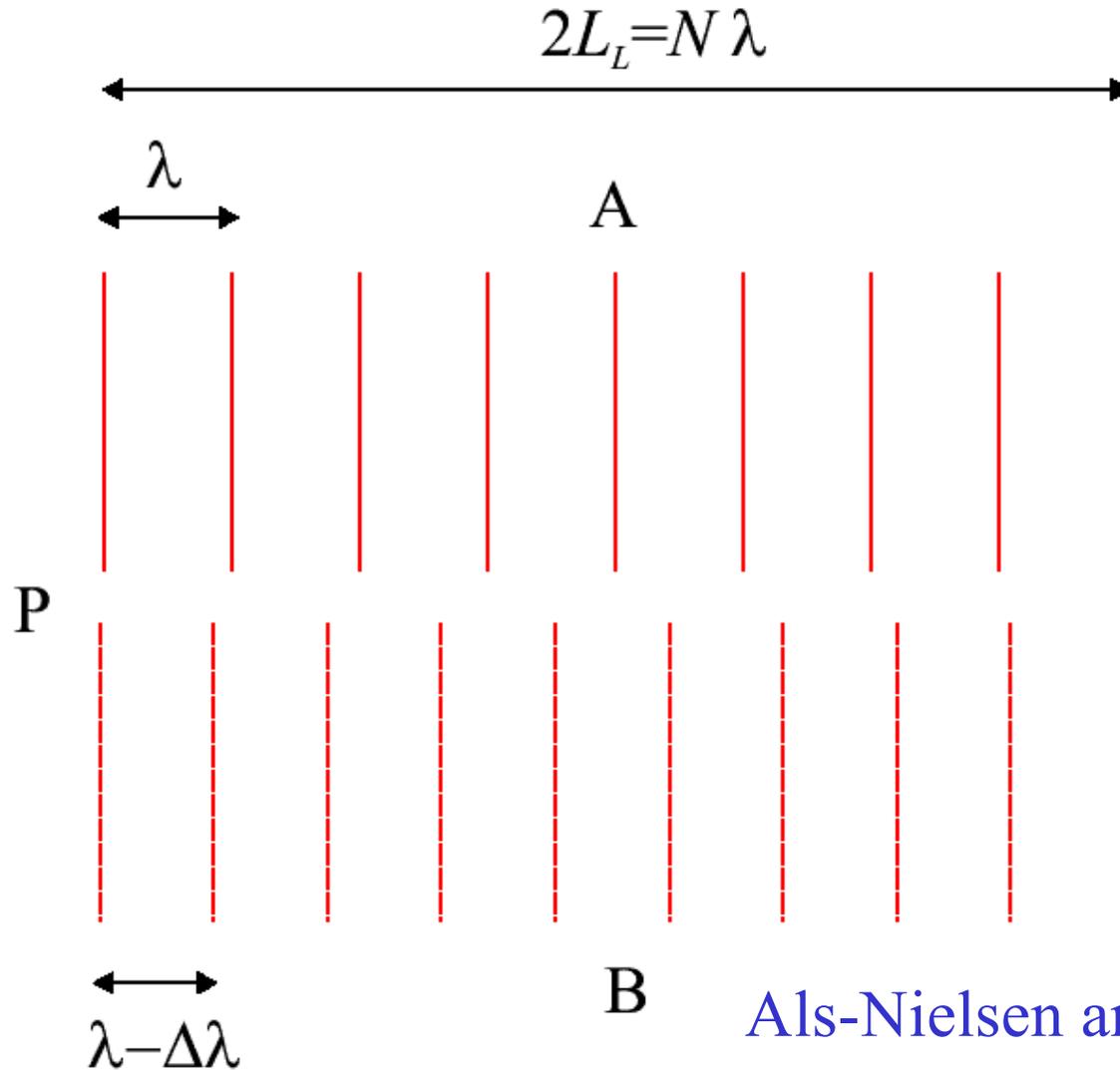
XTOP-04, Pruhonice

September 8, 2004

Outline

- Coherence in Diffraction
- How to Solve the **Phase** Problem
- Nanocrystal Shapes
- Use of Optics in CXD
- Diffraction from **Phase** Objects

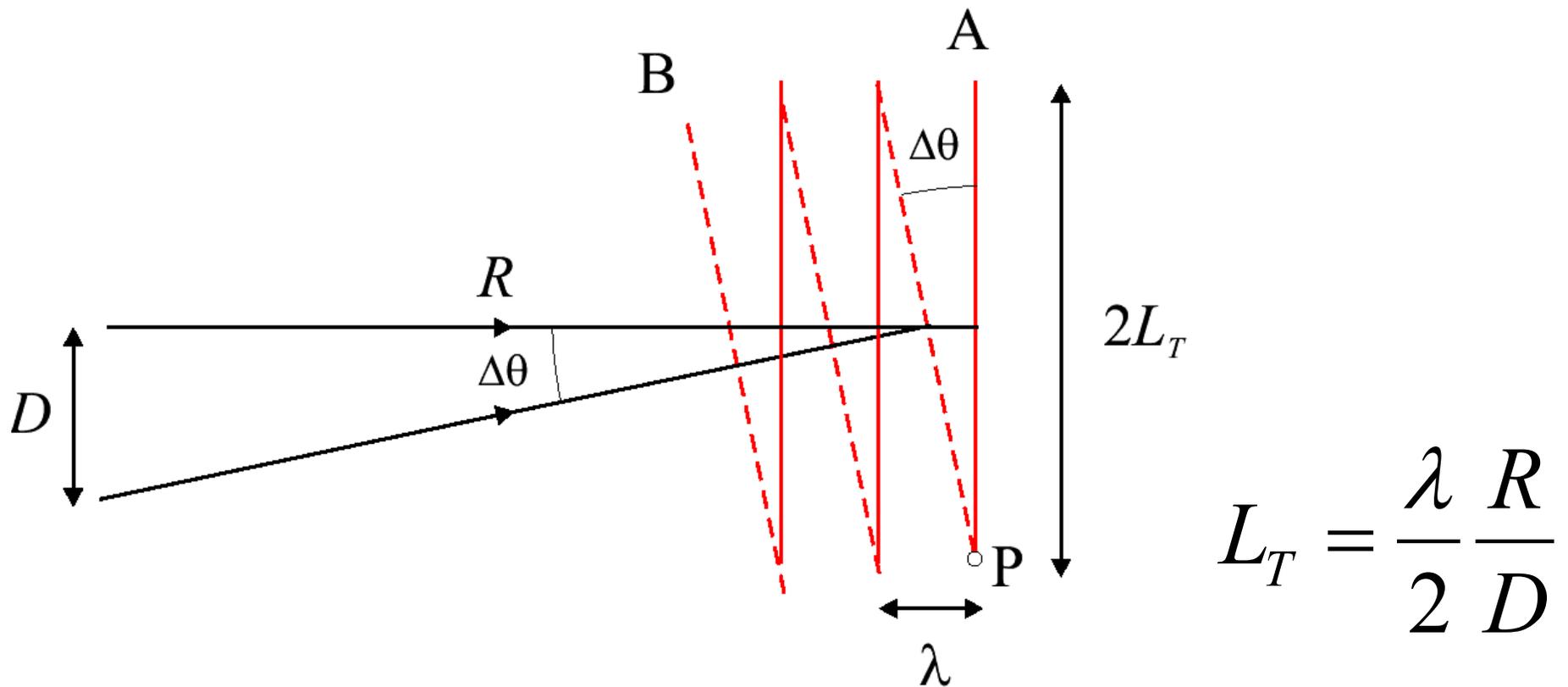
Longitudinal Coherence



$$L_L = \frac{1}{2} \frac{\lambda^2}{\Delta\lambda}$$

Als-Nielsen and McMorro (2001)

Lateral (Transverse) Coherence



$$L_T = \frac{\lambda R}{2 D}$$

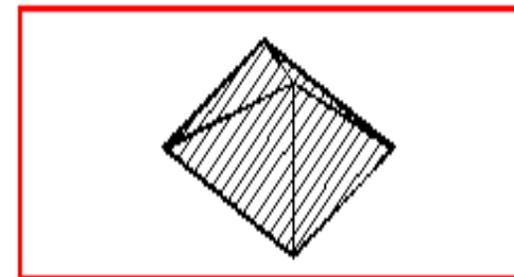
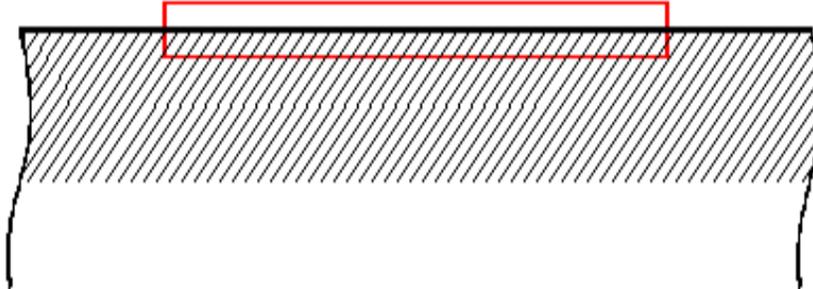
Als-Nielsen and McMorrow (2001)

Coherence at the APS or ESRF

Typical of 3rd Generation (undulator) Synchrotron Source

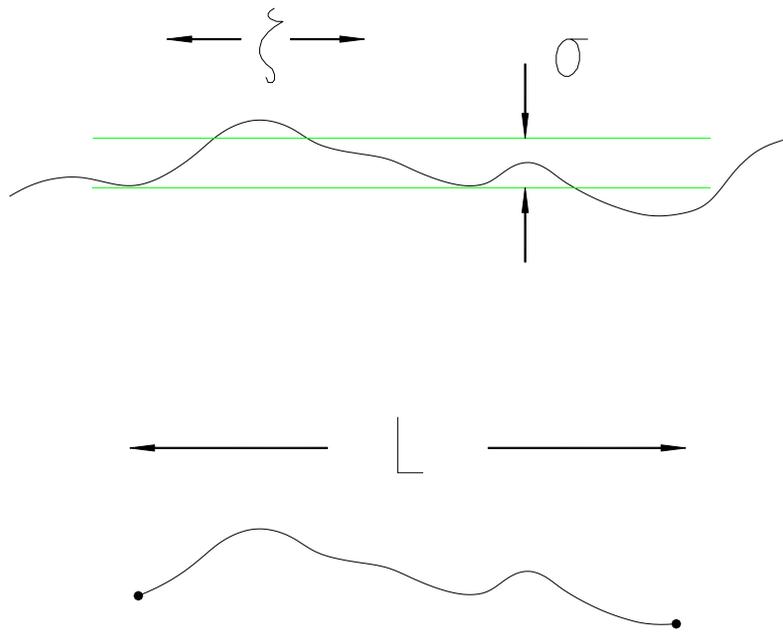
Coherence of	ξ_{VER}	ξ_{HORIZ}	ξ_{LONG}	Flux
Raw Undulator	35 μm	9 μm	0.004 μm	2×10^{12}
Si(111) Monochromator	35 μm	9 μm	1 μm	1×10^{10}
C(111) Monochromator	35 μm	9 μm	3 μm	3×10^9

Coherent region defined by slits

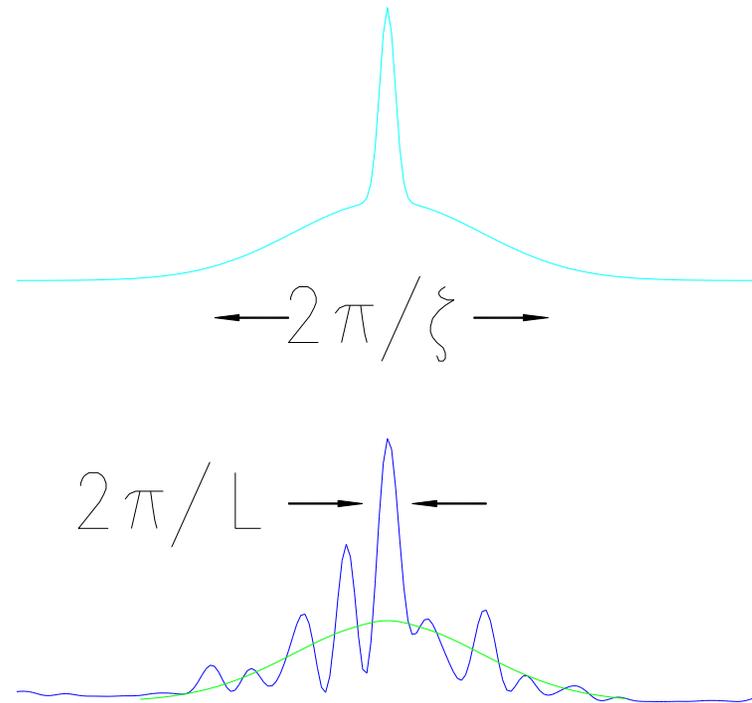


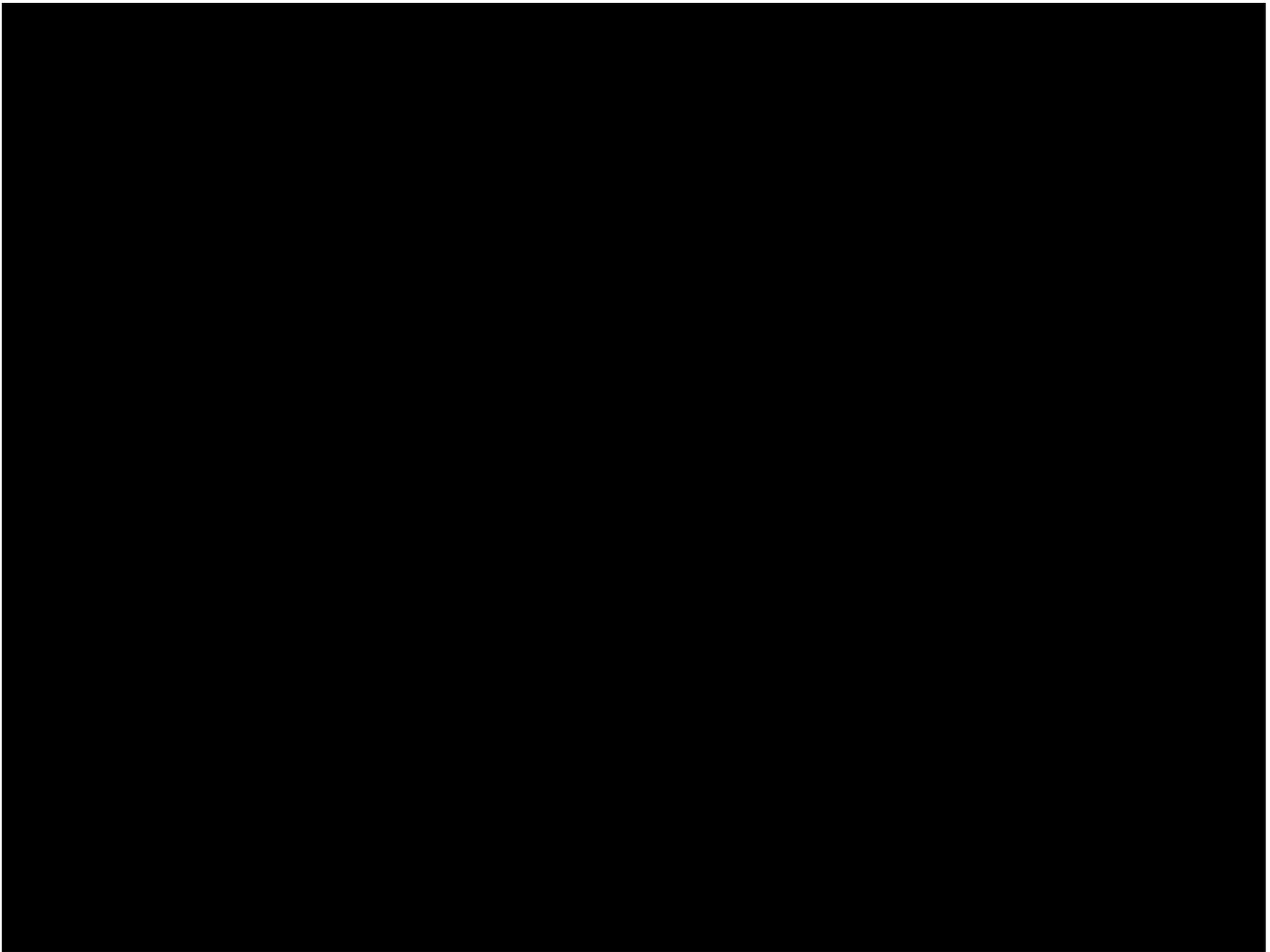
Diffuse Scattering acquires Structure using CXD

Real Space

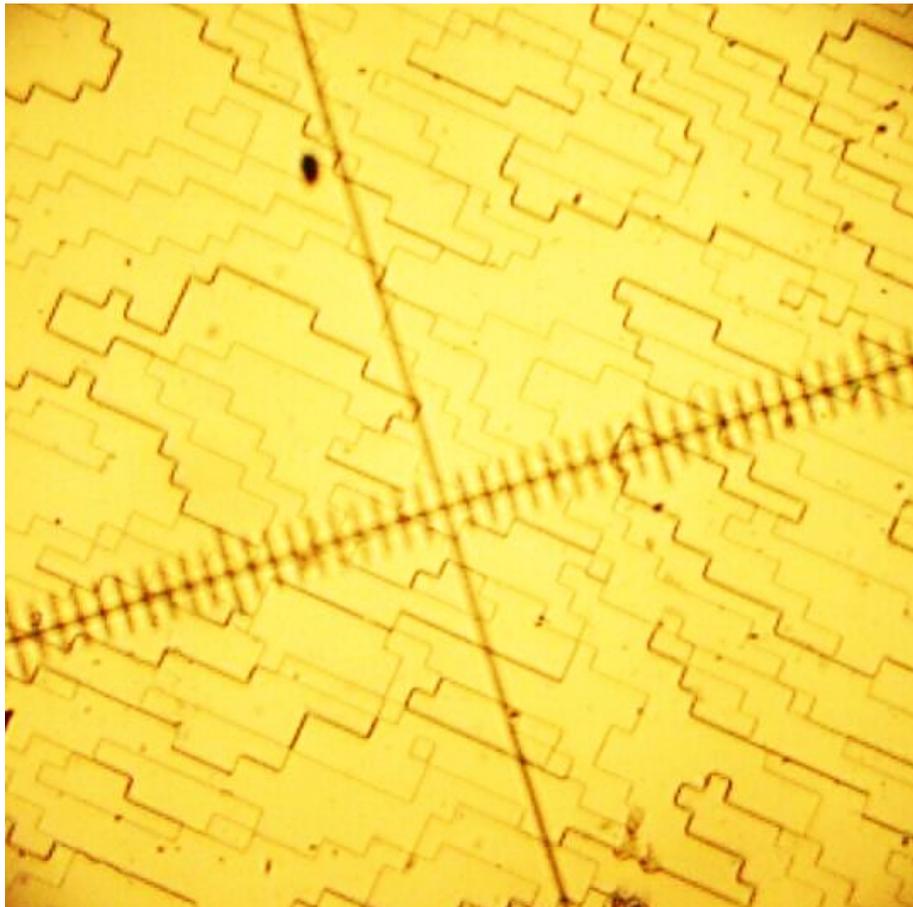


Reciprocal Space

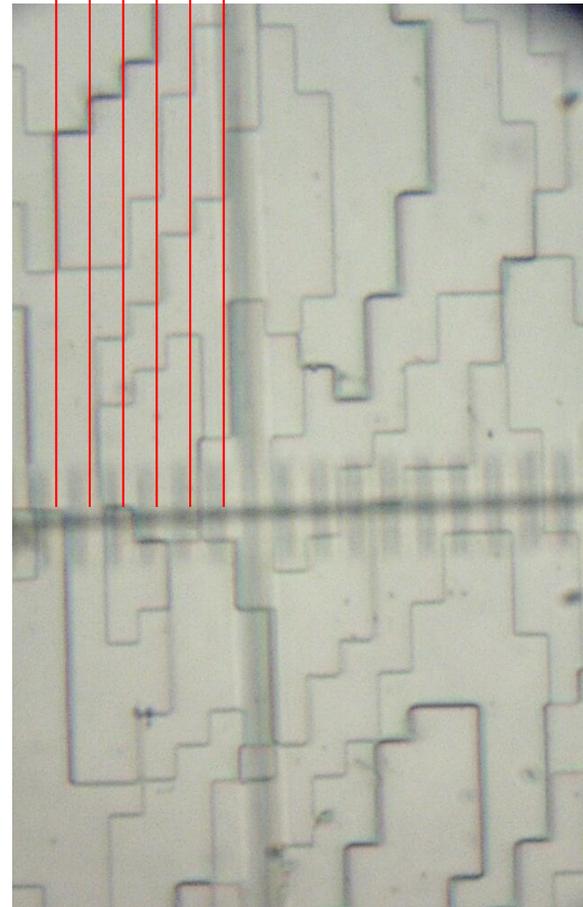


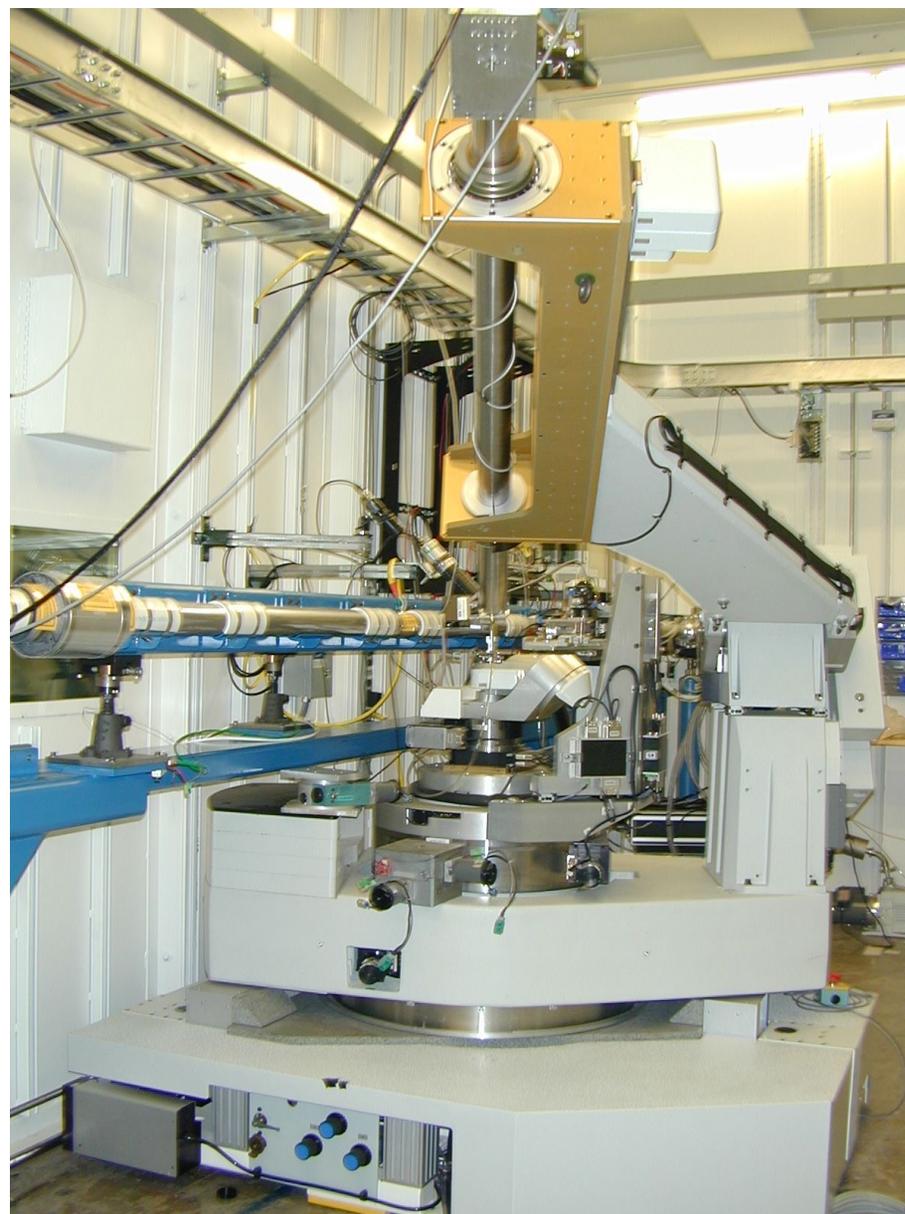
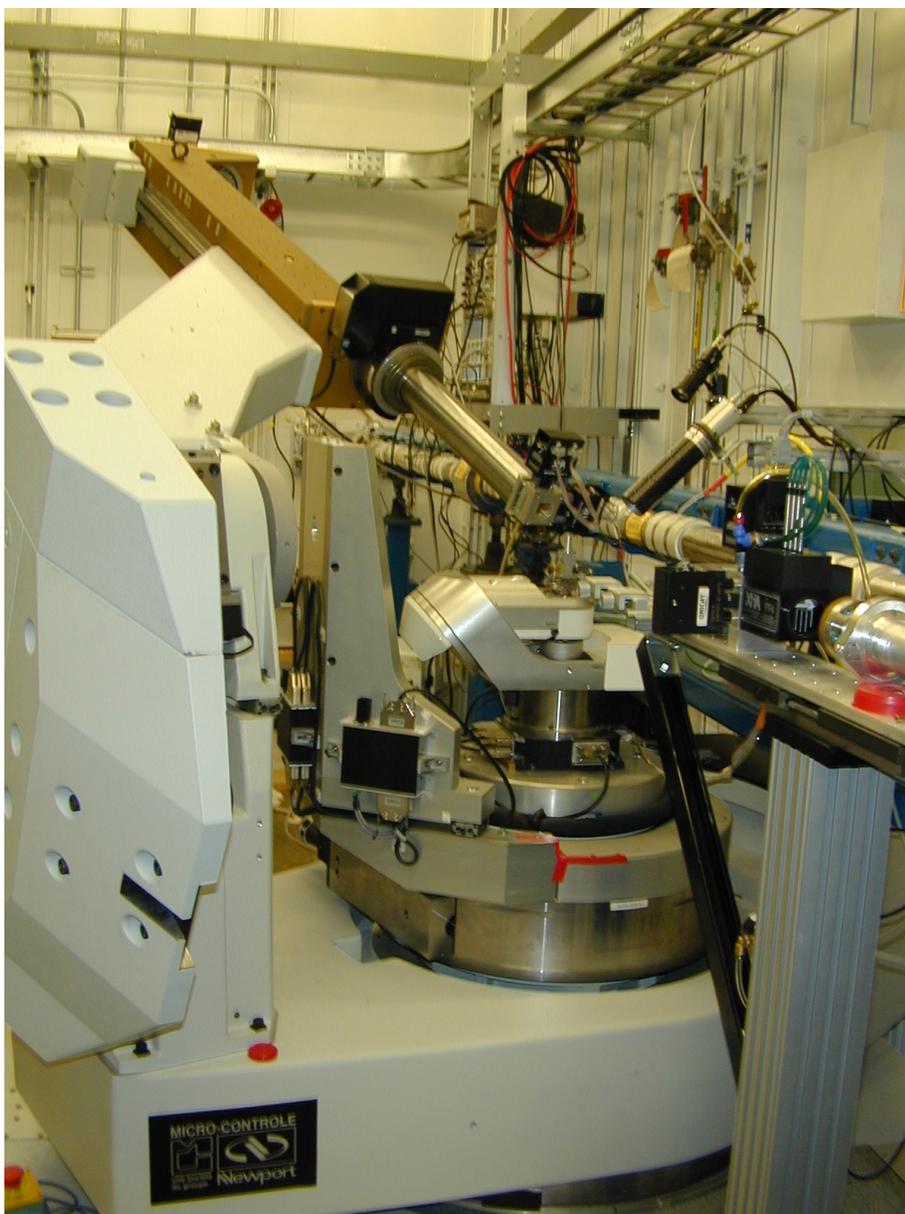


Microscope Images of Gratings

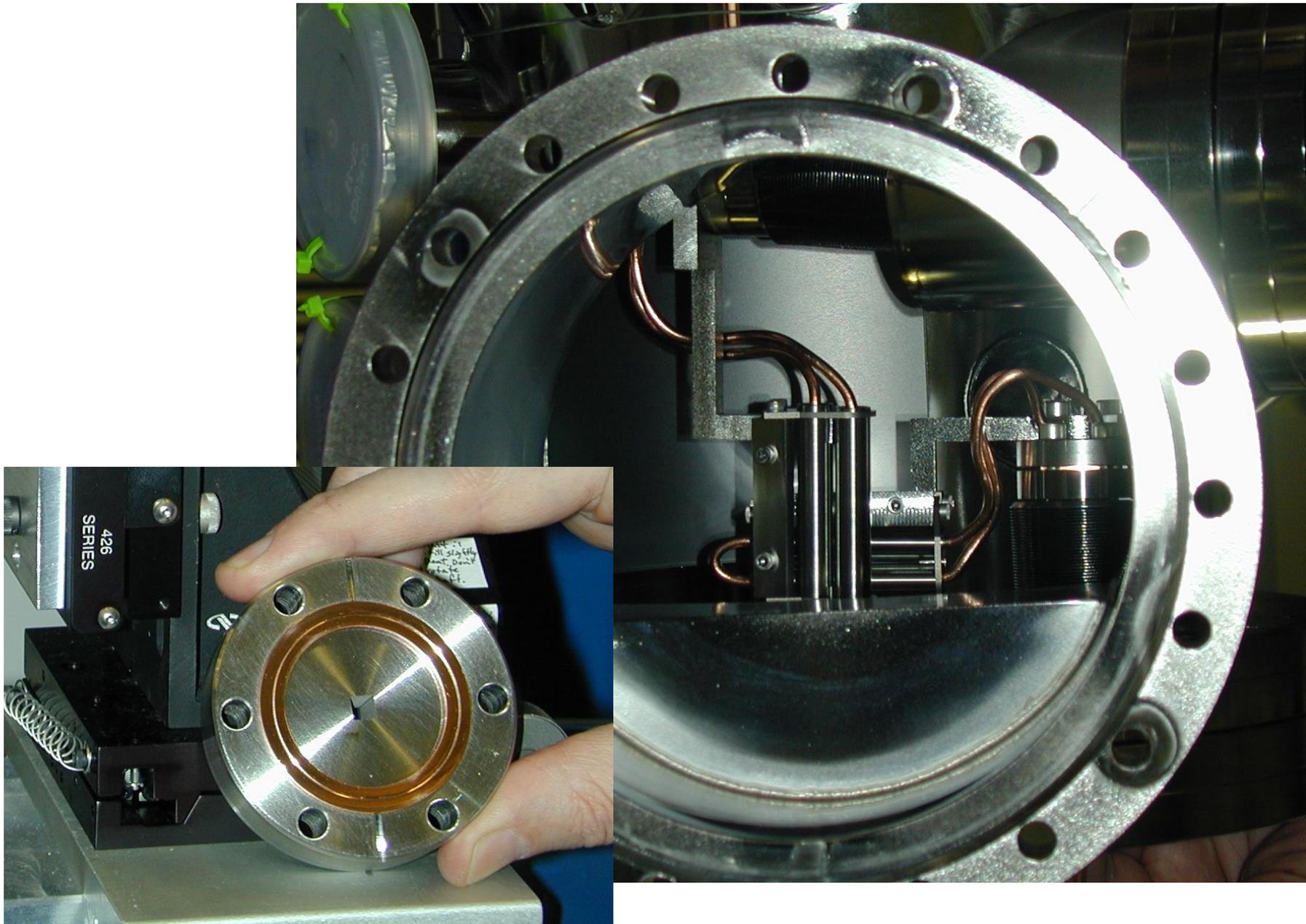


5 μ m grid lines



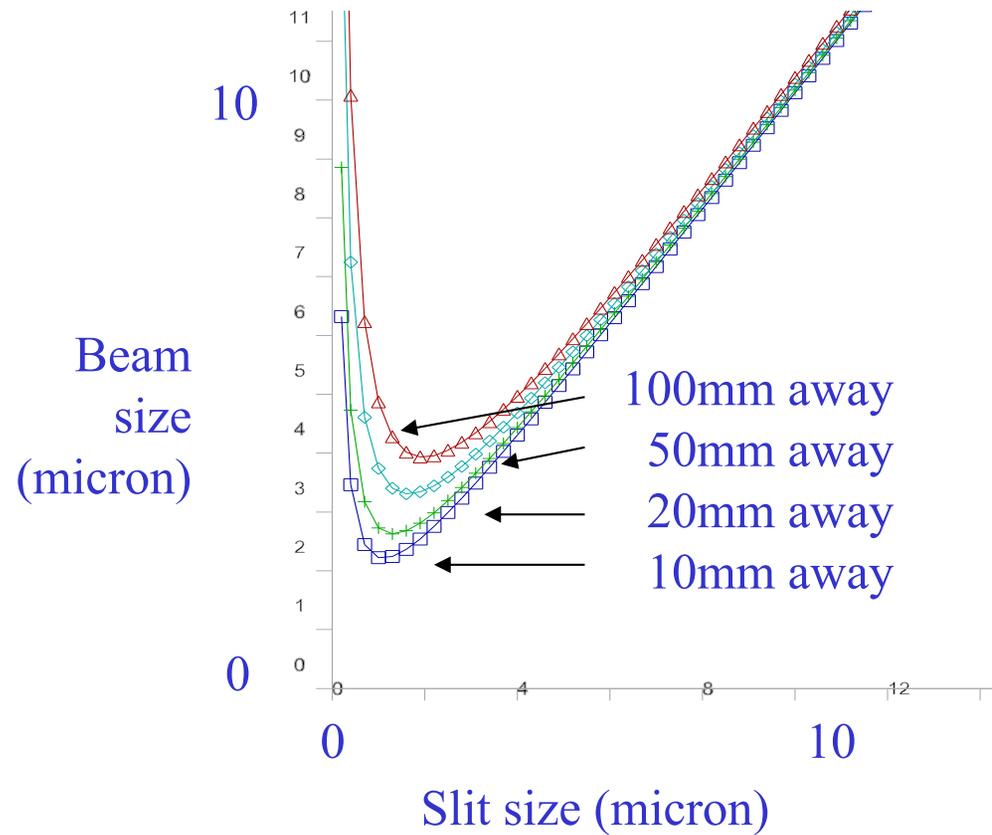


I. K. Robinson, XTOP-04, Sept 2004

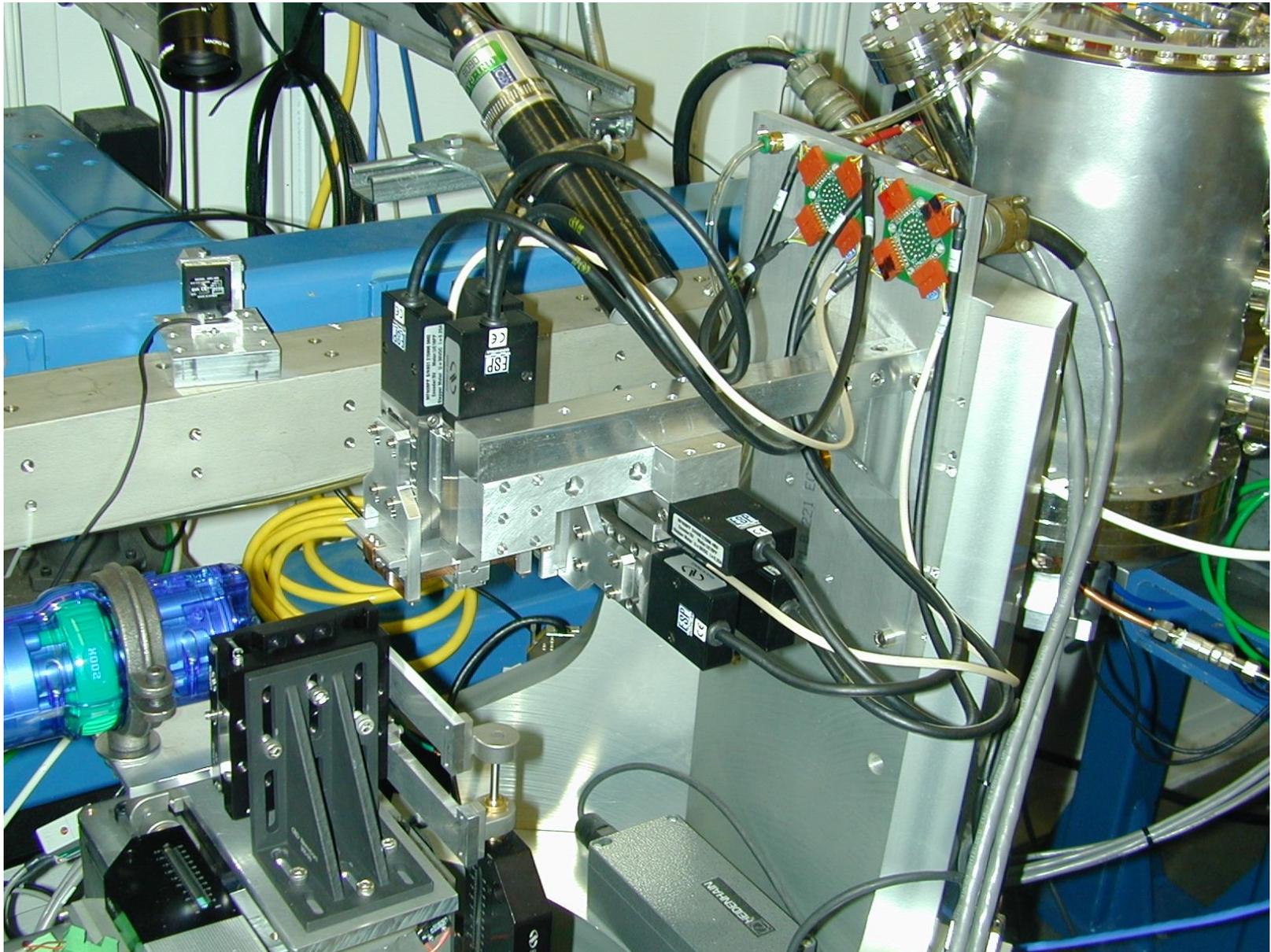


I. K. Robinson, XTOP-04, Sept 2004

Smallest Beam using Slits (9keV)



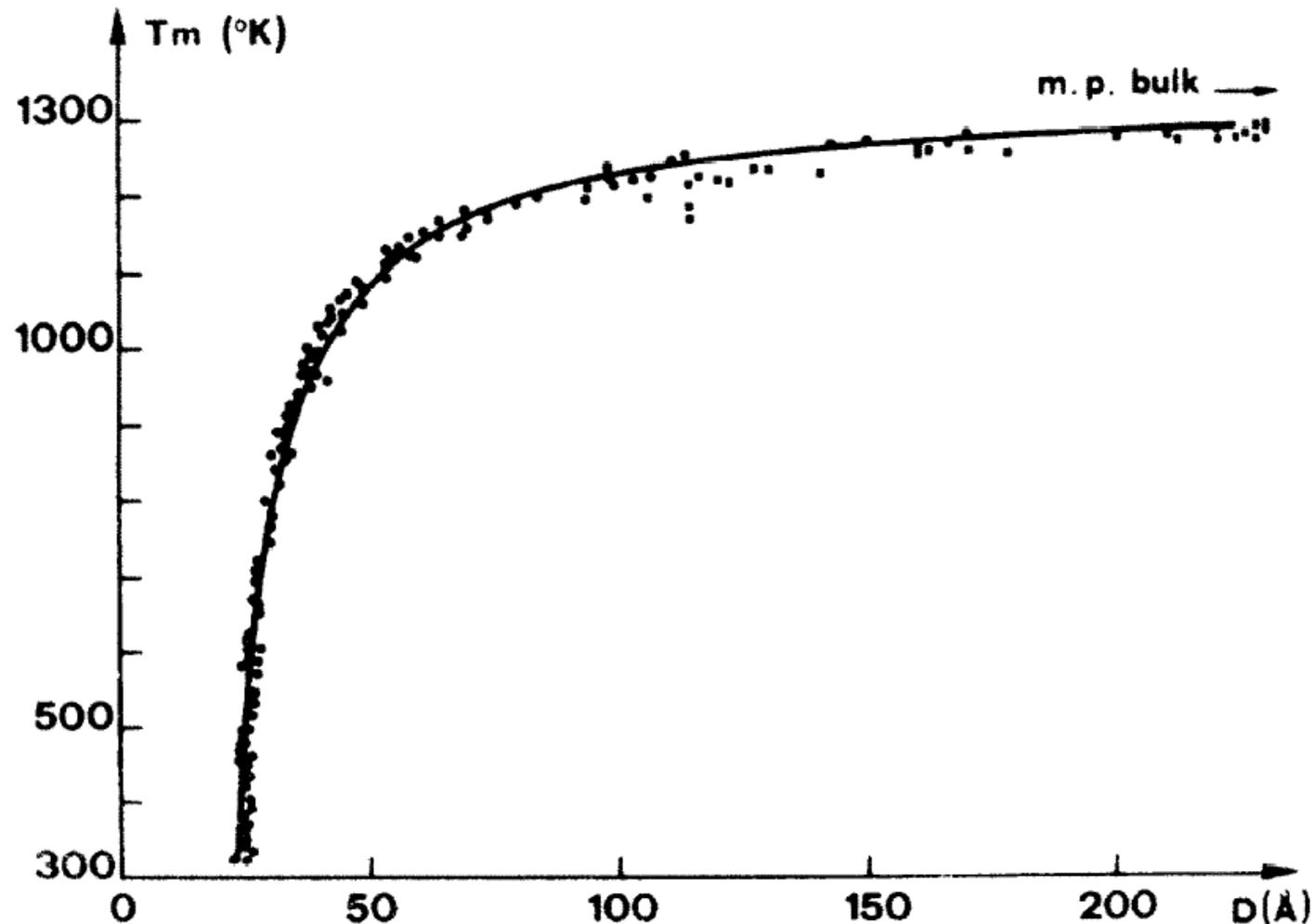
$$y(x) = x + \frac{\lambda d}{x}$$



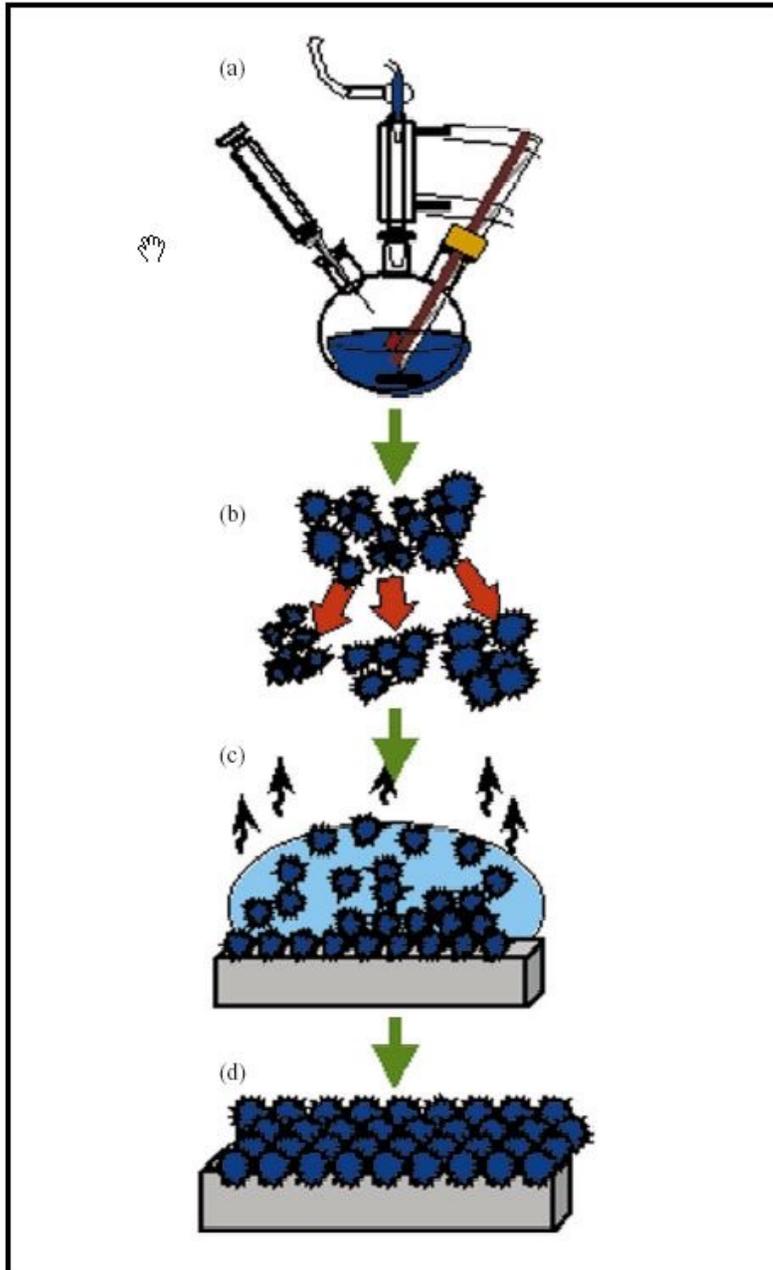
I. K. Robinson, XTOP-04, Sept 2004

Size-dependent Melting of Au Particles

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

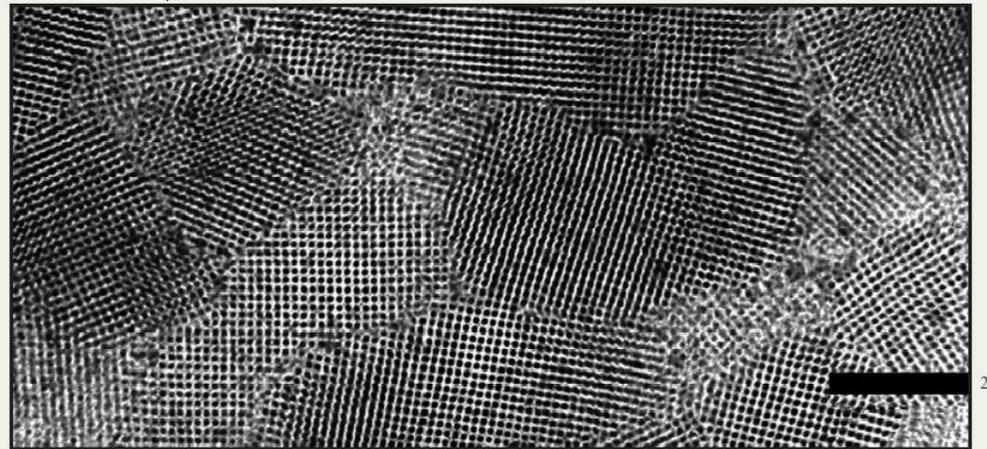


Chemical Synthesis of Nanocrystals



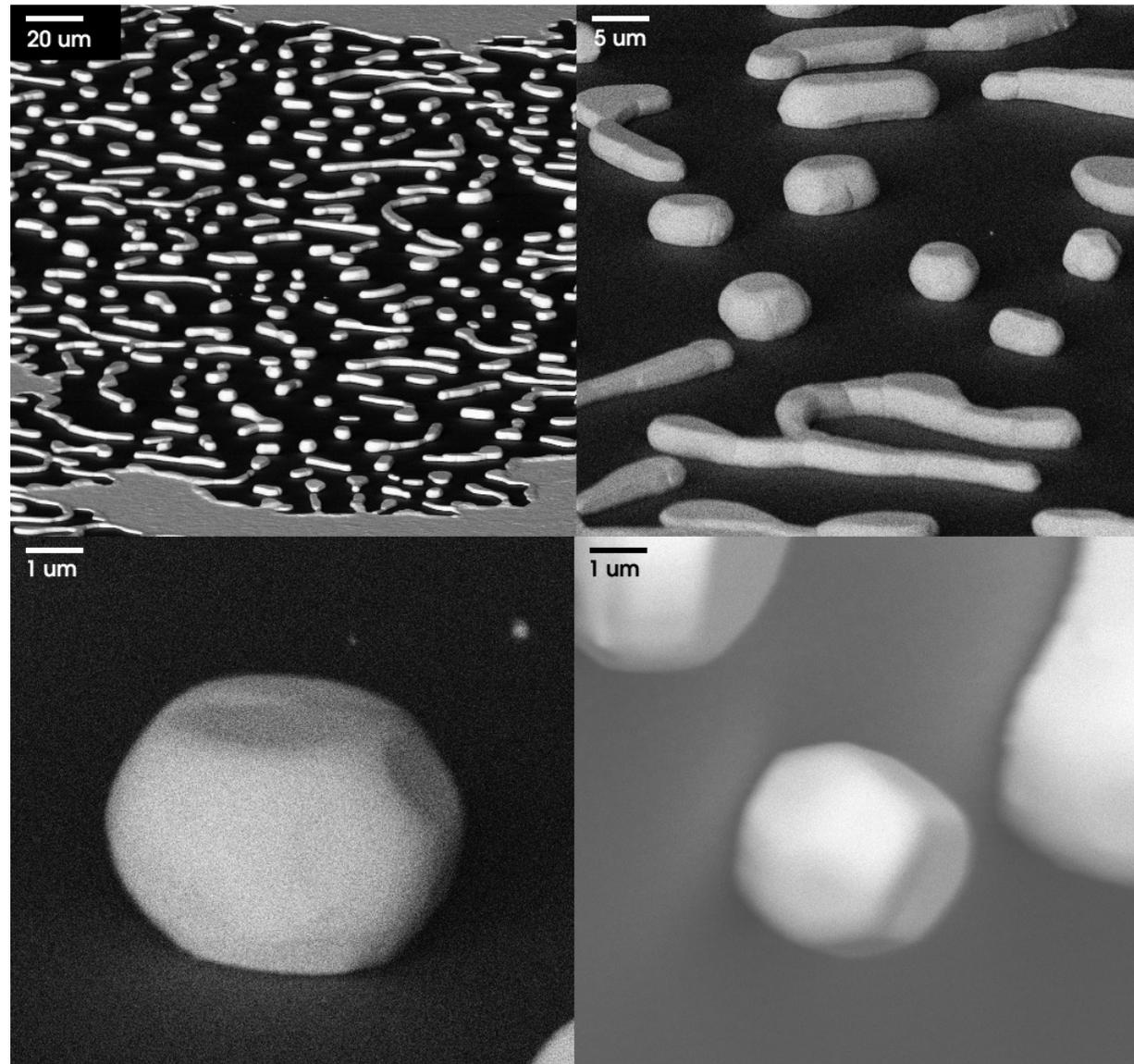
- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

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

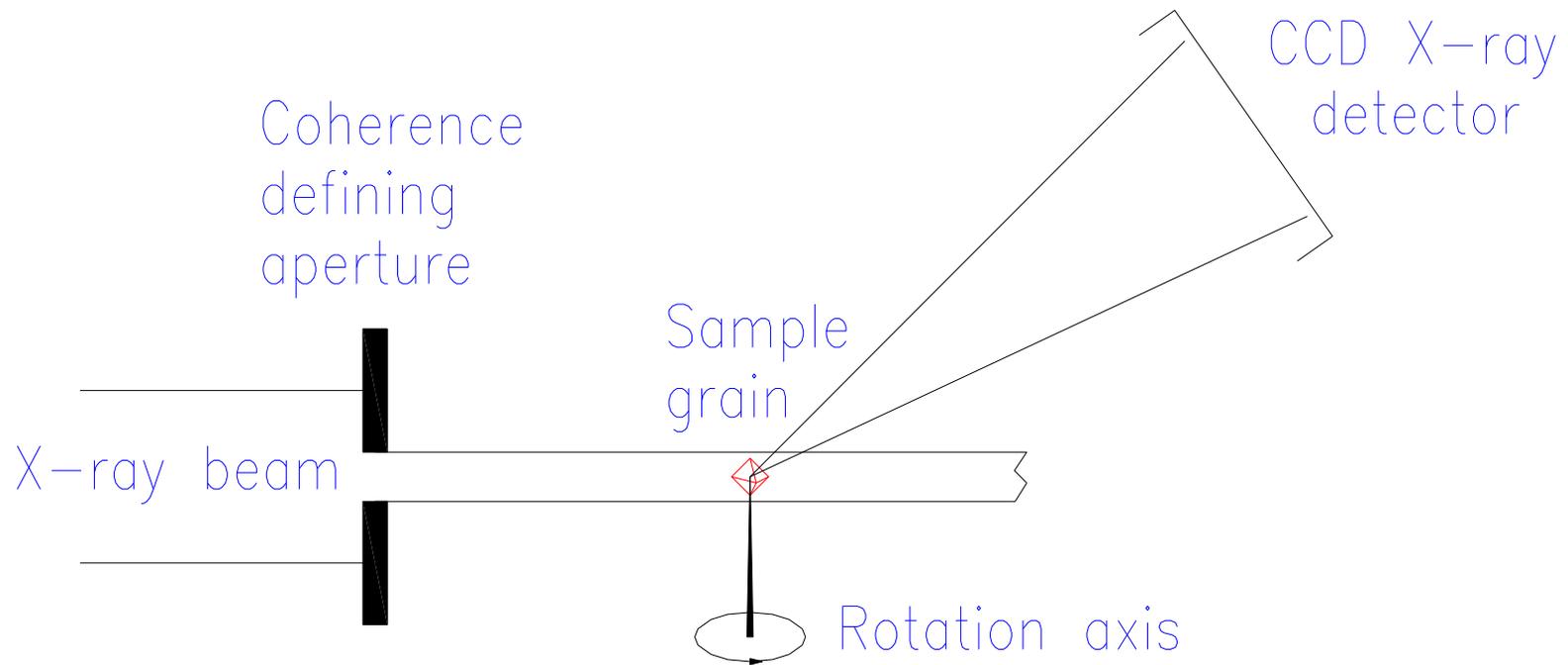


SEMS

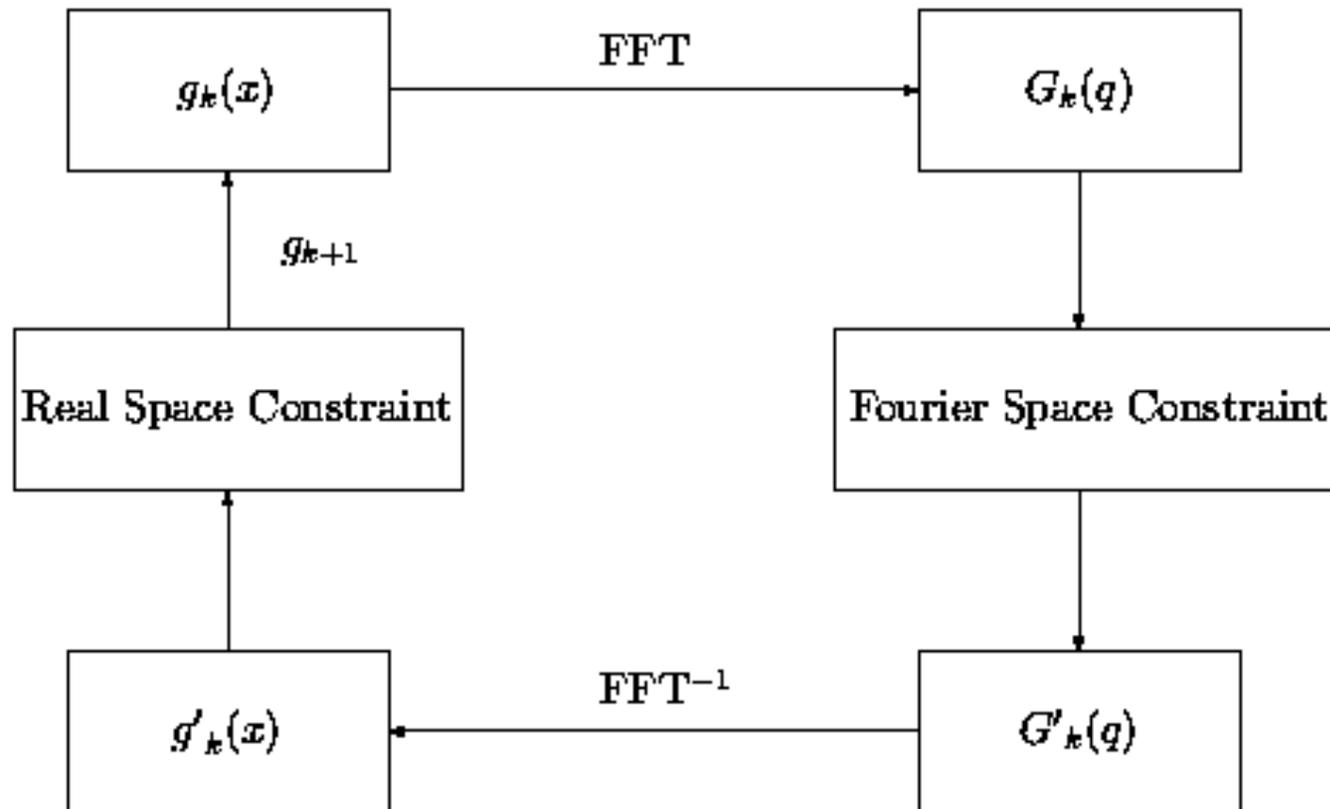
- Au blanket film
- Quartz substrate
- Annealed at 950°C for 70 hrs.



Lensless X-ray Microscope



Generic “Error Reduction” method



J. R. Fienup *Appl. Opt.* 21 2758 (1982)

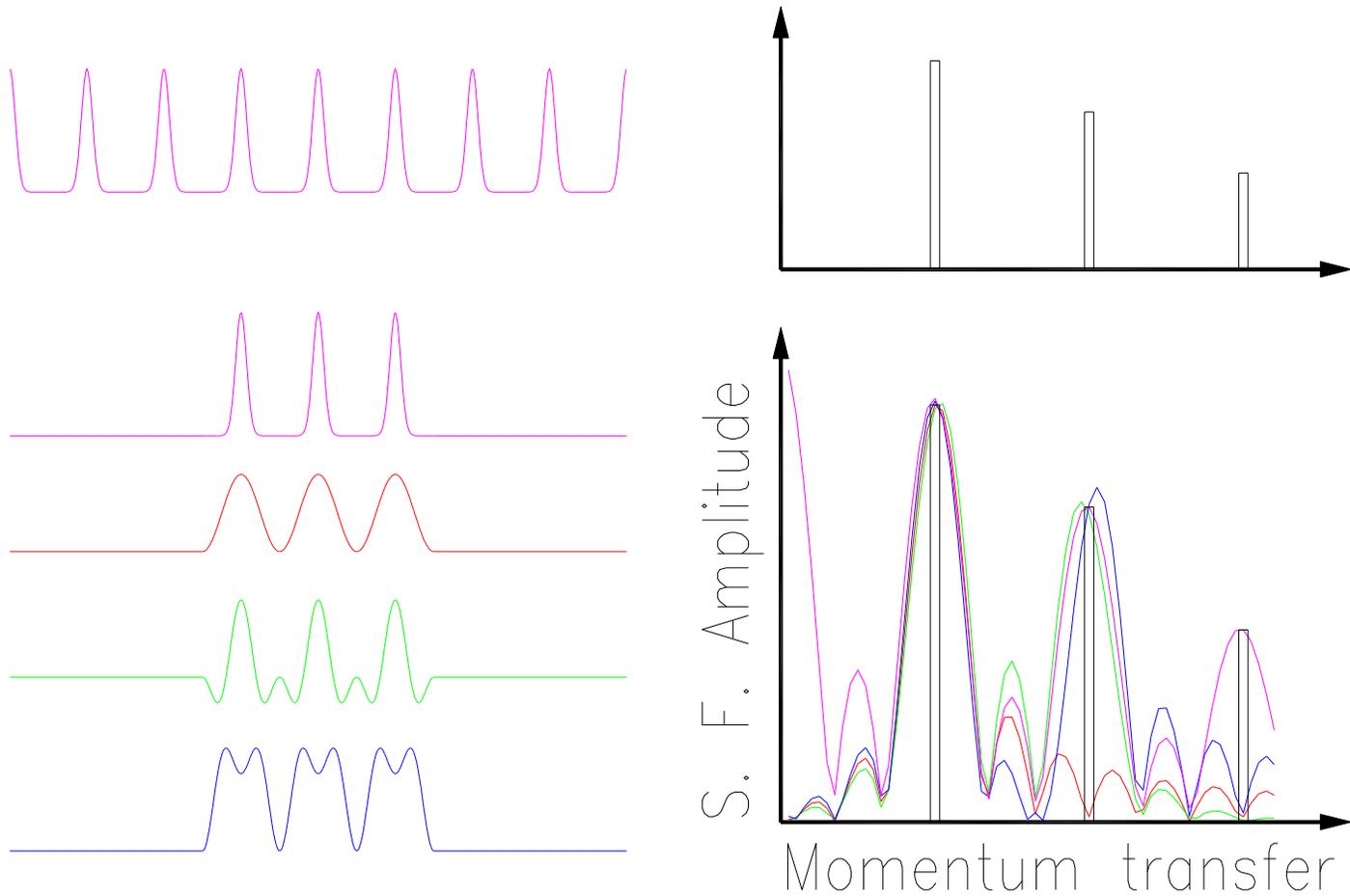
R. W. Gerchberg and W. O. Saxton *Optik* 35 237 (1972)

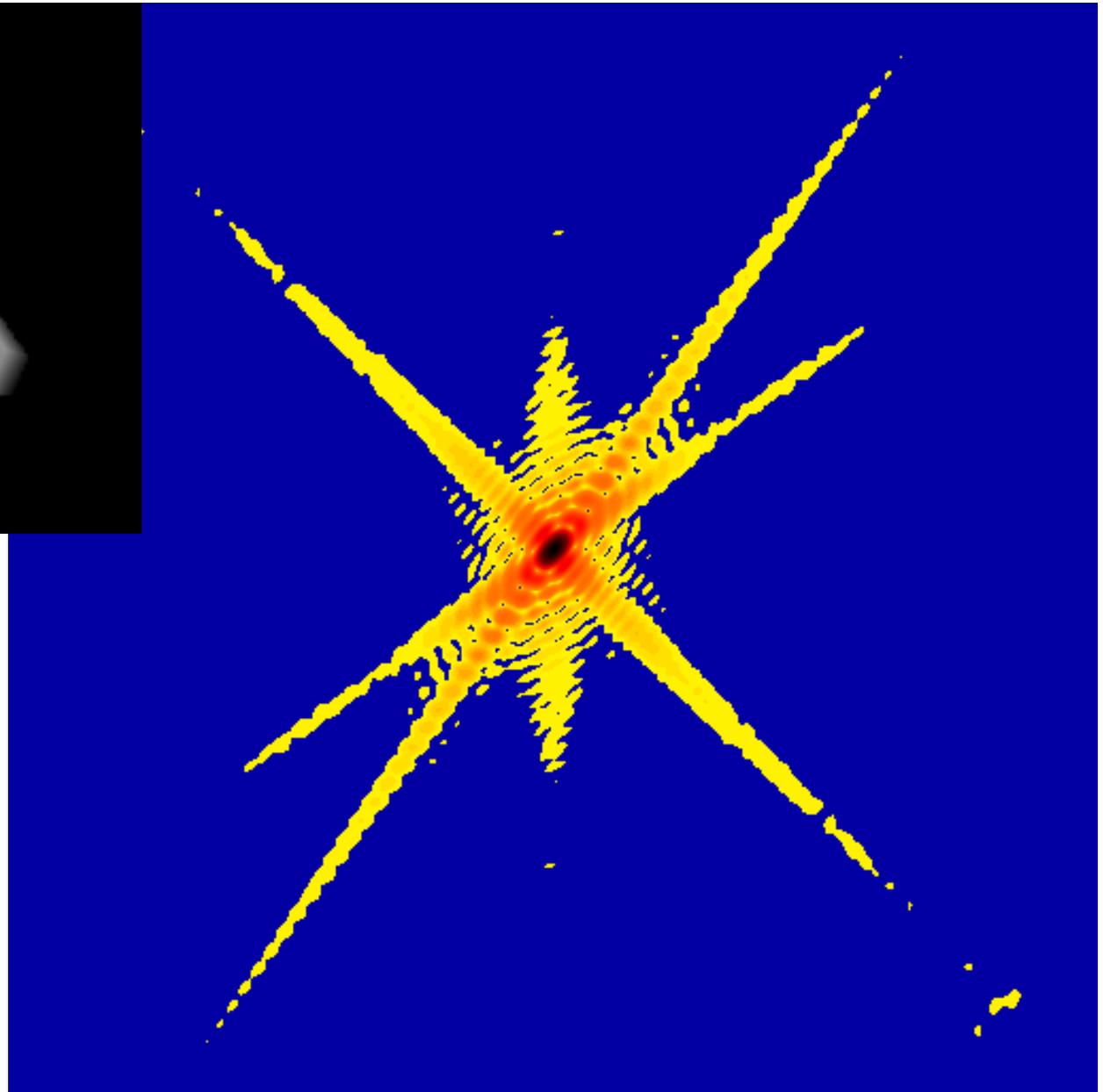
Real-space Constraints in Crystallography

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)

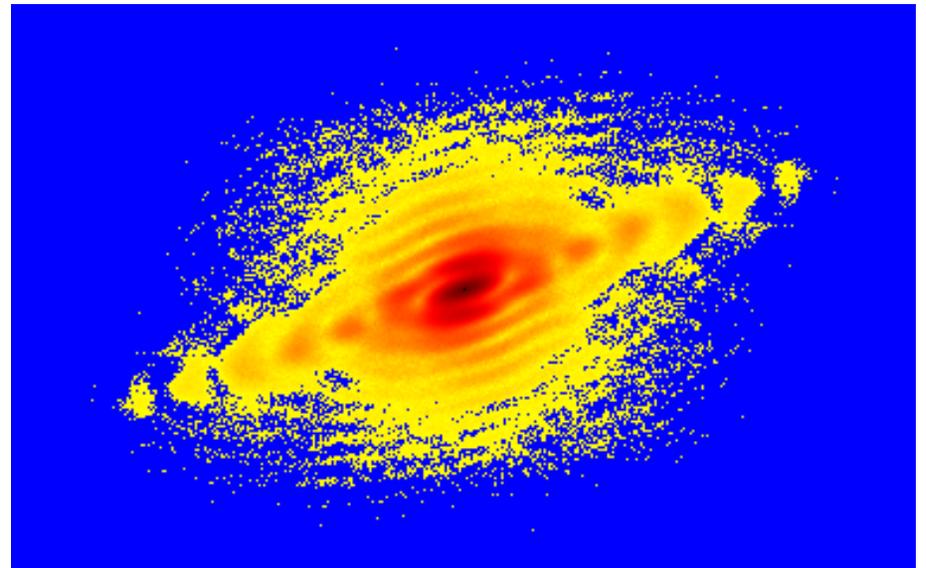
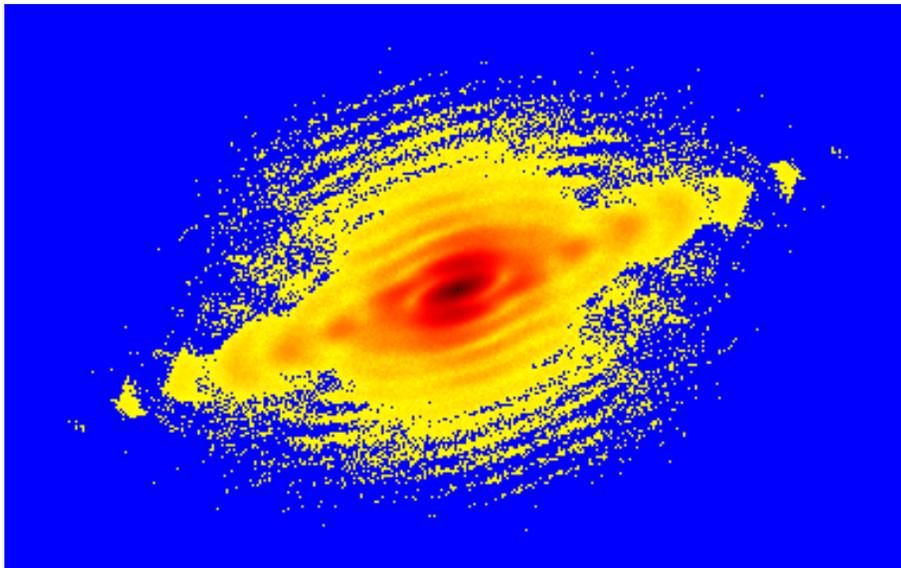
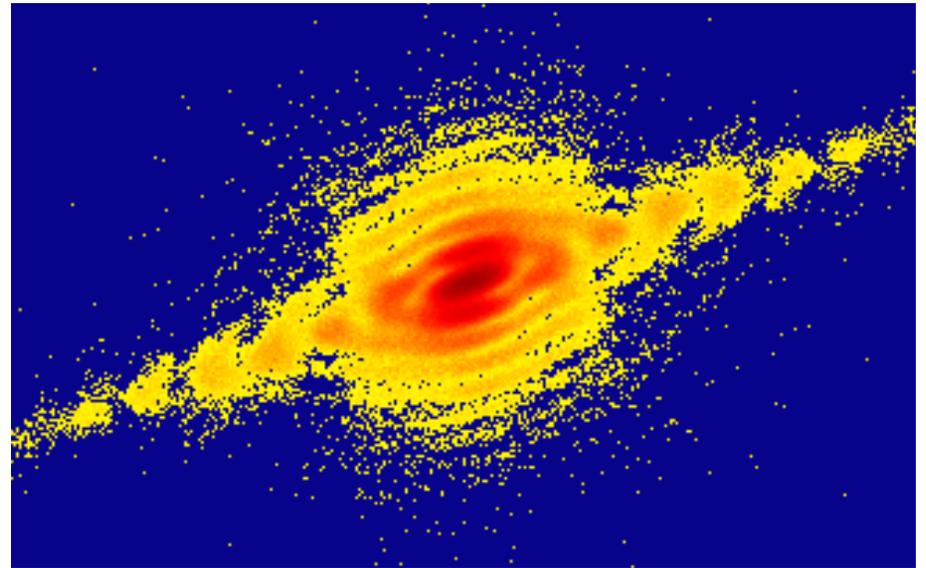
Phase Problem: Finite-size Effect





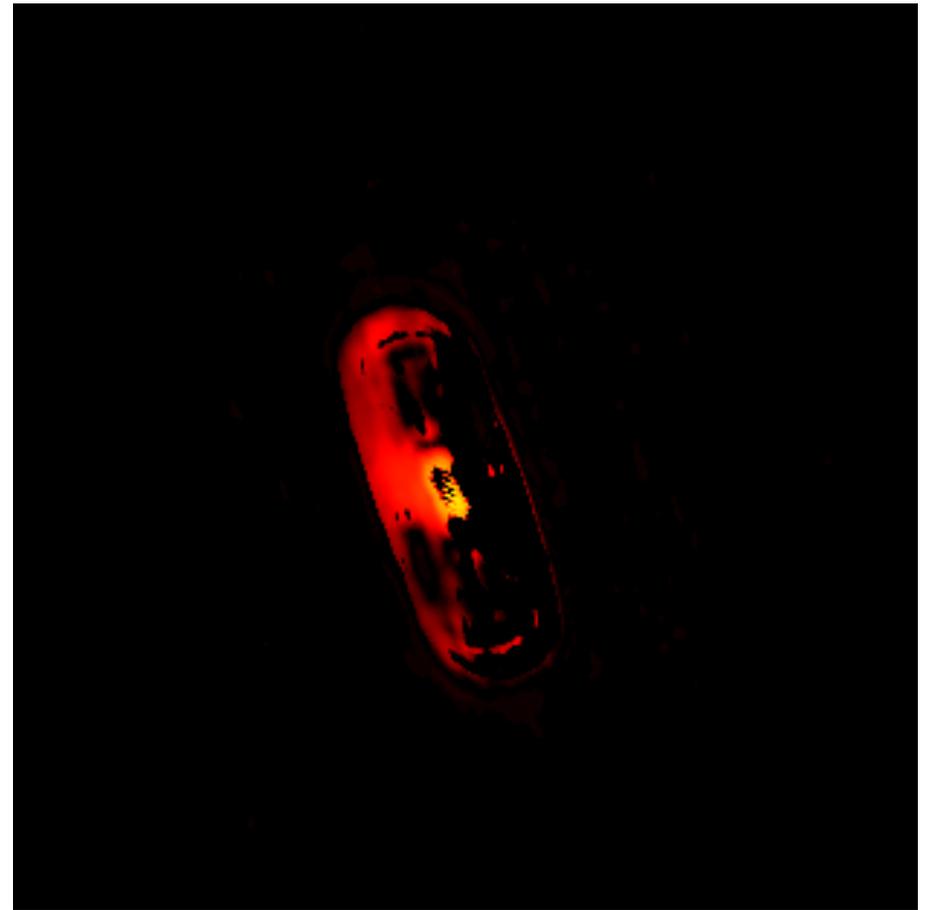
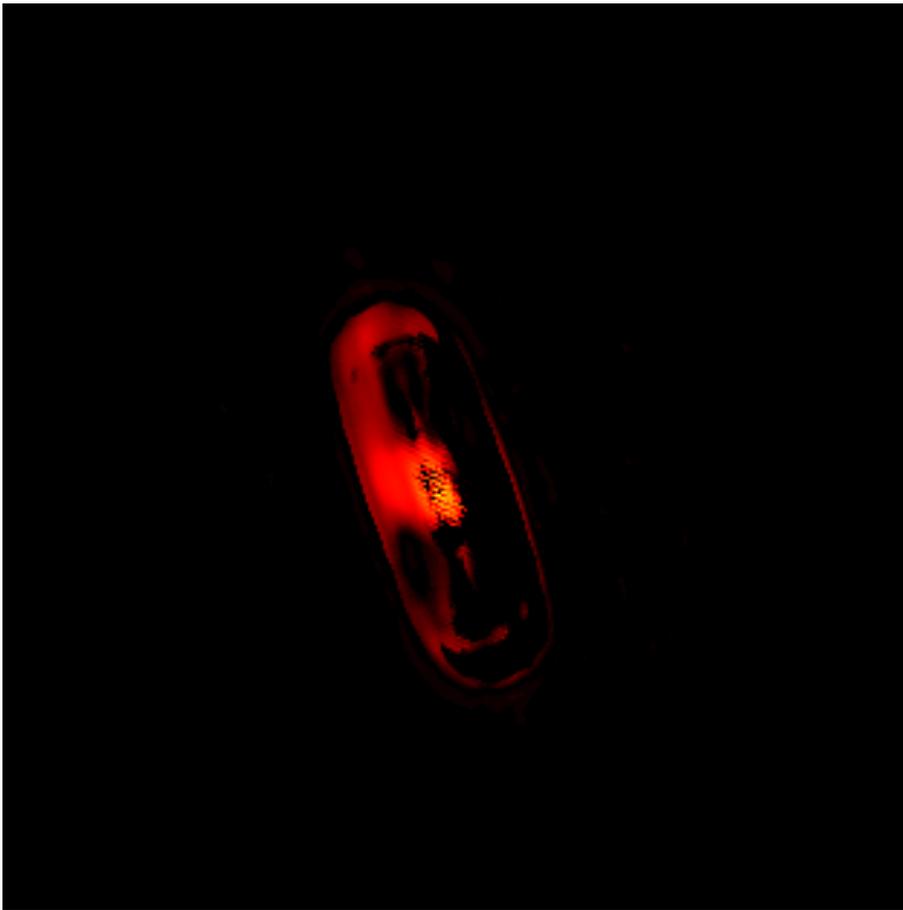
Symmetrized Data and two best fits

Chisq=0.0005

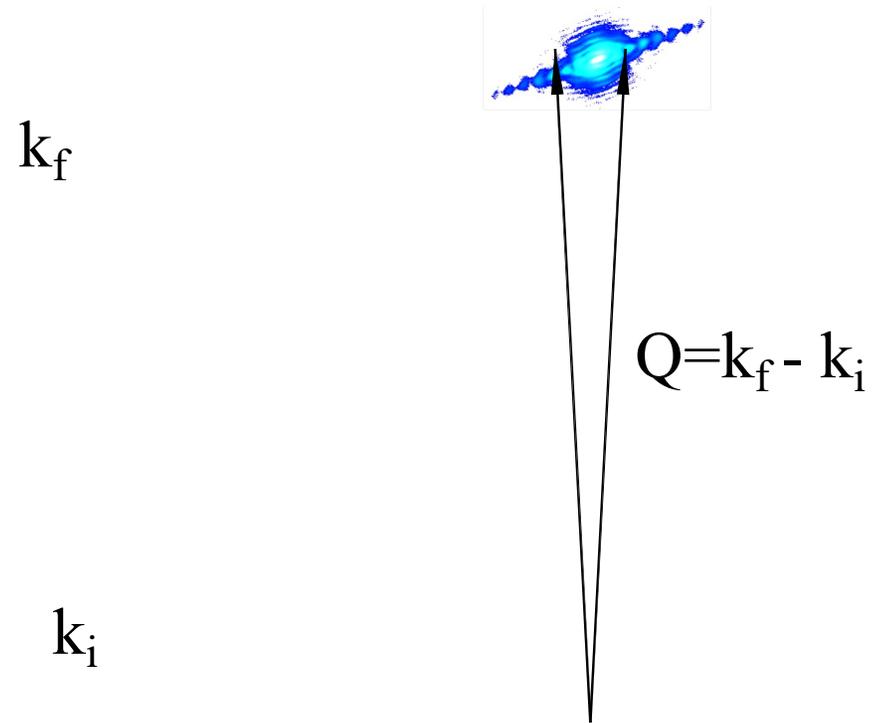


2D Reconstructions

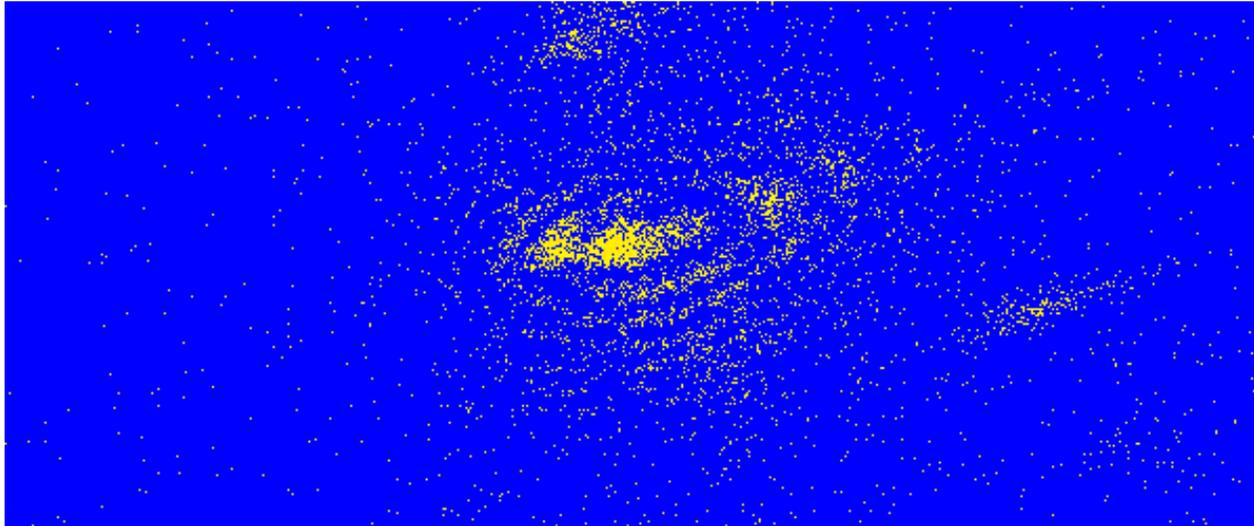
chisquare = 0.0005

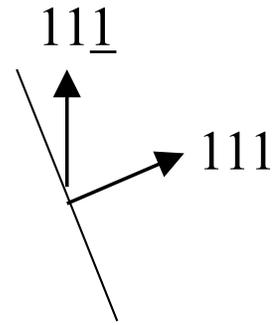
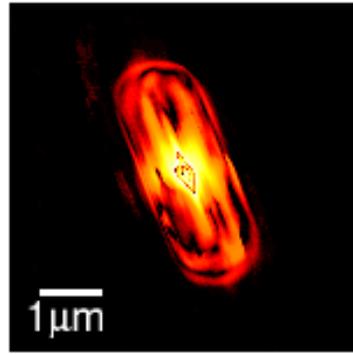
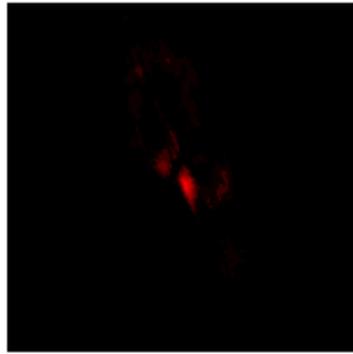


3D Diffraction Method

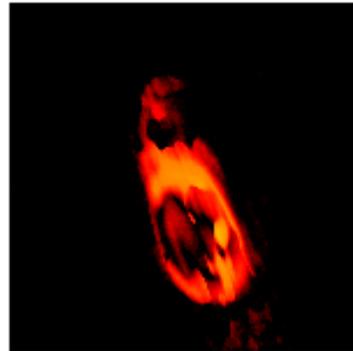
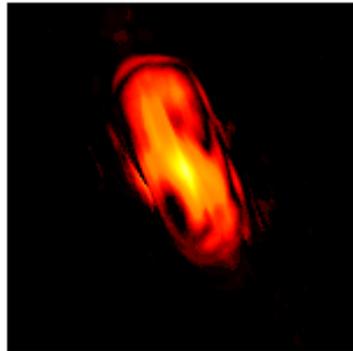
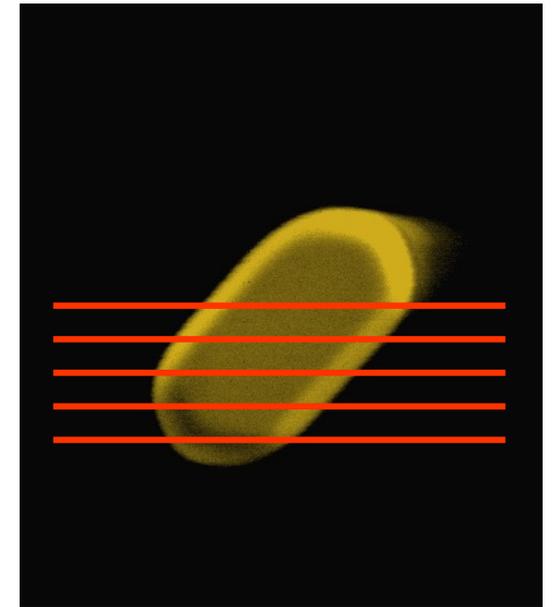
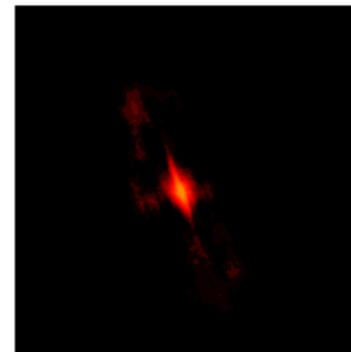
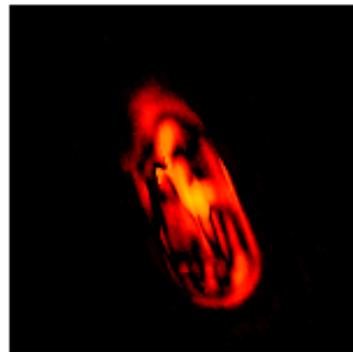
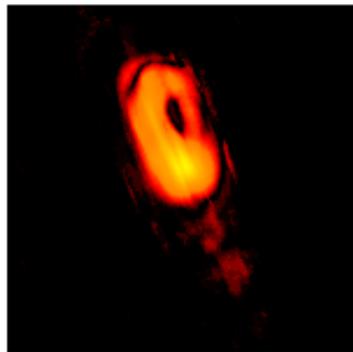
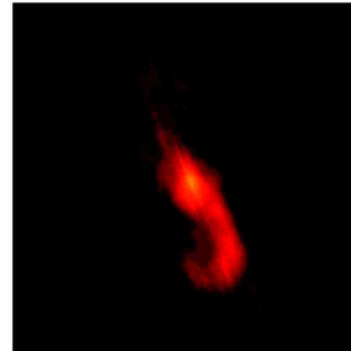
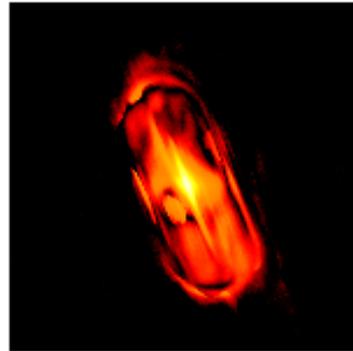
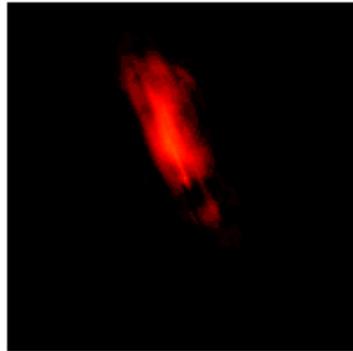


3D Diffraction Data 1 micron Au crystal



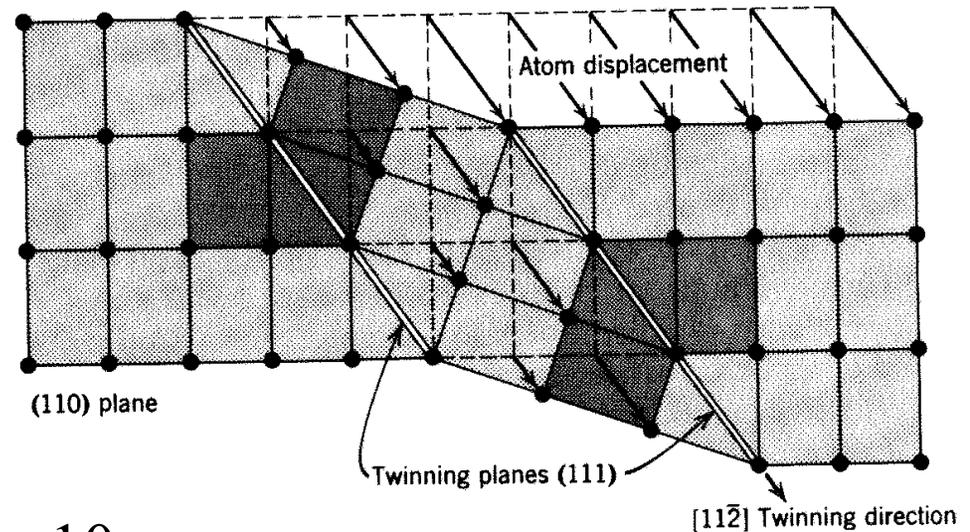
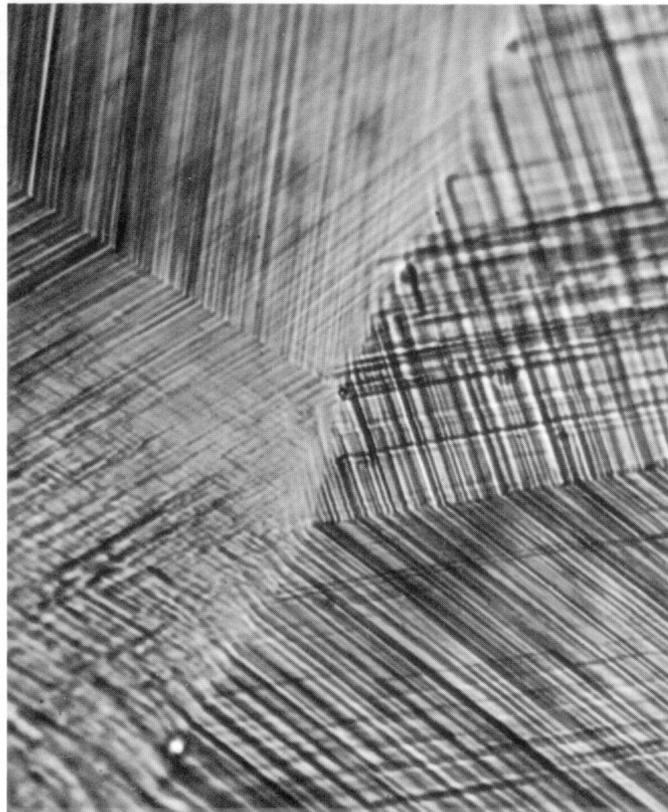


Slices through
plan view SEM:



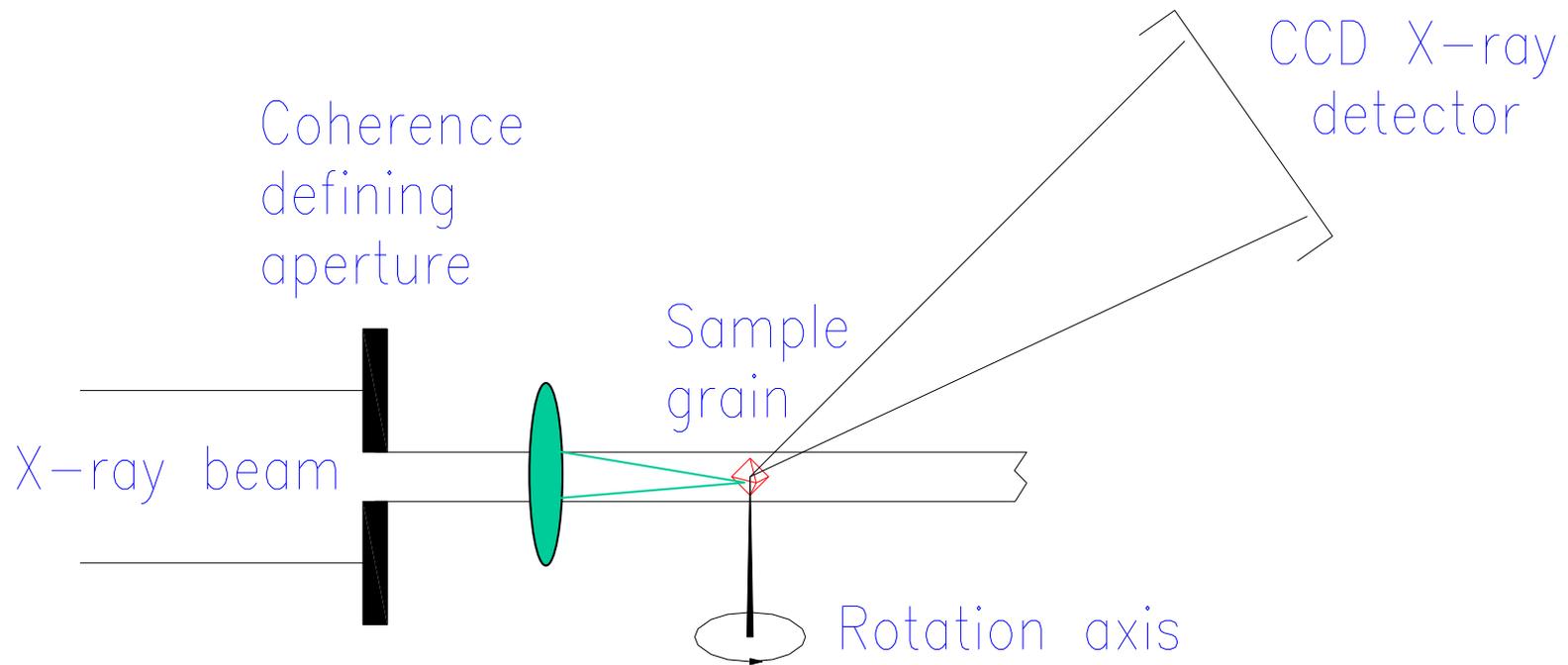
Twinning in deformed FCC metals

J. Wulff, "Structure and Property of Materials III" (1965)

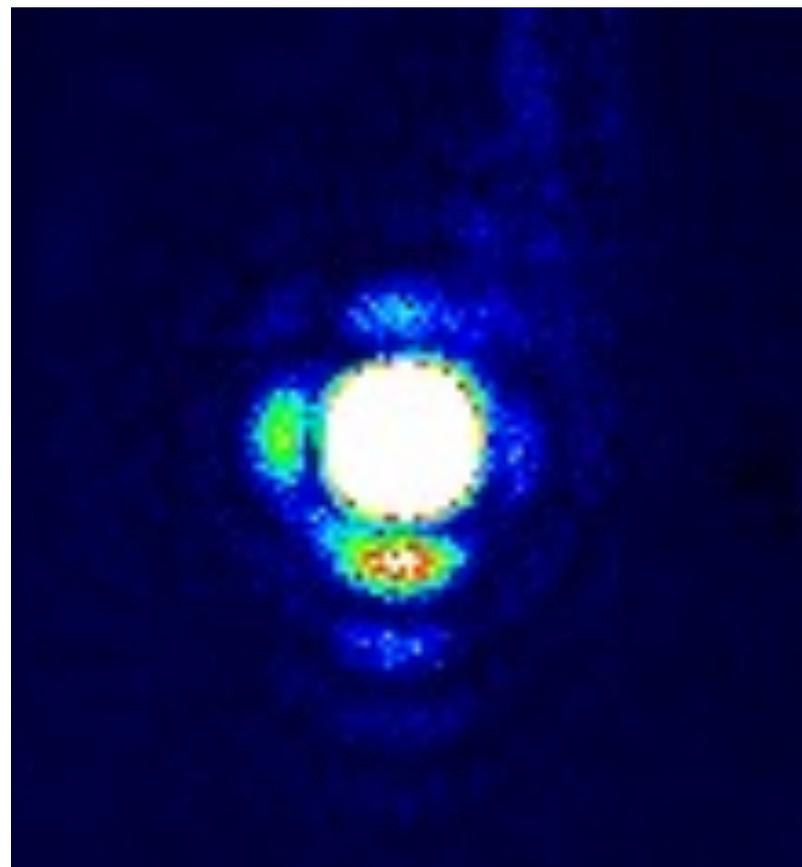
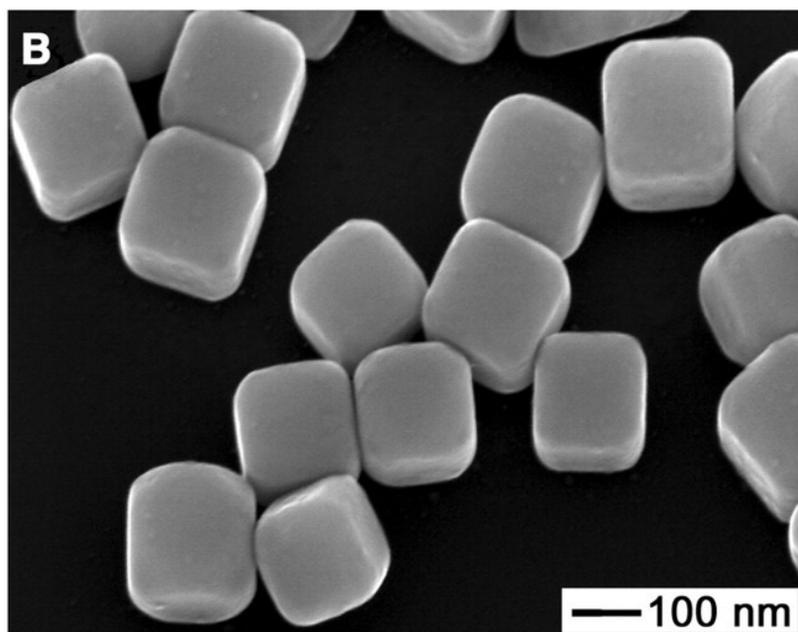


■ $\sim 10\mu\text{m}$
Cu

Lensless X-ray Microscope

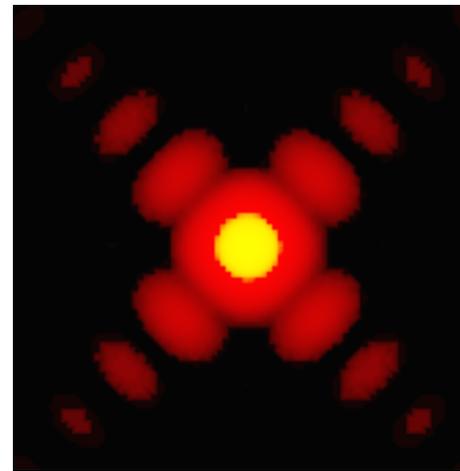
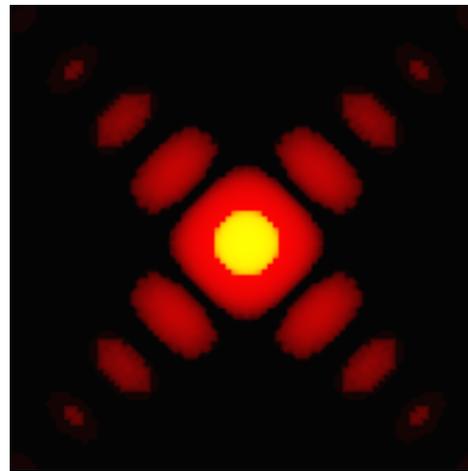


Chemically Synthesized Silver Nanocubes



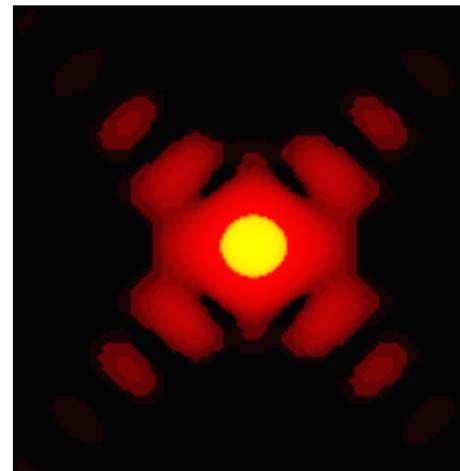
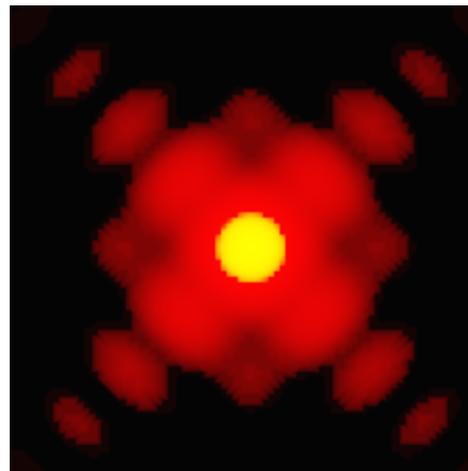
Yugang Sun and Younan Xia,
Science 298 2177 (2003)

Spherical and cylindrical waves



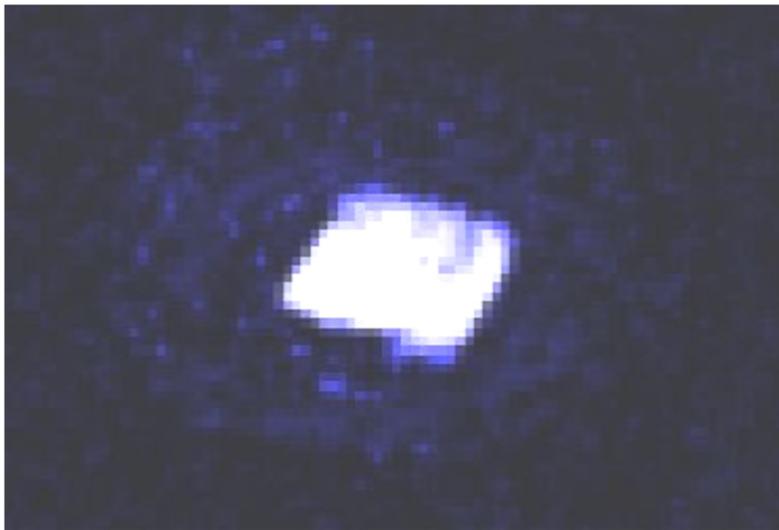
$\pi/4$

$\pi/2$

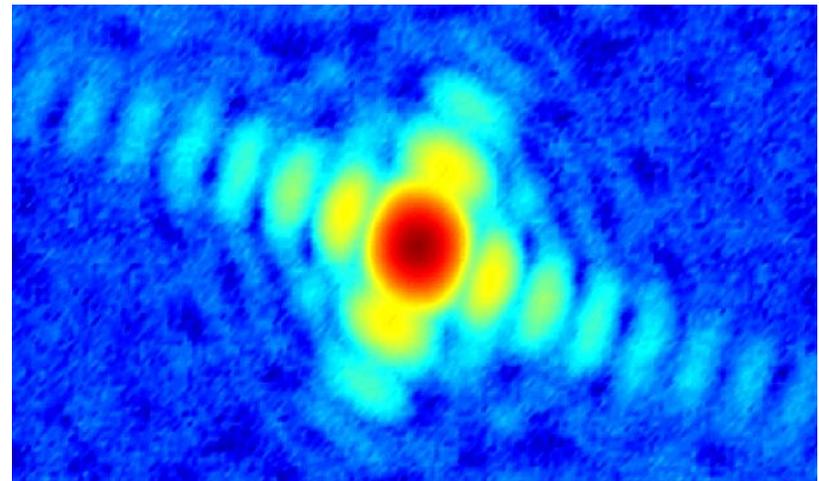
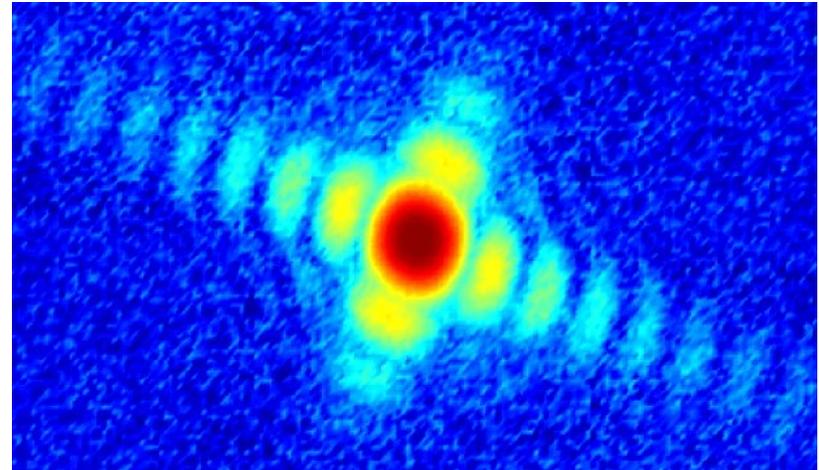


$\pi/4$ (x)

Reconstruction of Ag Nanocrystal



←→
200nm

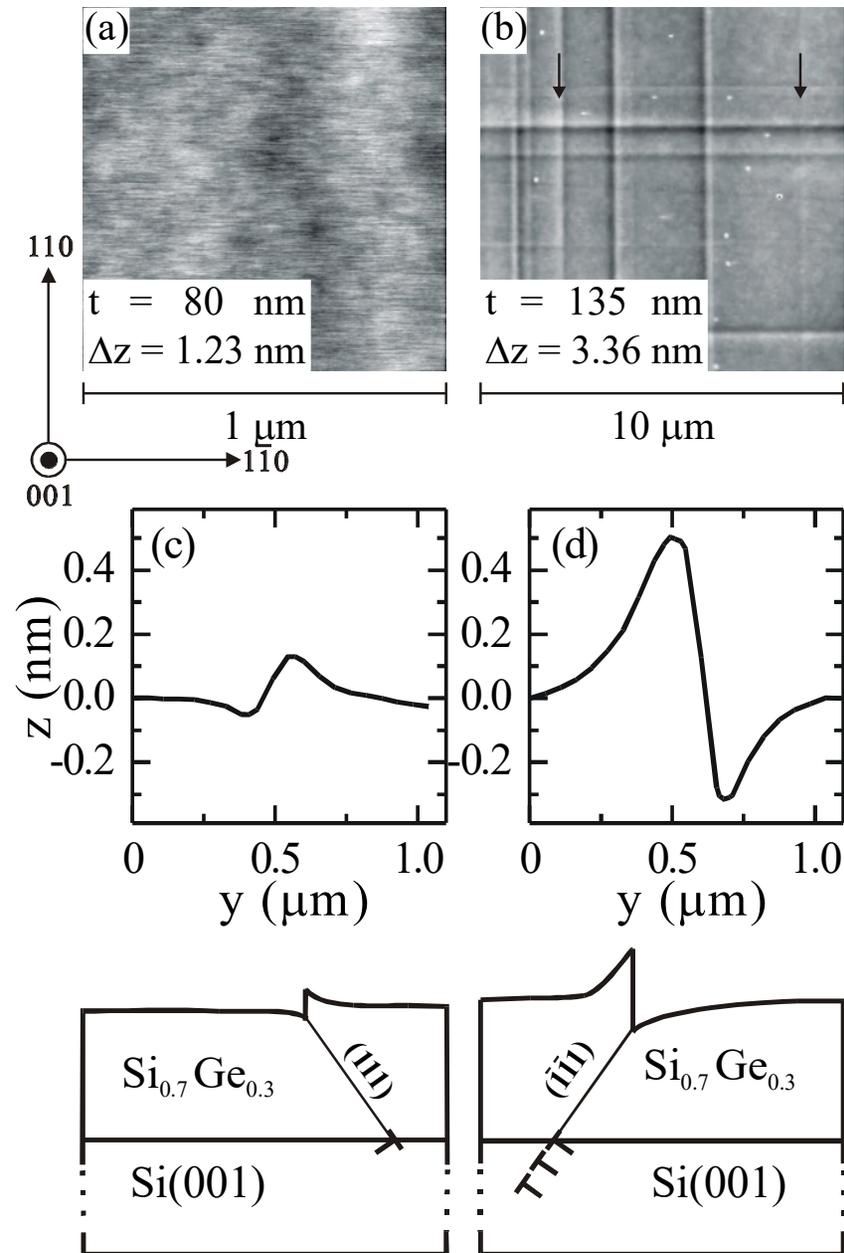


Low dislocation density GeSi films

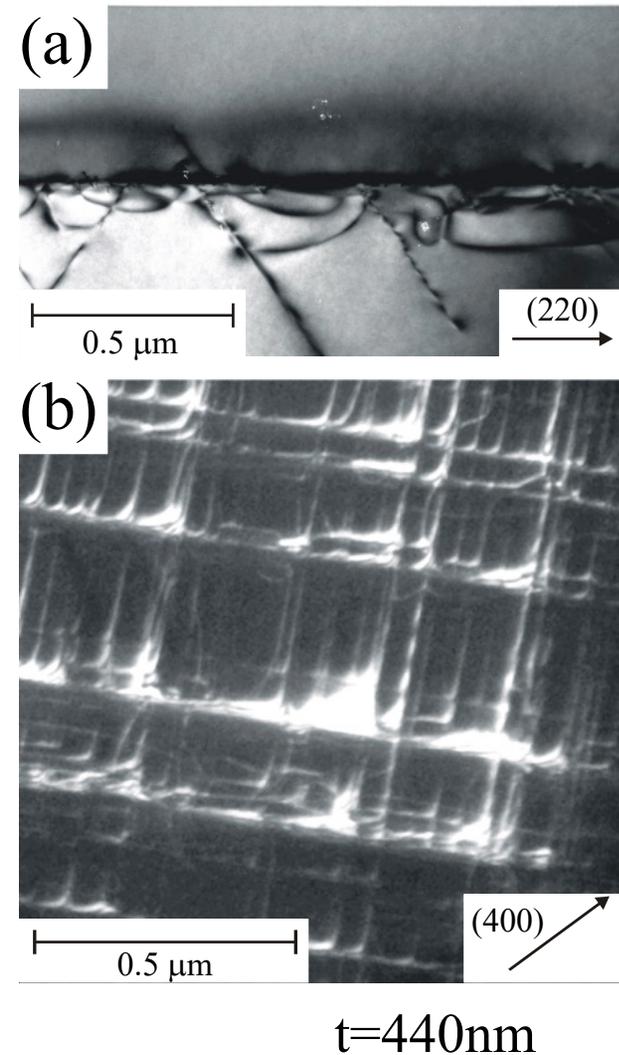
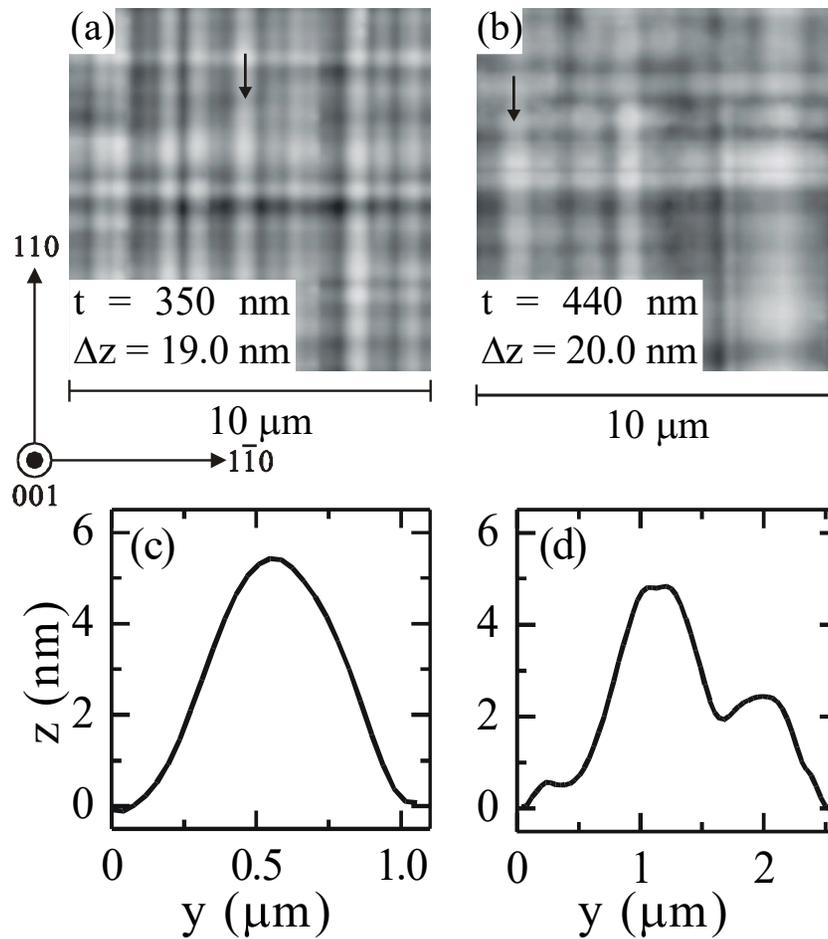
Thickness close to critical thickness

Dislocations aggregate at interface and glide to surface along $\{111\}$

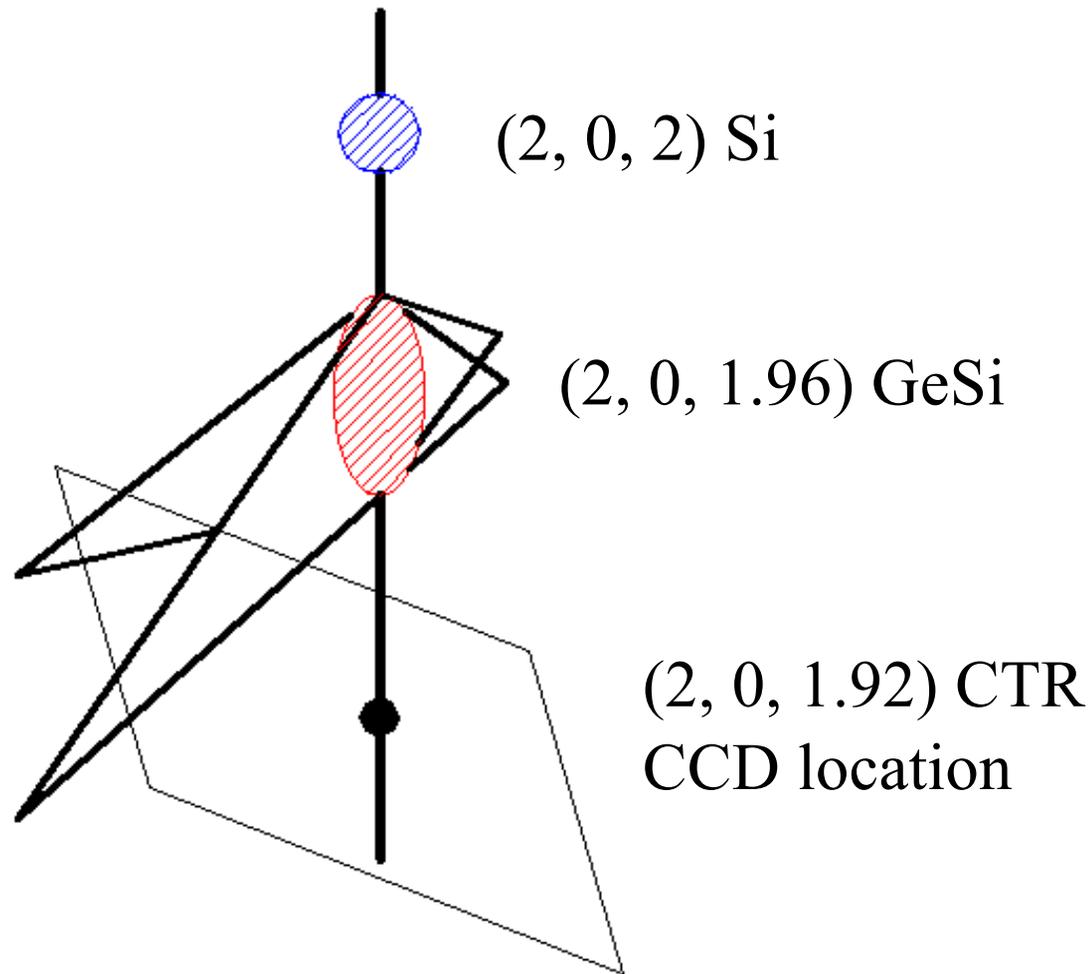
T. Spila, UIUC Thesis



Higher Dislocation Density $\text{Ge}_{0.3}\text{Si}_{0.7}$

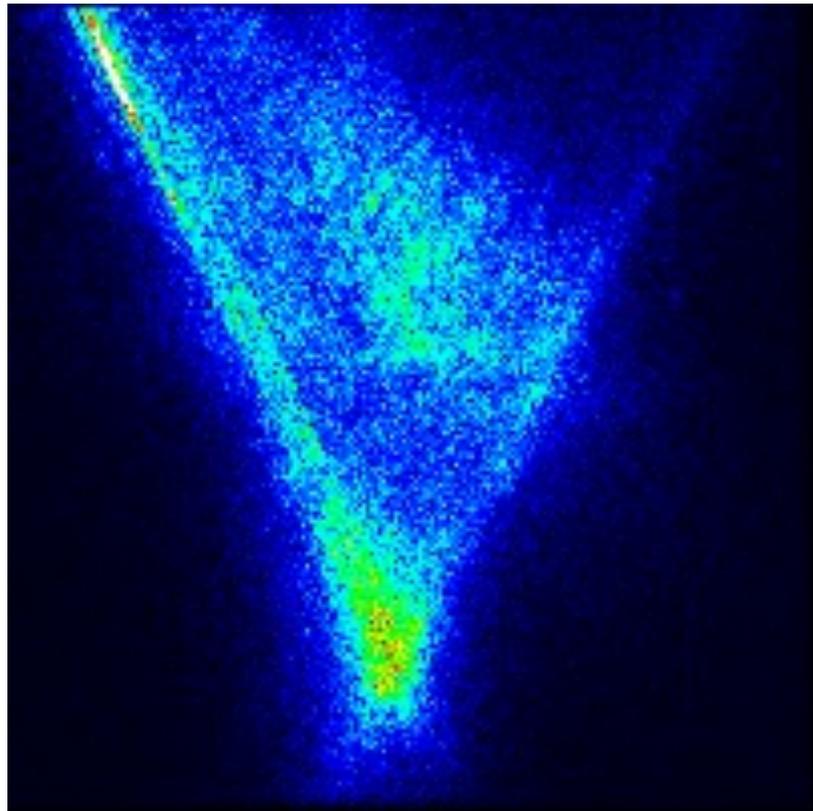


Dislocations in Reciprocal Space

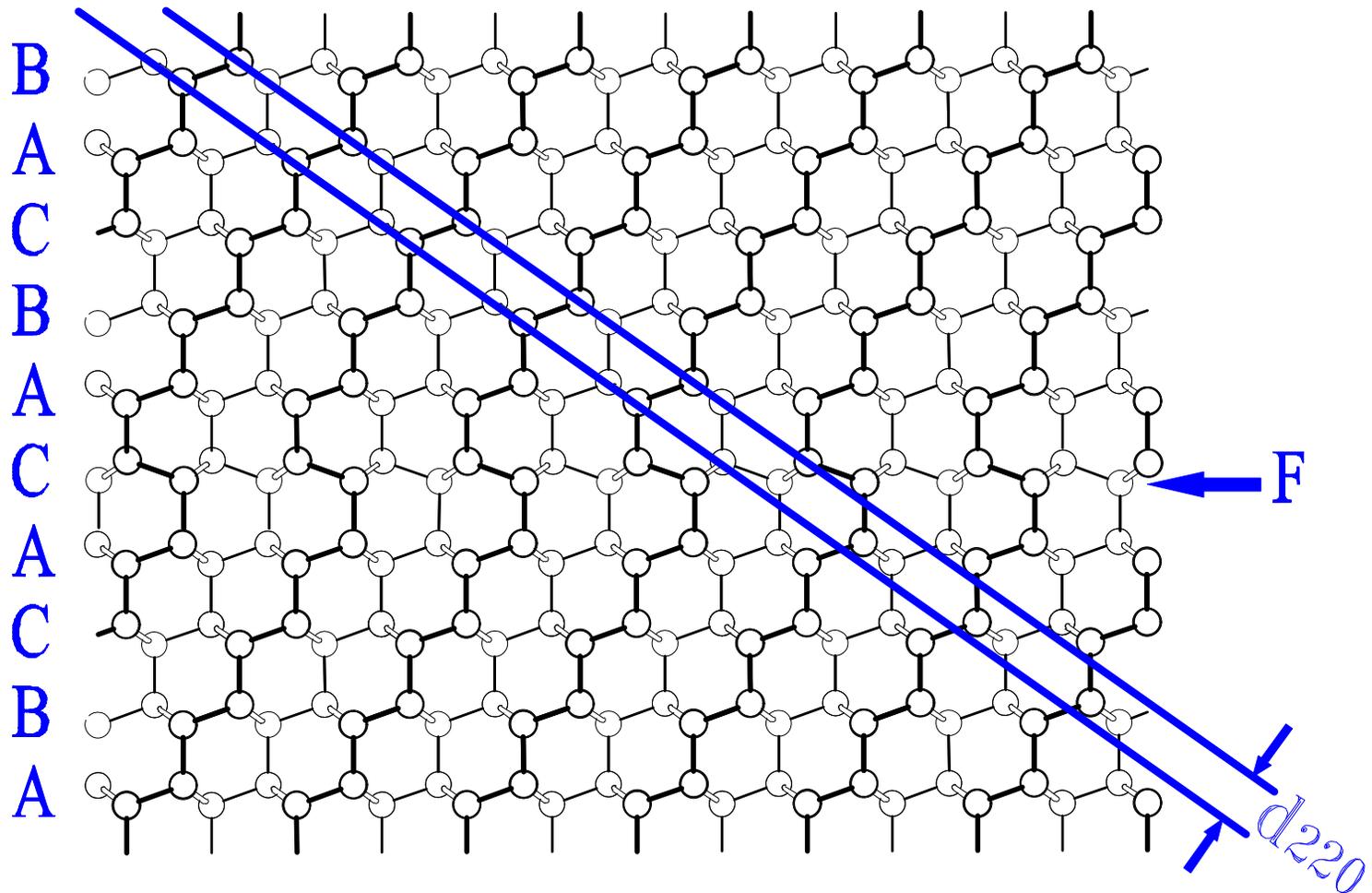


Use CCD and scan sample position

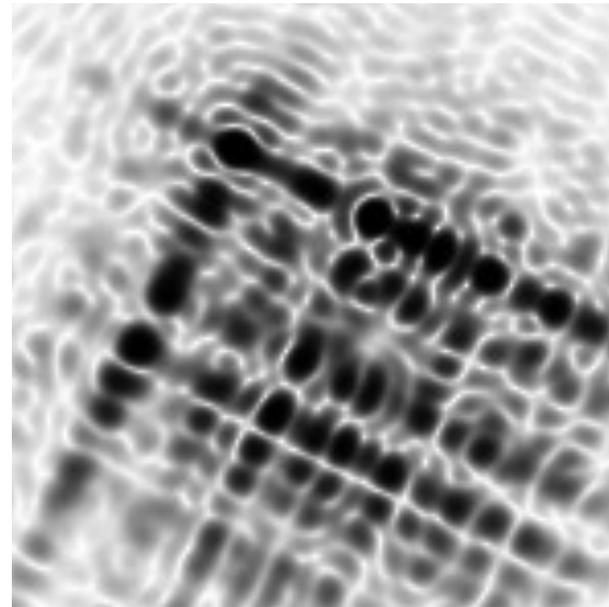
(2,0,1.92) 280nm thick $\text{Ge}_{0.3}\text{Si}_{0.7}$



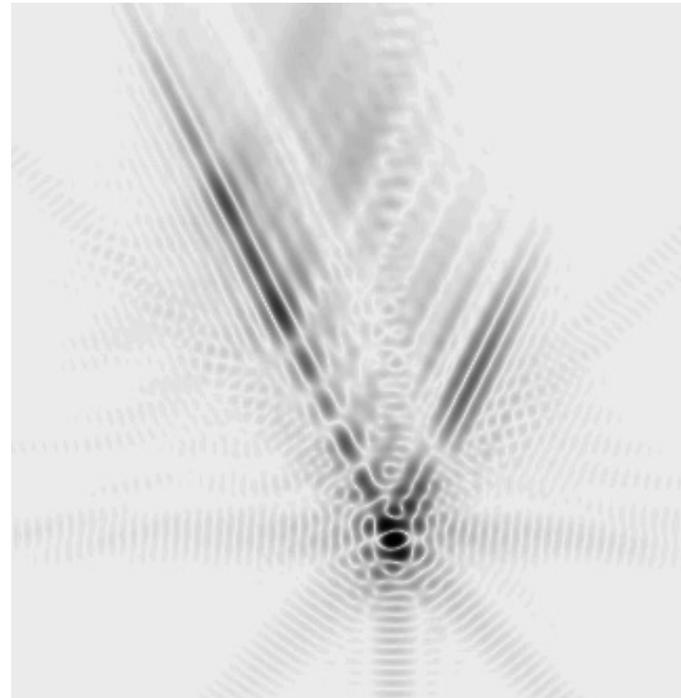
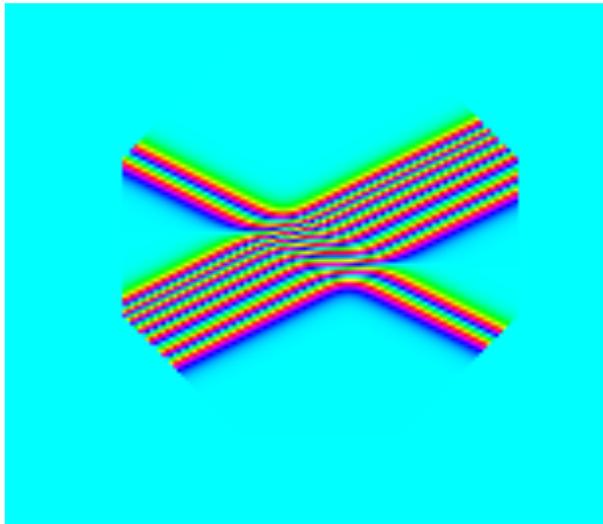
Deformation fault in Silicon



Dislocation Diffraction



Simulation of GeSi data



Conclusions and Outlook

- Inversion of CXD demonstrated
- Internal structure of Au Nanocrystals
- Phasing by computation instead of lens
- Preservation of coherence upon focussing
- Dislocations give asymmetric patterns
- Strain fields should be accessible by inversion