Coherent Hard X-ray Scattering and Imaging

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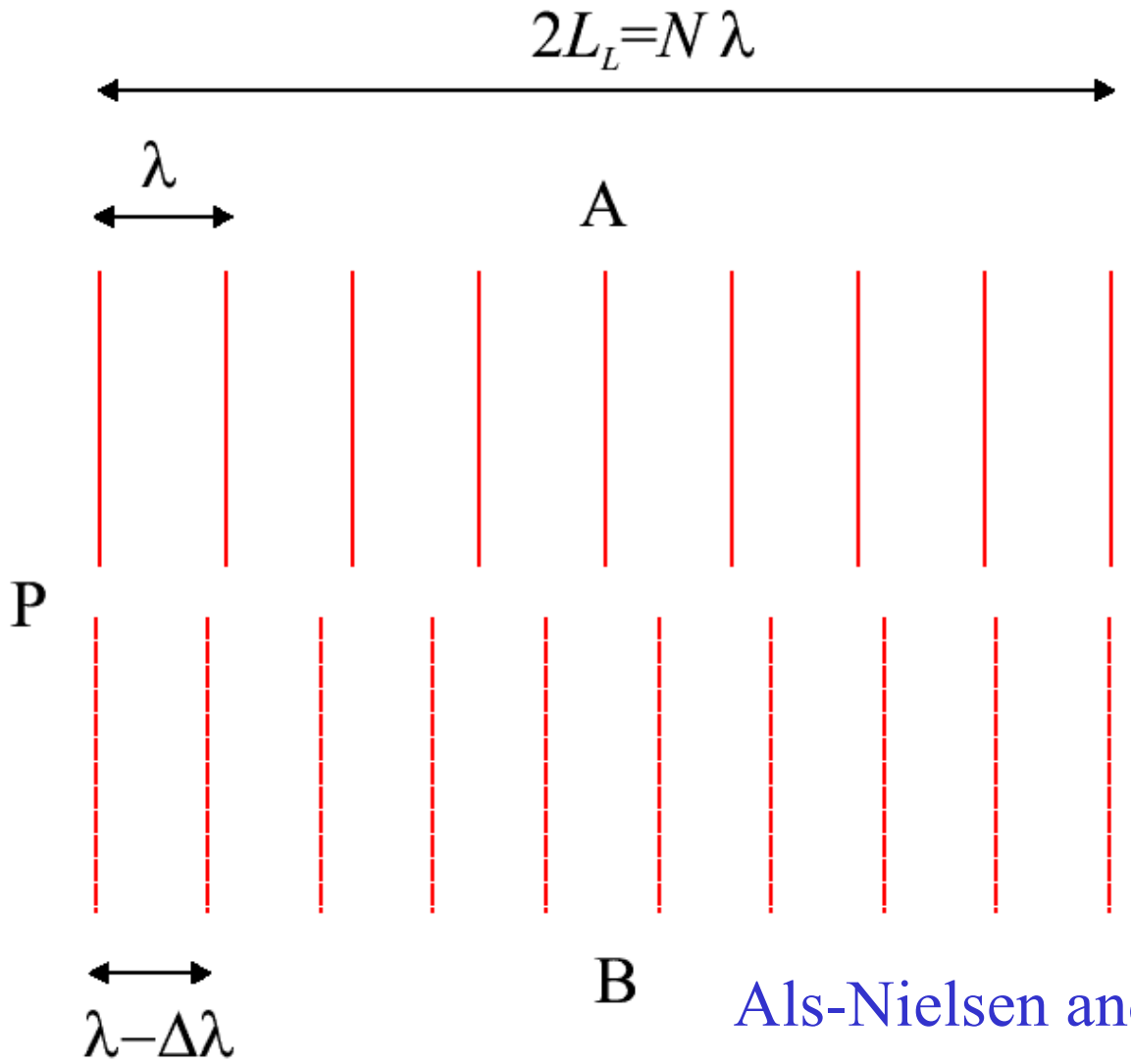
Workshop on emerging new directions of synchrotron research with soft X-rays VUV and Infrared

SRC, Madison, September 2004

Outline

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

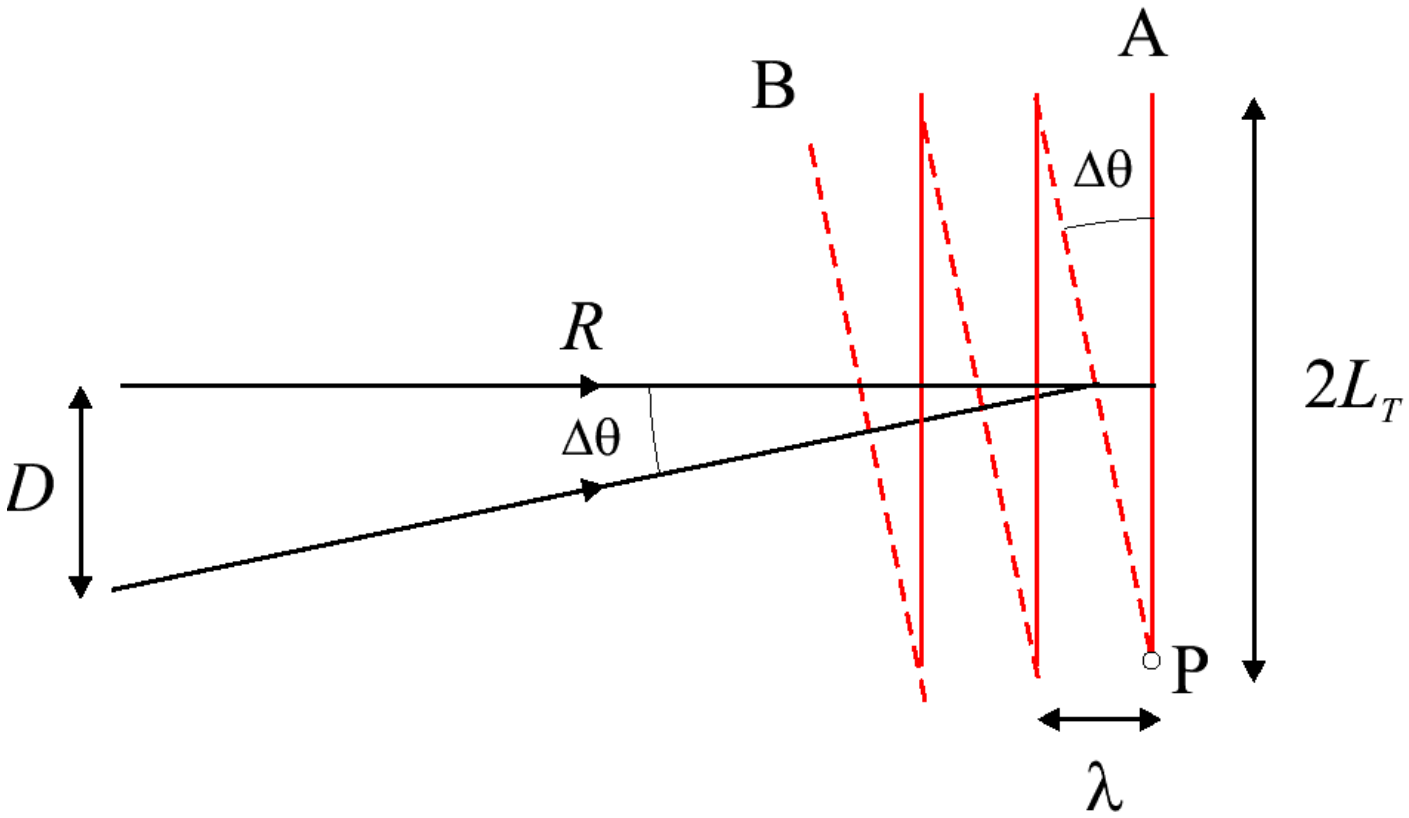
Longitudinal Coherence



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

Als-Nielsen and McMorrow (2001)

Lateral (Transverse) Coherence



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

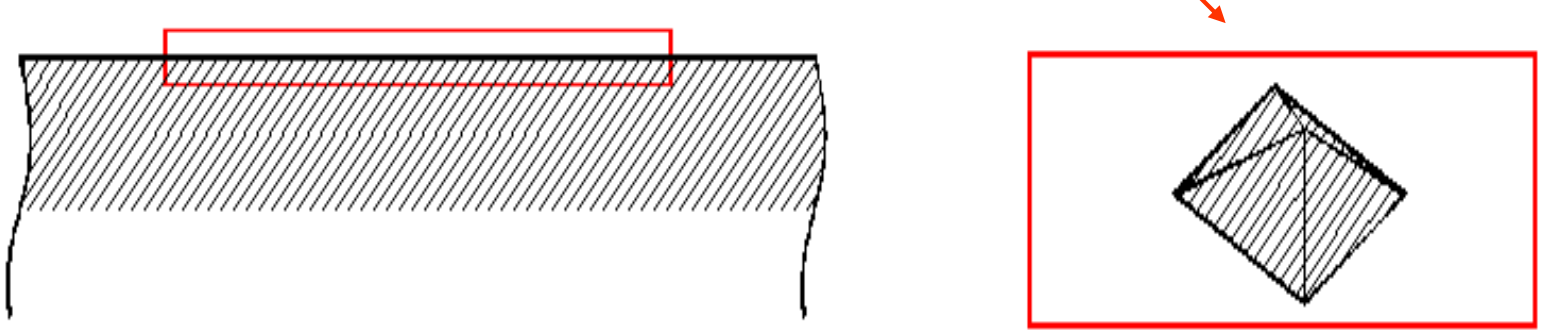
Als-Nielsen and McMorrow (2001)

Coherence at the APS or ESRF

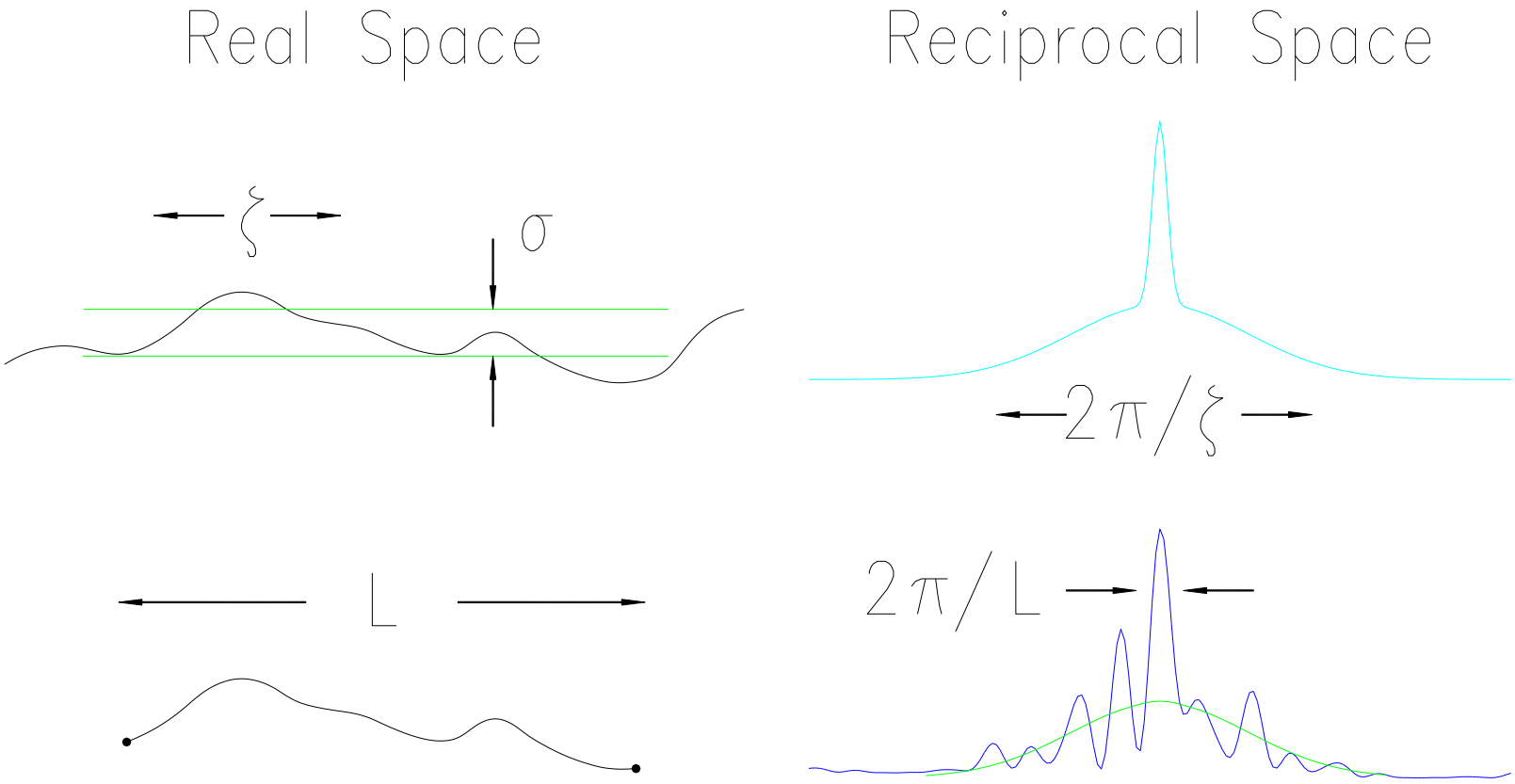
Typical of 3rd Generation (undulator) Synchrotron Source

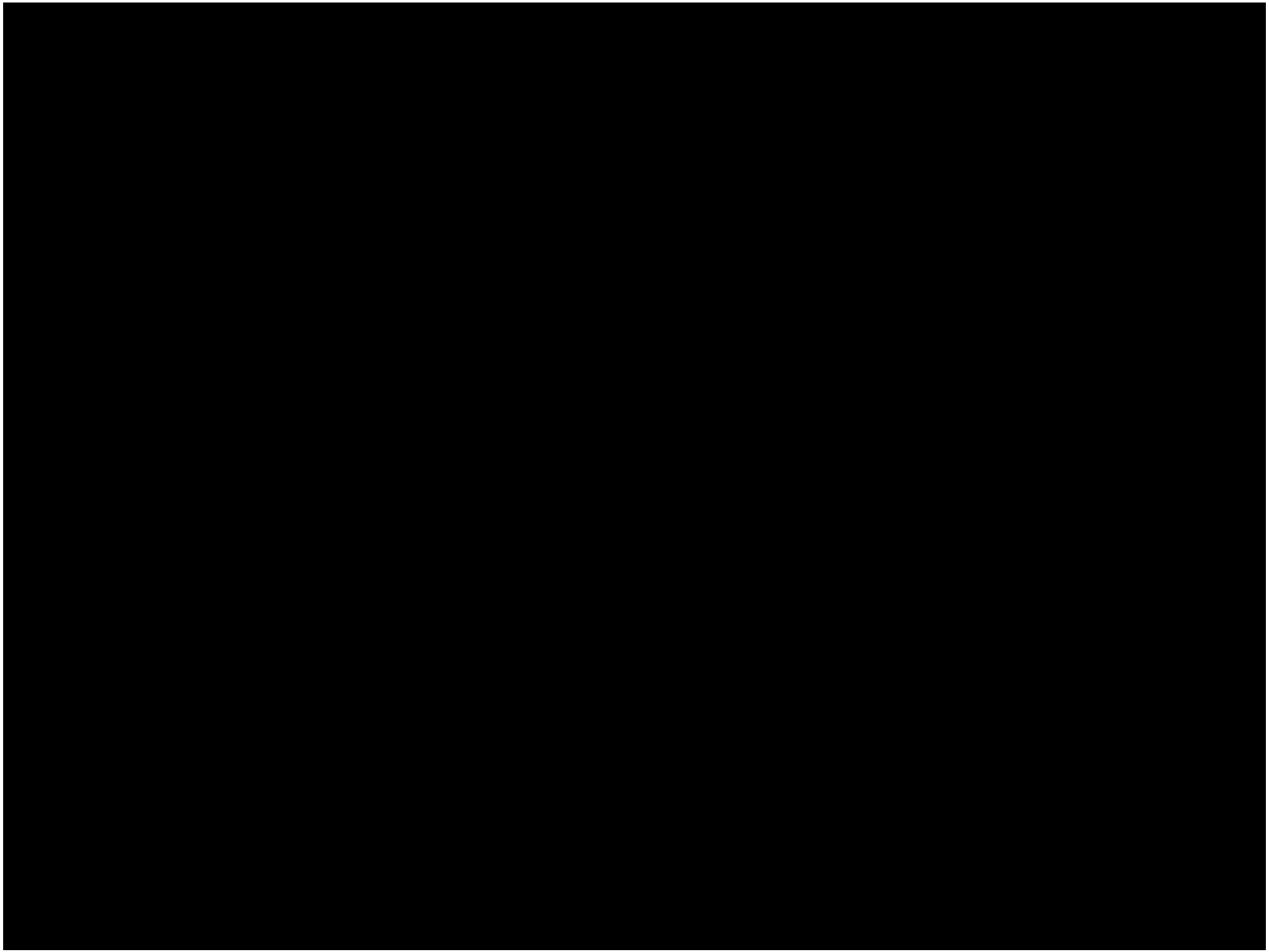
Coherence of	ξ_{VER}	ξ_{HORIZ}	ξ_{LONG}	Flux
Raw Undulator	35μm	9μm	0.004μm	2×10^{12}
Si(111) Monochromator	35μm	9μm	1μm	1×10^{10}
C(111) Monochromator	35μm	9μm	3μm	3×10^{9}

Coherent region defined by slits

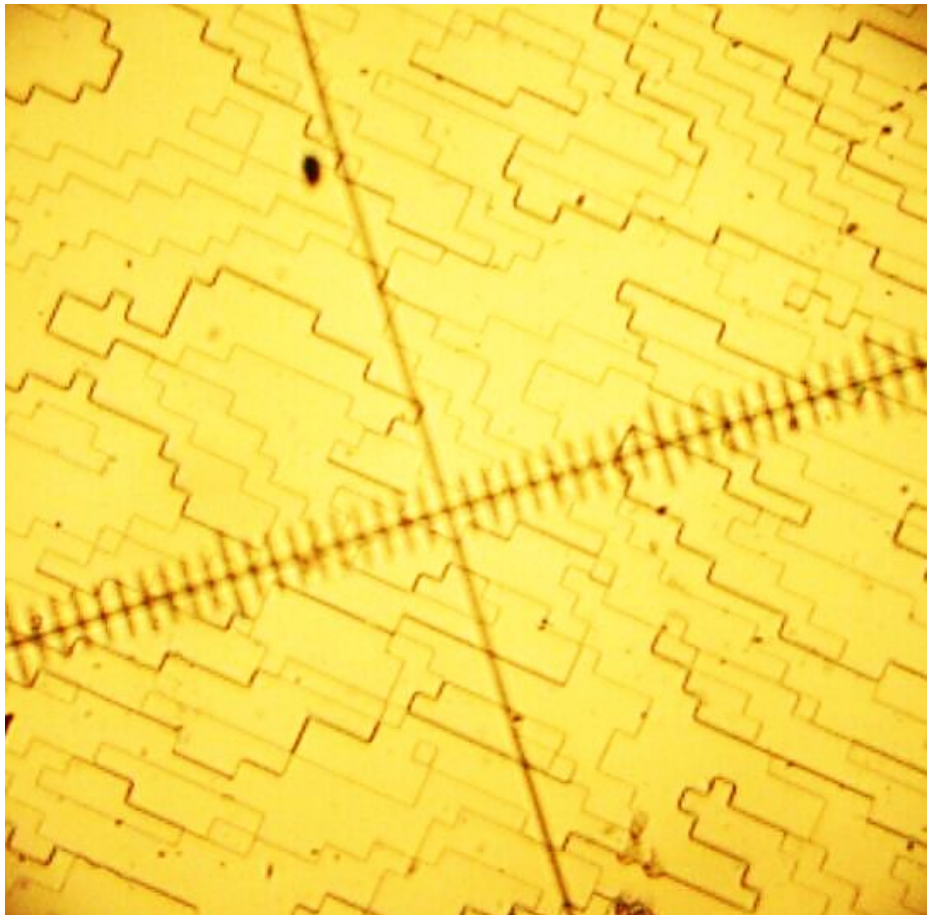


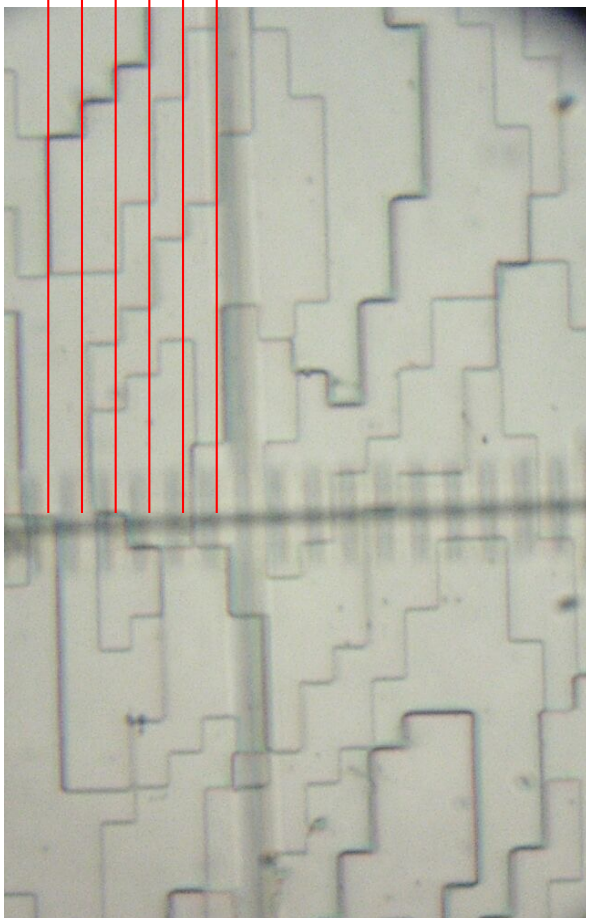
Diffuse Scattering acquires Structure using CXD

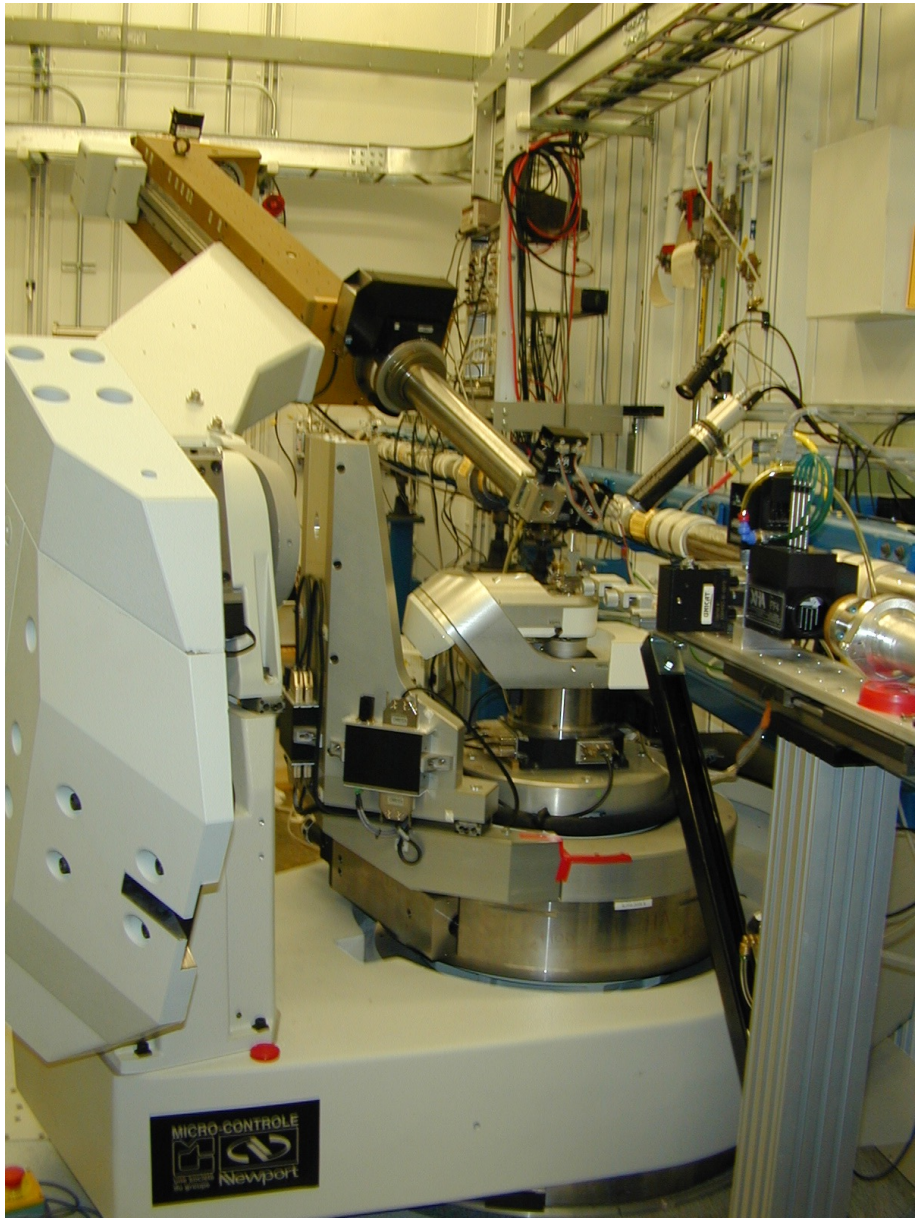


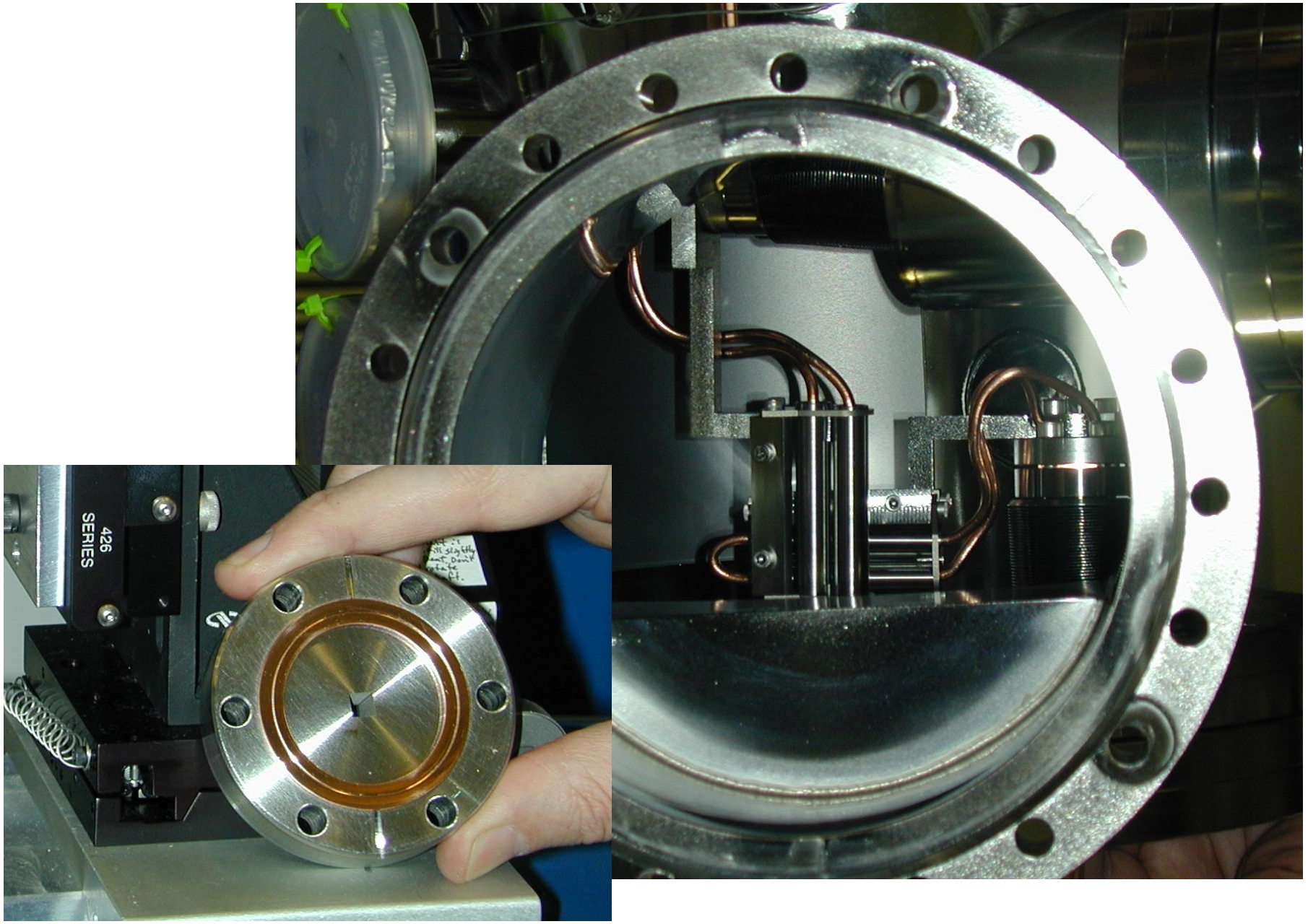


Microscope Images of Gratings

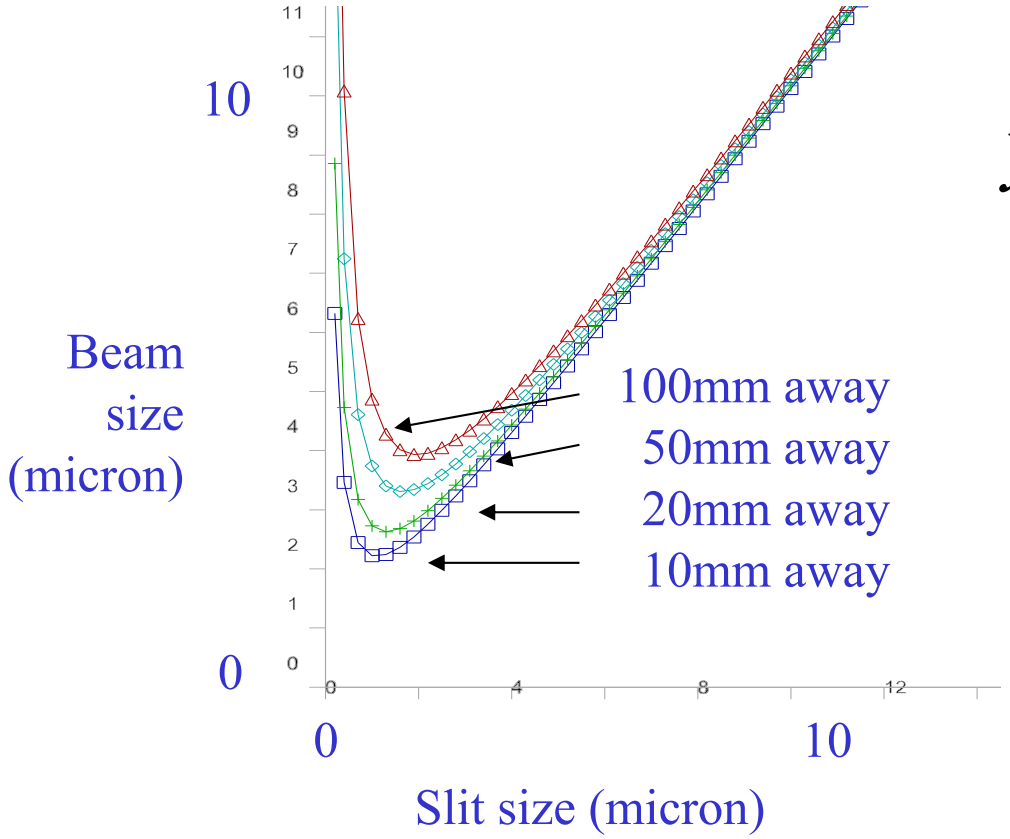




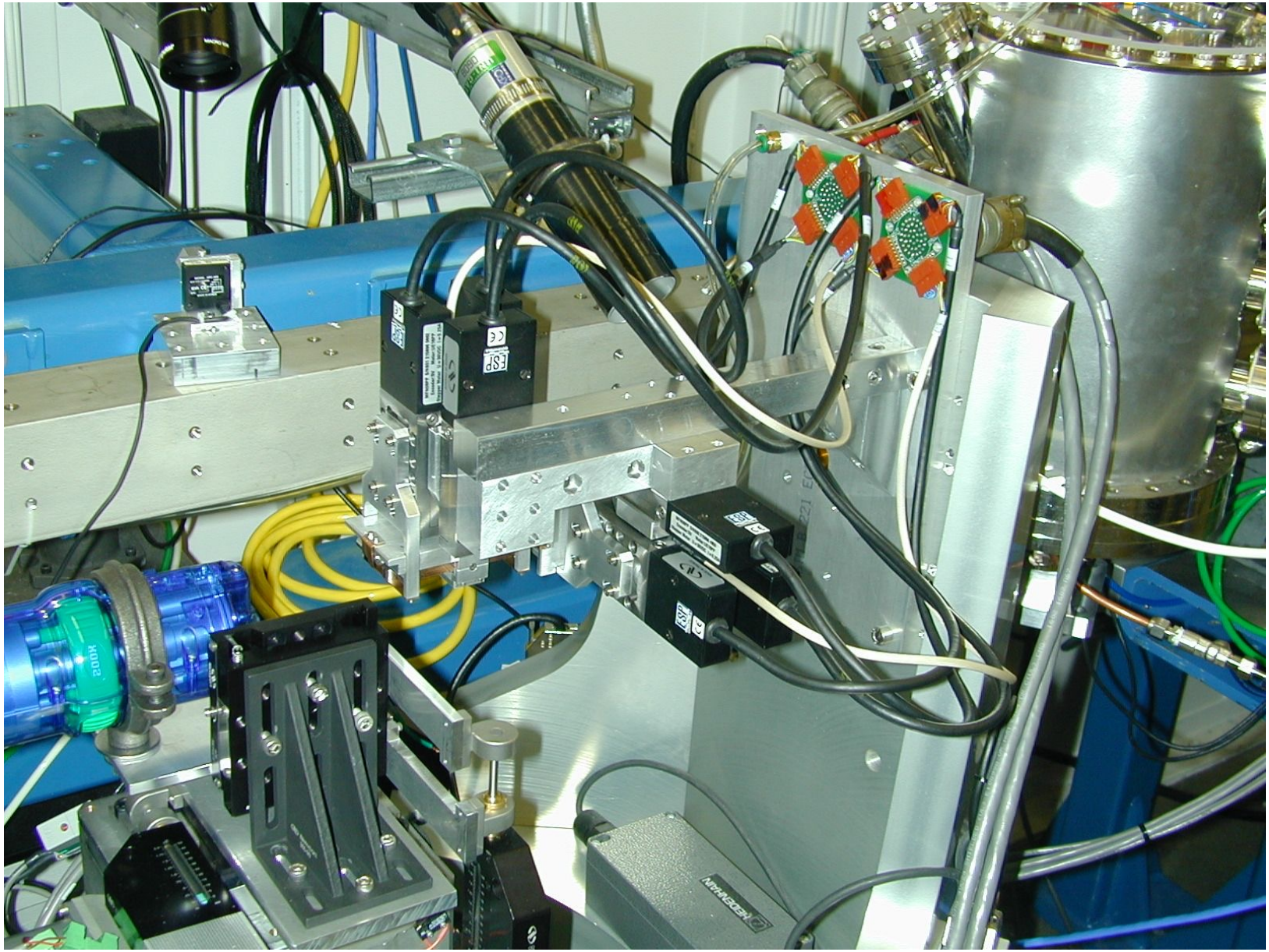

MICRO-CONTROLE
Newport


426
SERIES

Smallest Beam using Slits (9keV)

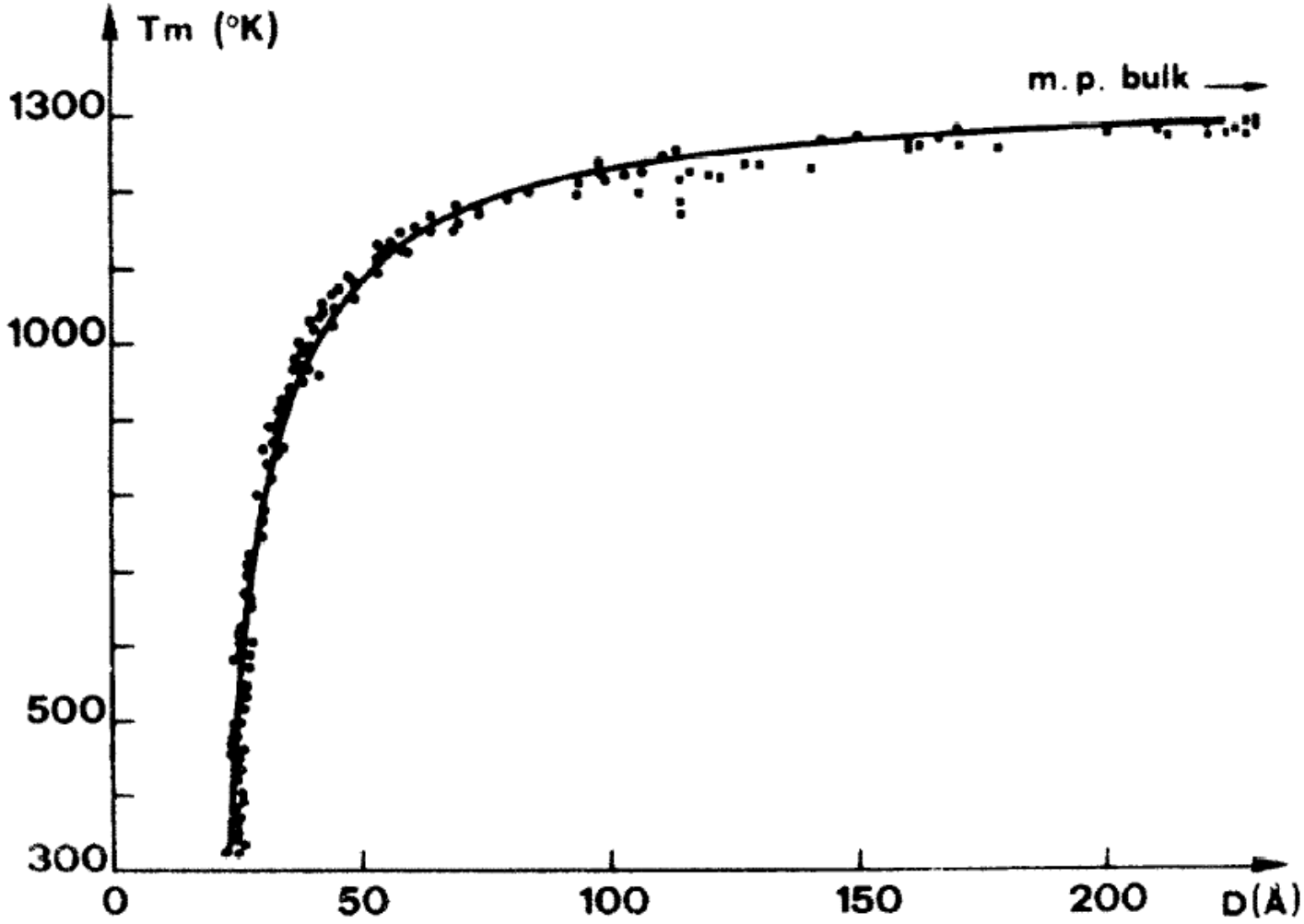


$$y(x) = x + \frac{\lambda d}{x}$$

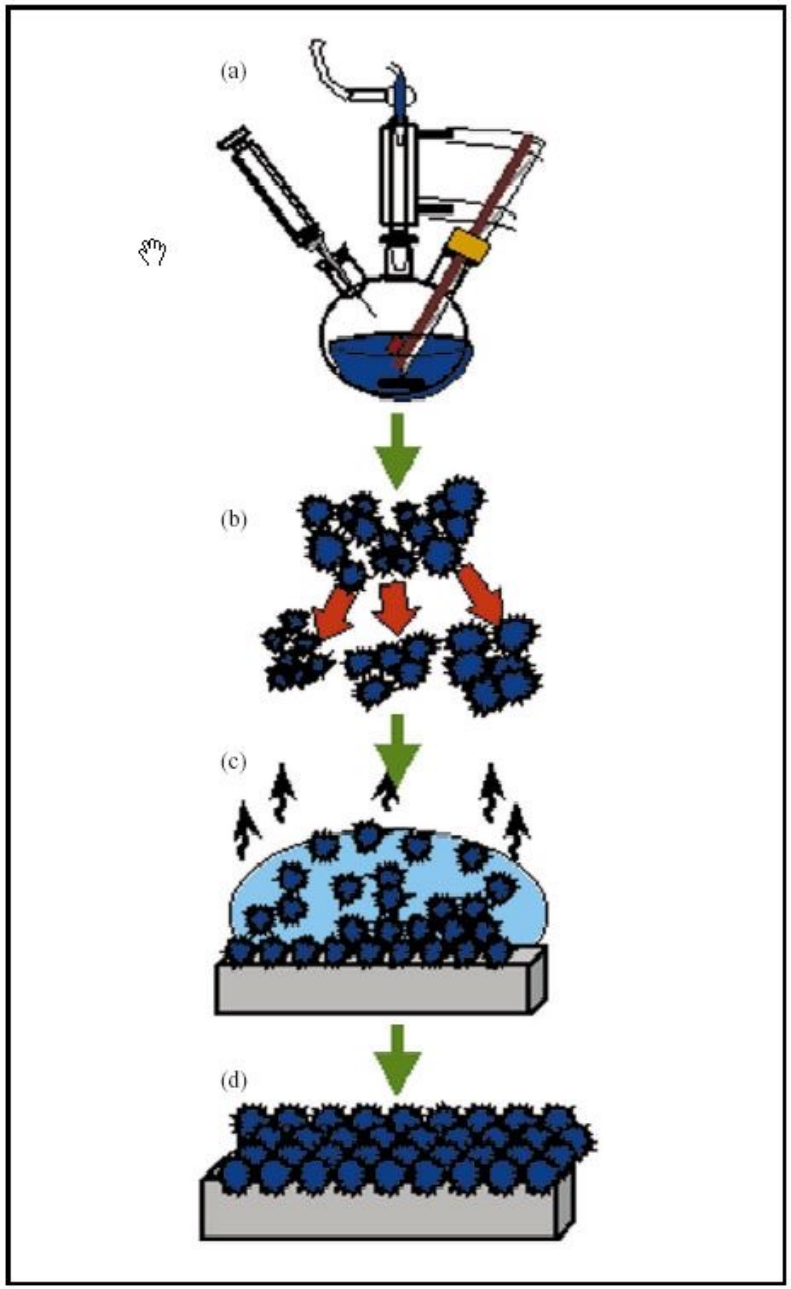

ESP
CE
200W

Size-dependent Melting of Au Particles

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

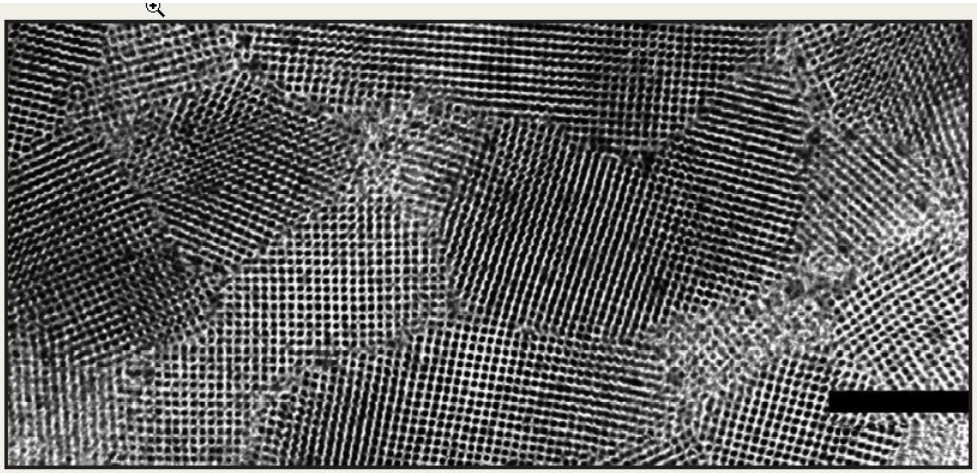


Chemical Synthesis of Nanocrystals



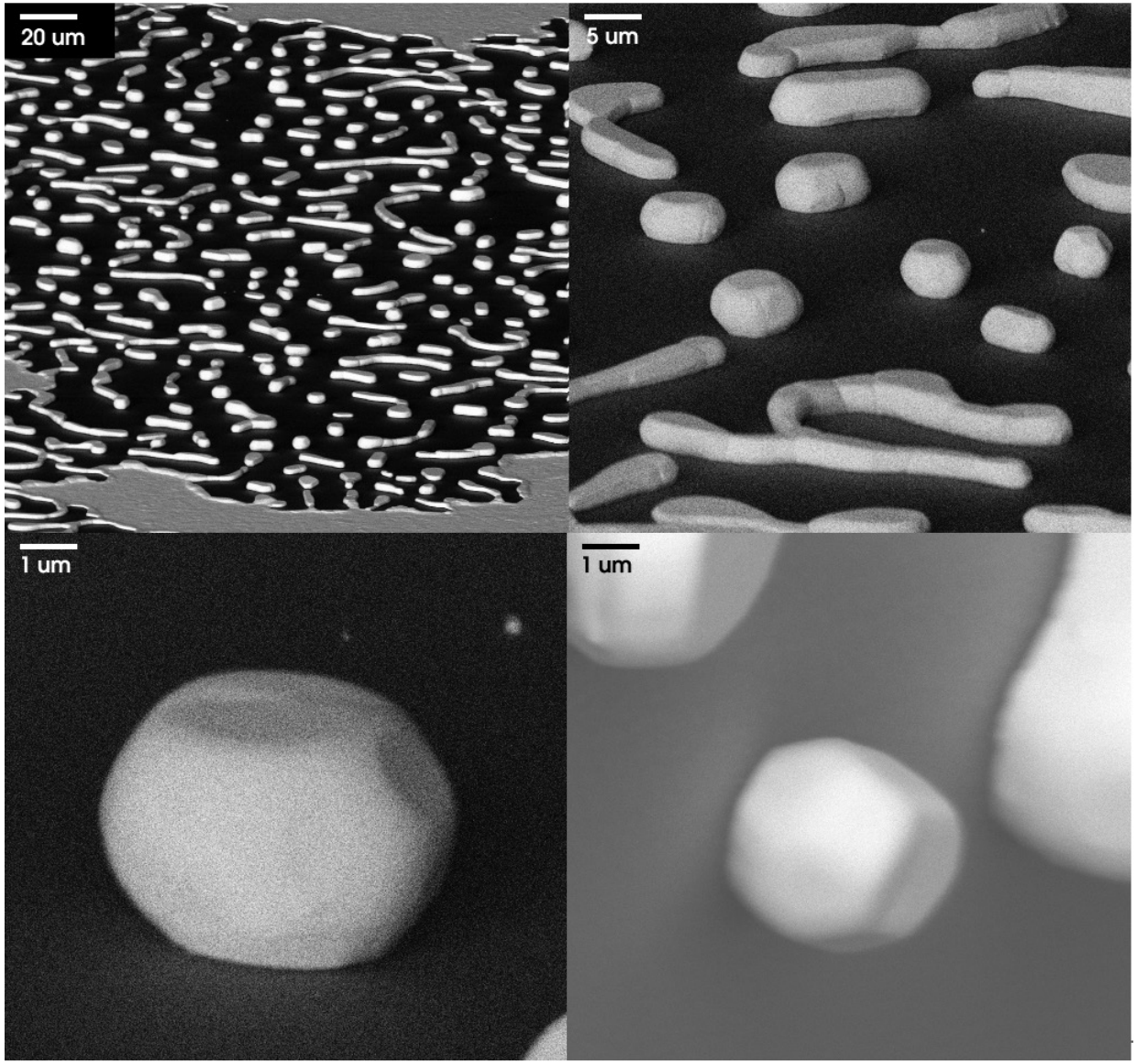
- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

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

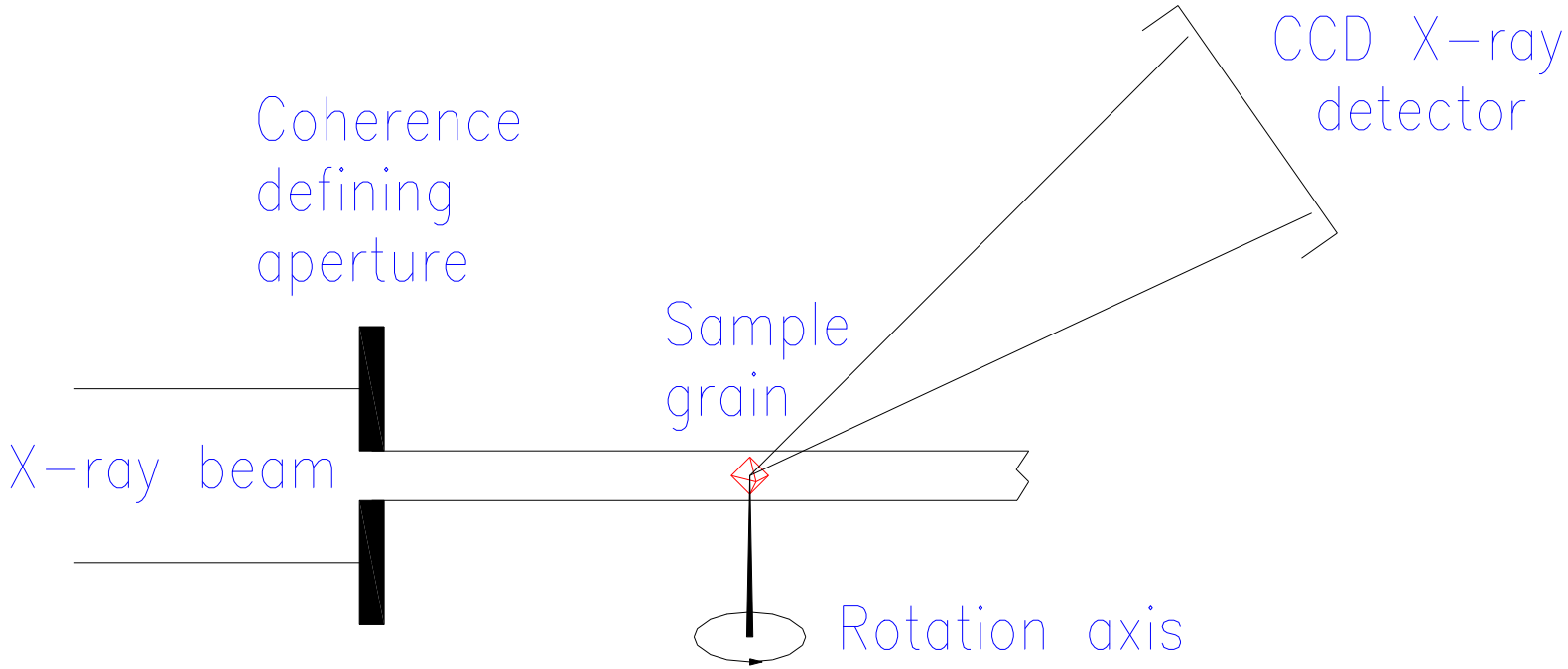


SEMS

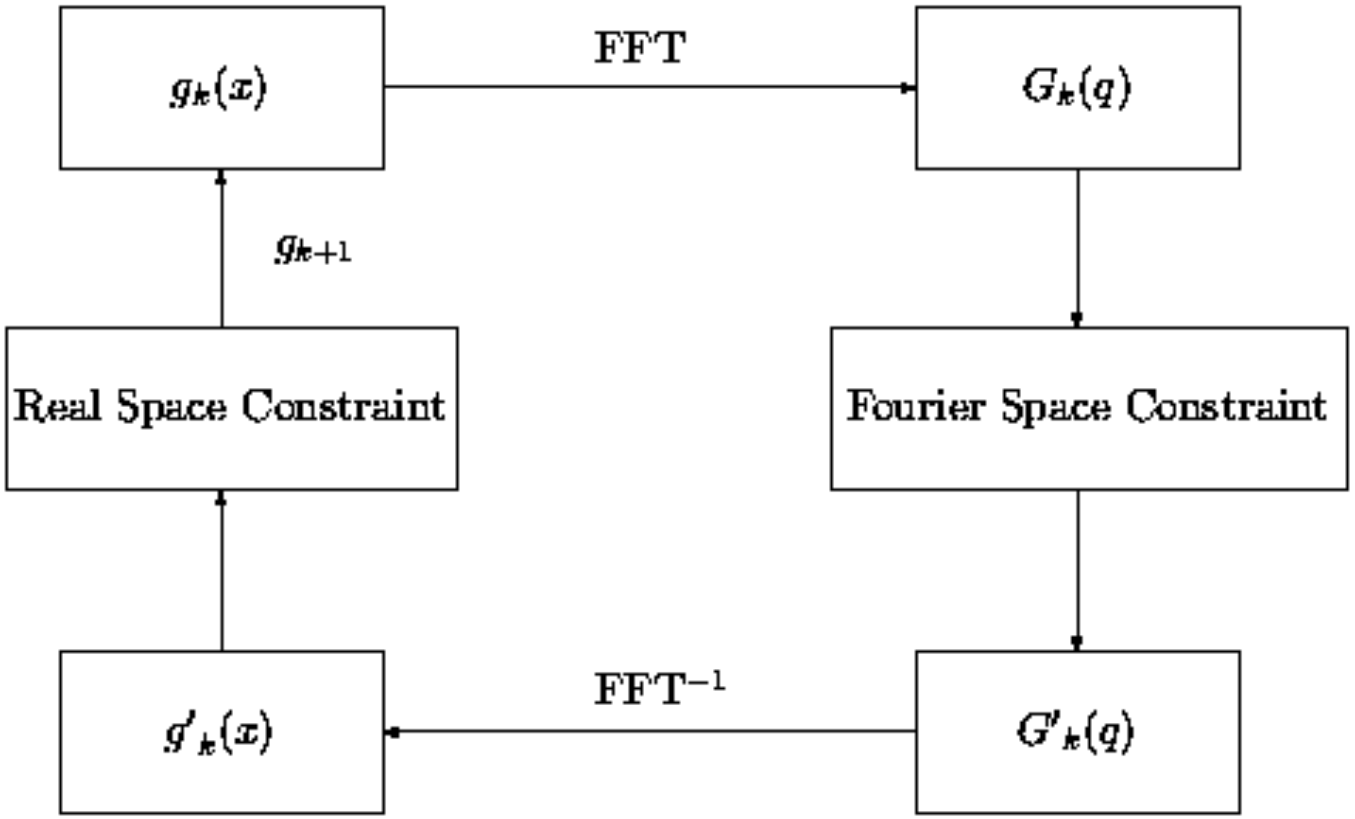
- Au blanket film
- Quartz substrate
- Annealed at 950°C for 70 hrs.



Lensless X-ray Microscope



Generic "Error Reduction" method

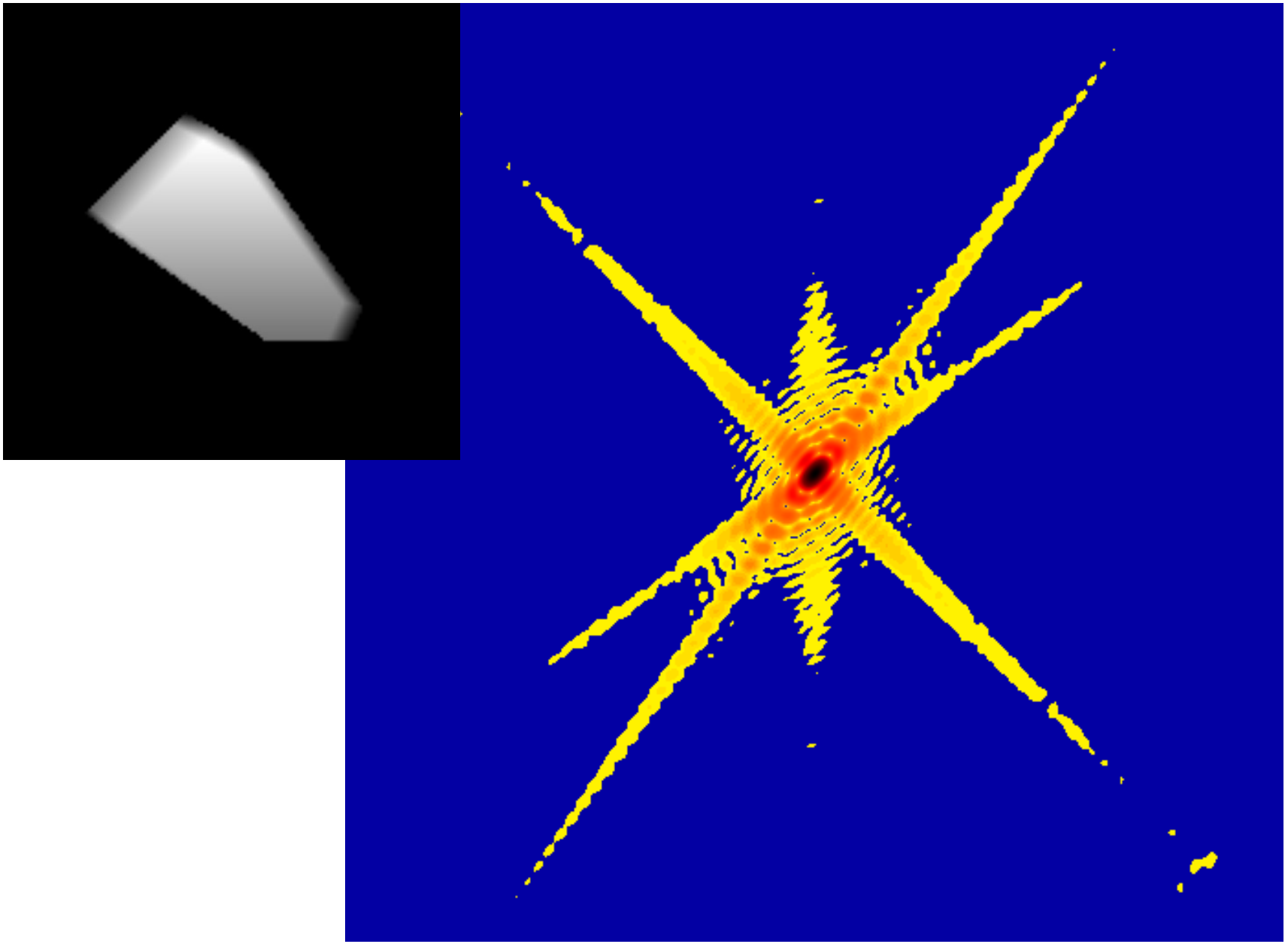


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

Real-space Constraints in Crystallograhy

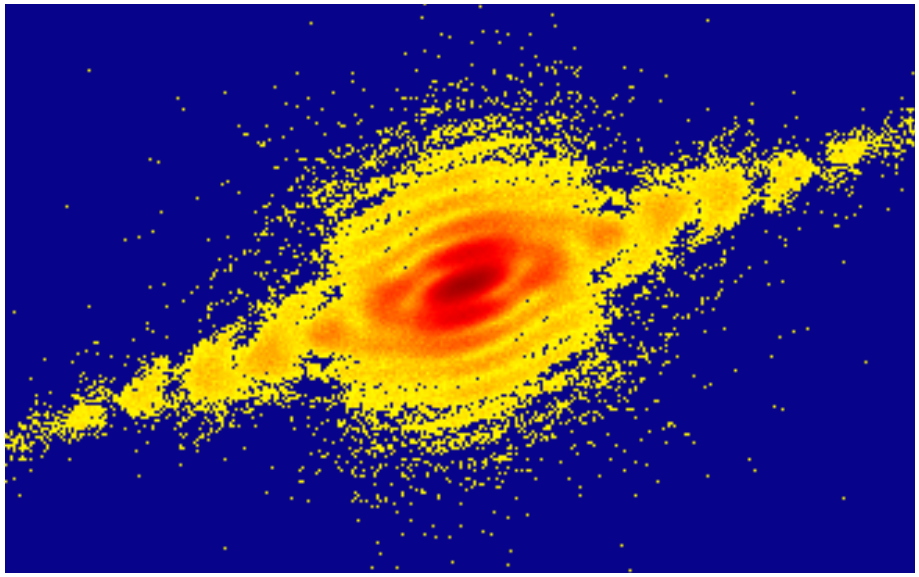
R. P. Millane, J. Opt. Soc Am. A 13 725 (1996)

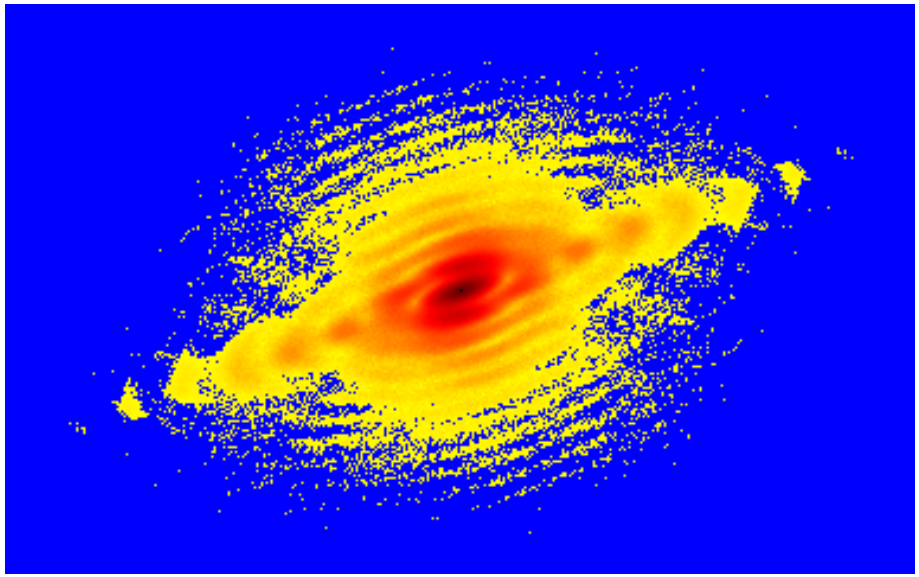
- 'Positivity' and 'Atomicity' constraints (Sayre)
- Finite support, molecular envelope
- Solvent flattening/Molecular replacement
- Non-crystallographic symmetry
- Non-uniqueness is 'pathologically rare' (d>1)
- Uses memory to avoid stagnation (Fienup HIO)

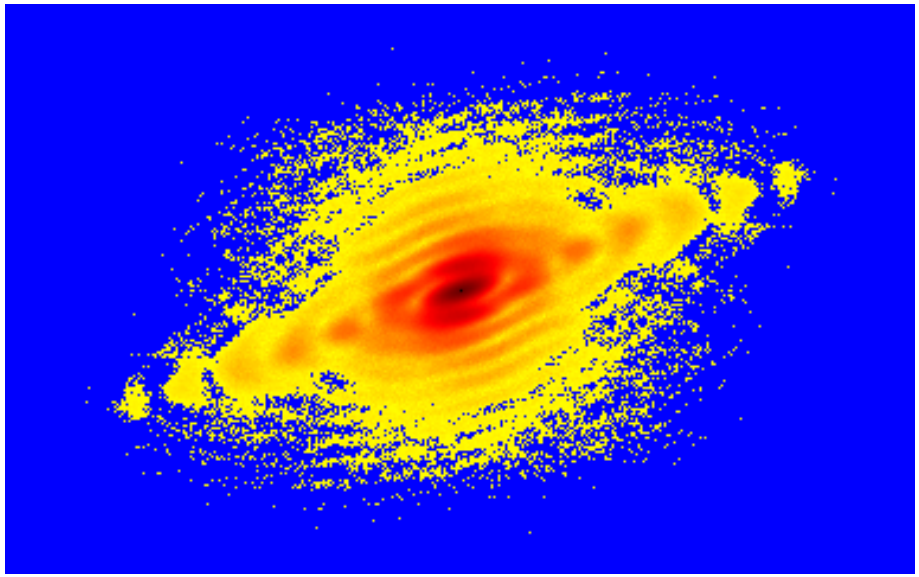


Symmetrized Data and two best fits

Chisq=0.0005

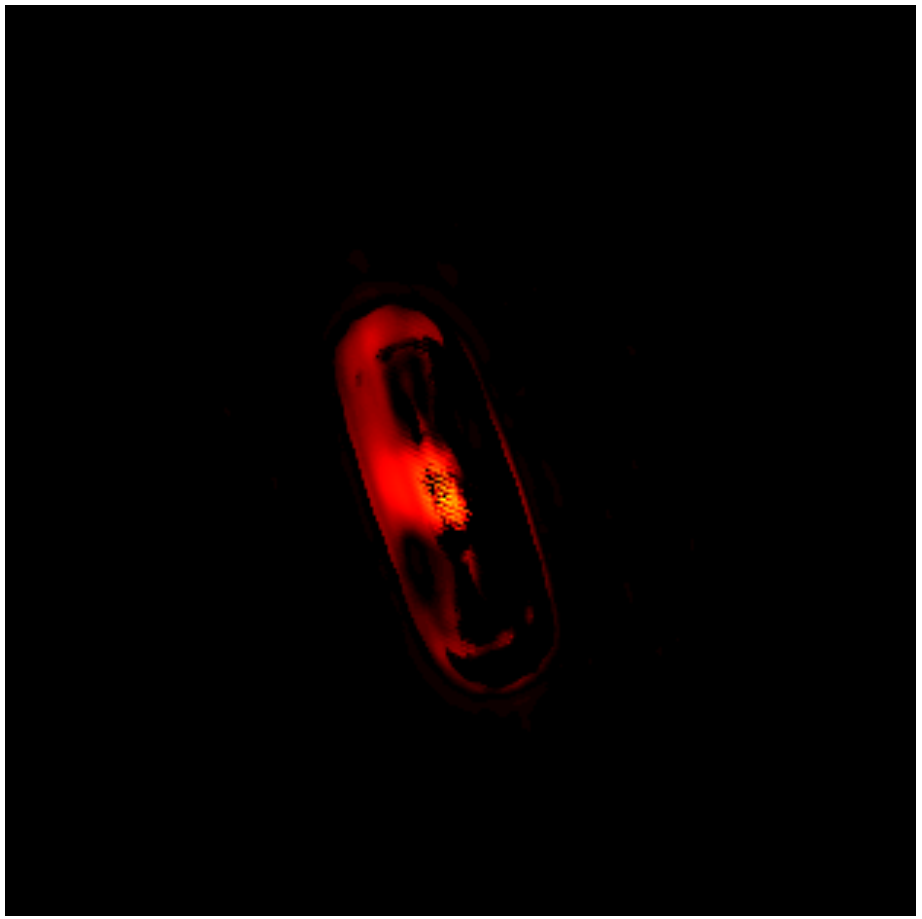


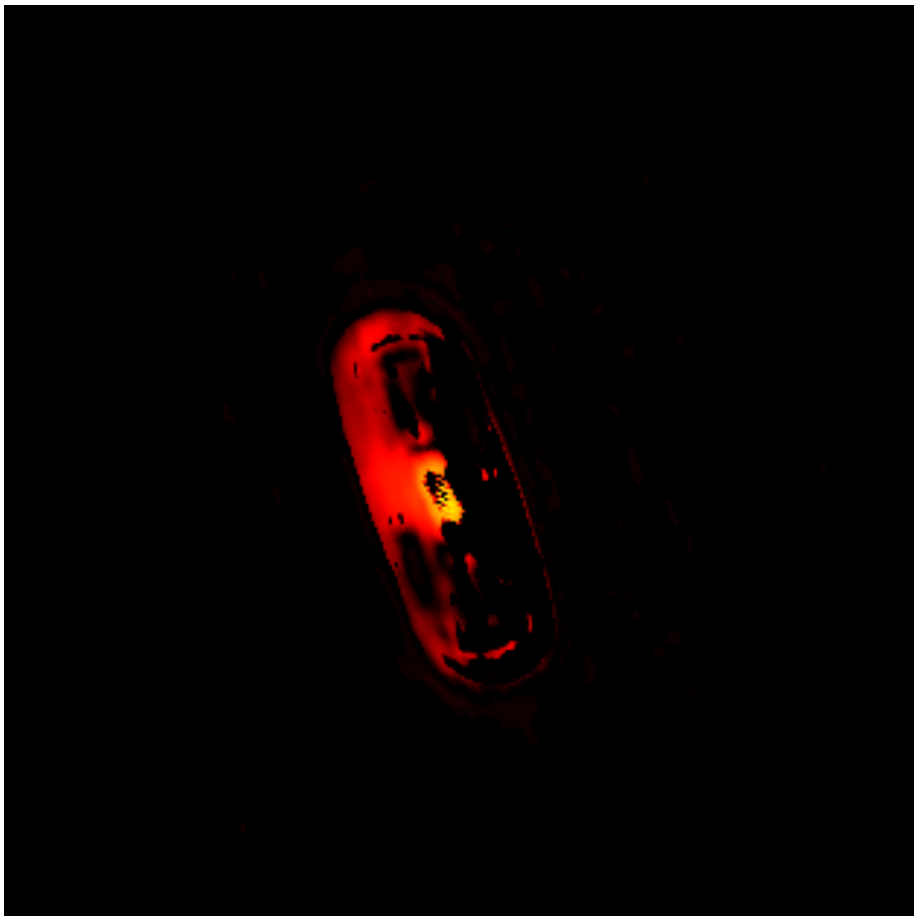




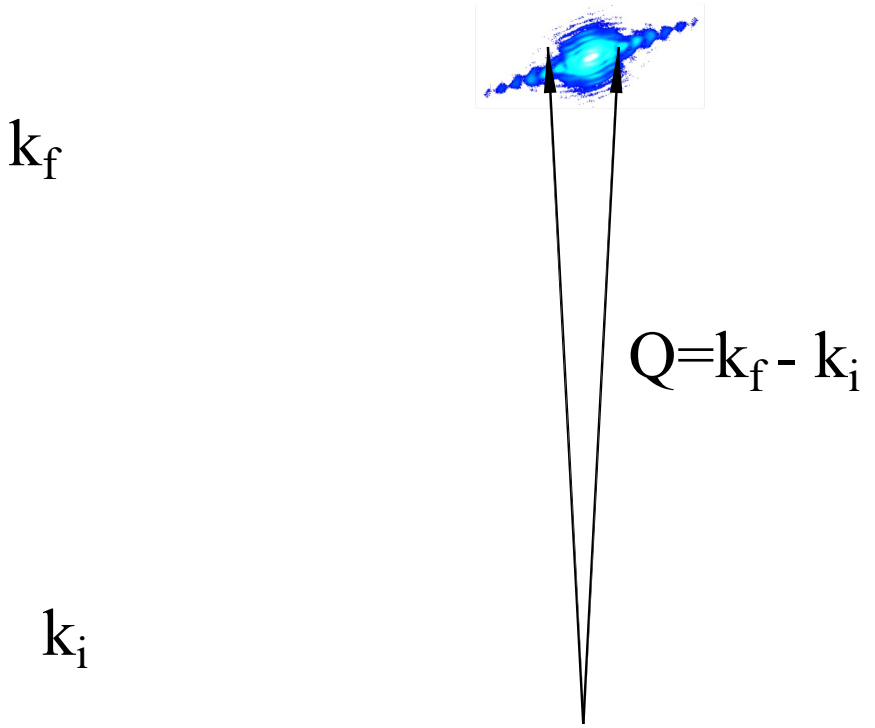
2D Reconstructions

chisquare = 0.0005

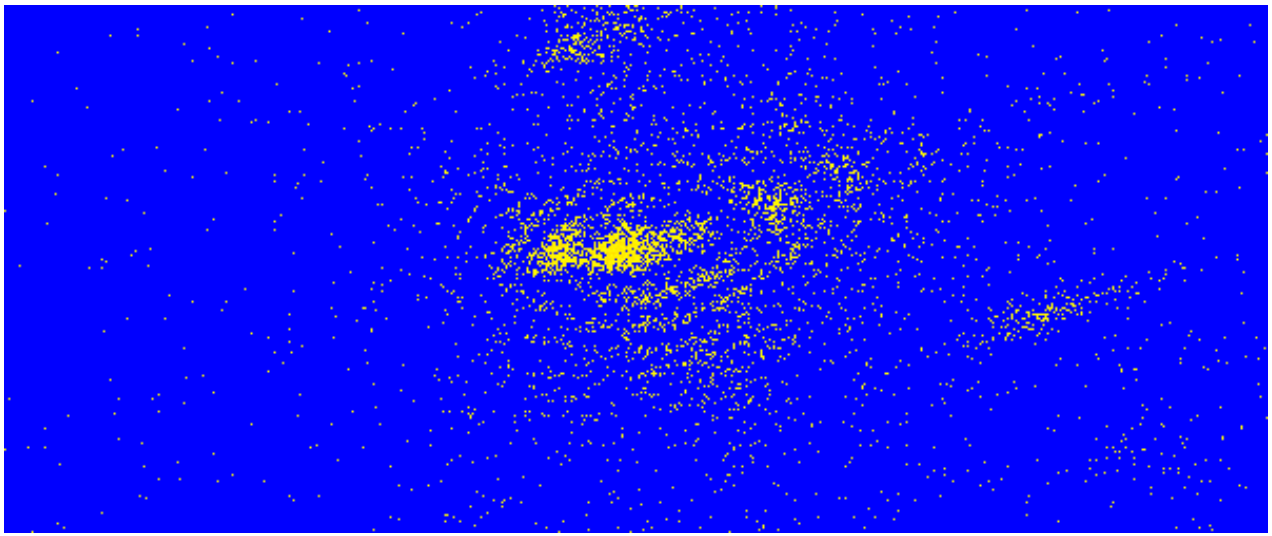


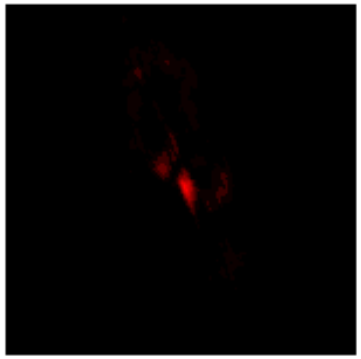
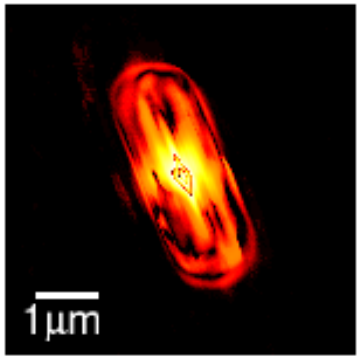


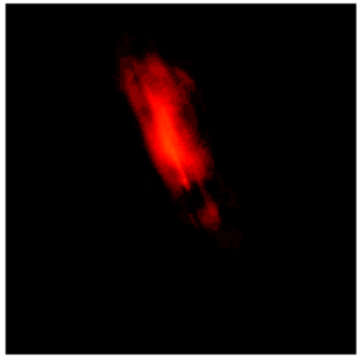
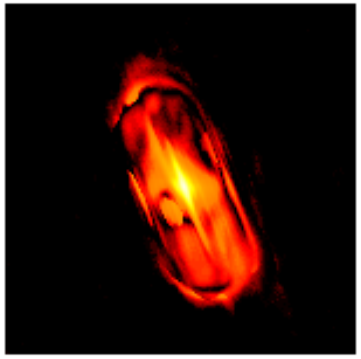
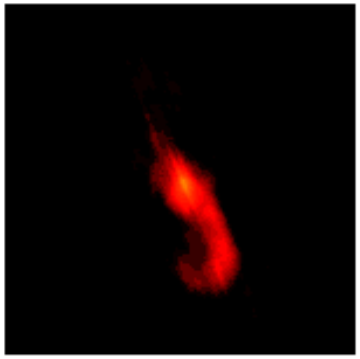
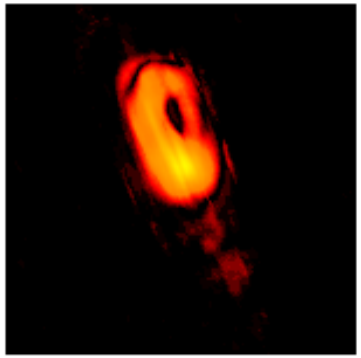
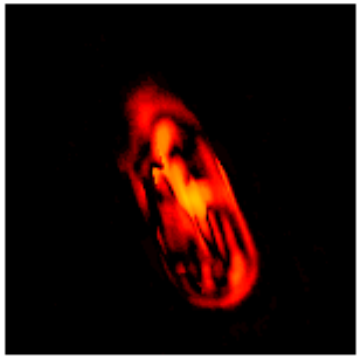
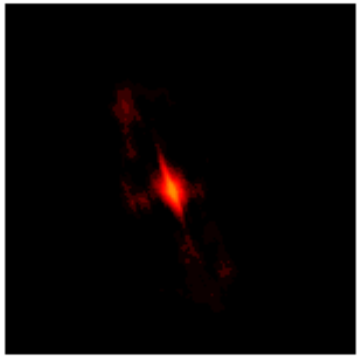
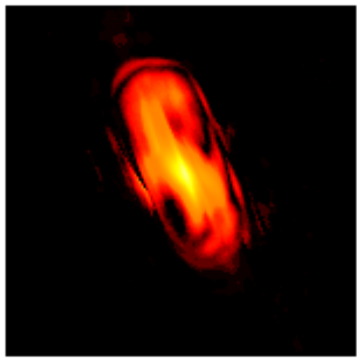
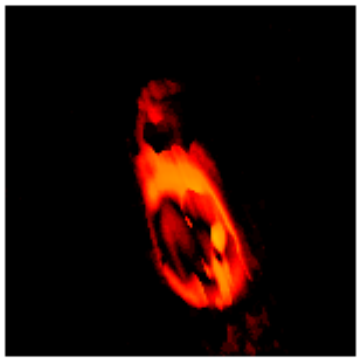
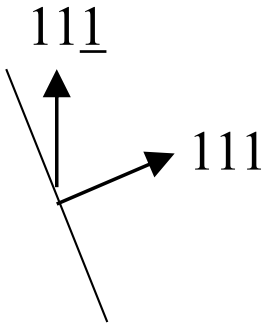
3D Diffraction Method



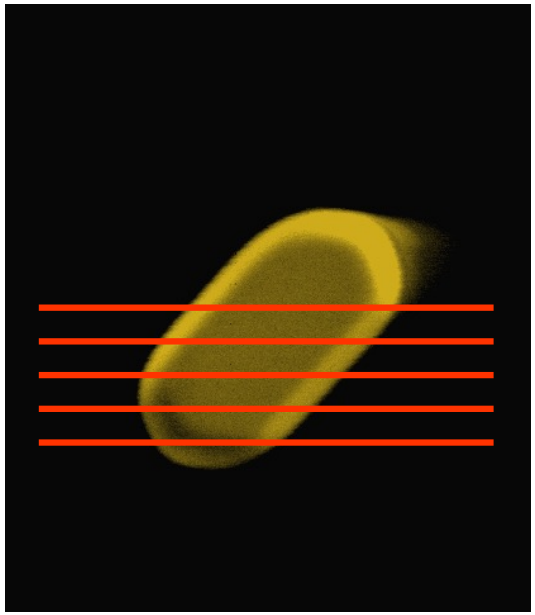
3D Diffraction Data
1 micron Au crystal



Slices through plan view SEM:

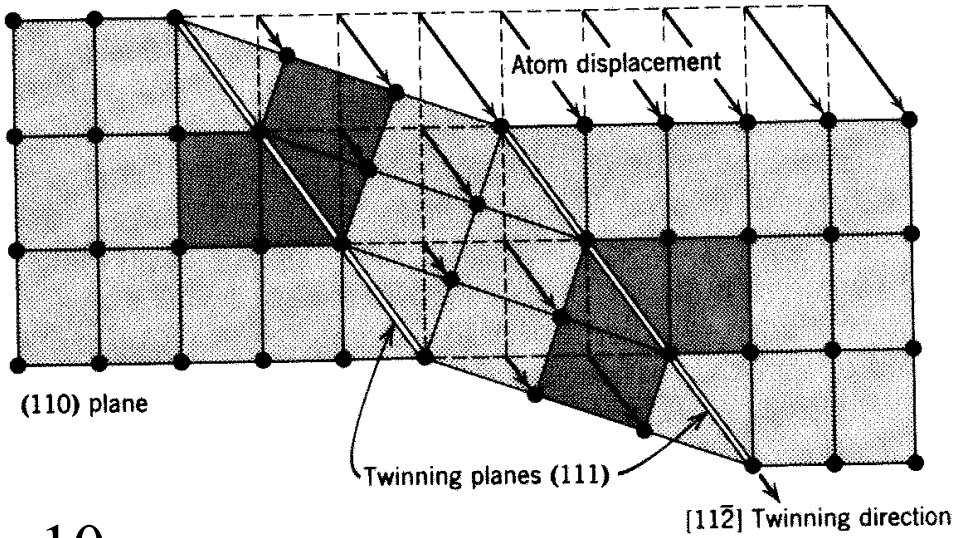


Twinning in deformed FCC metals

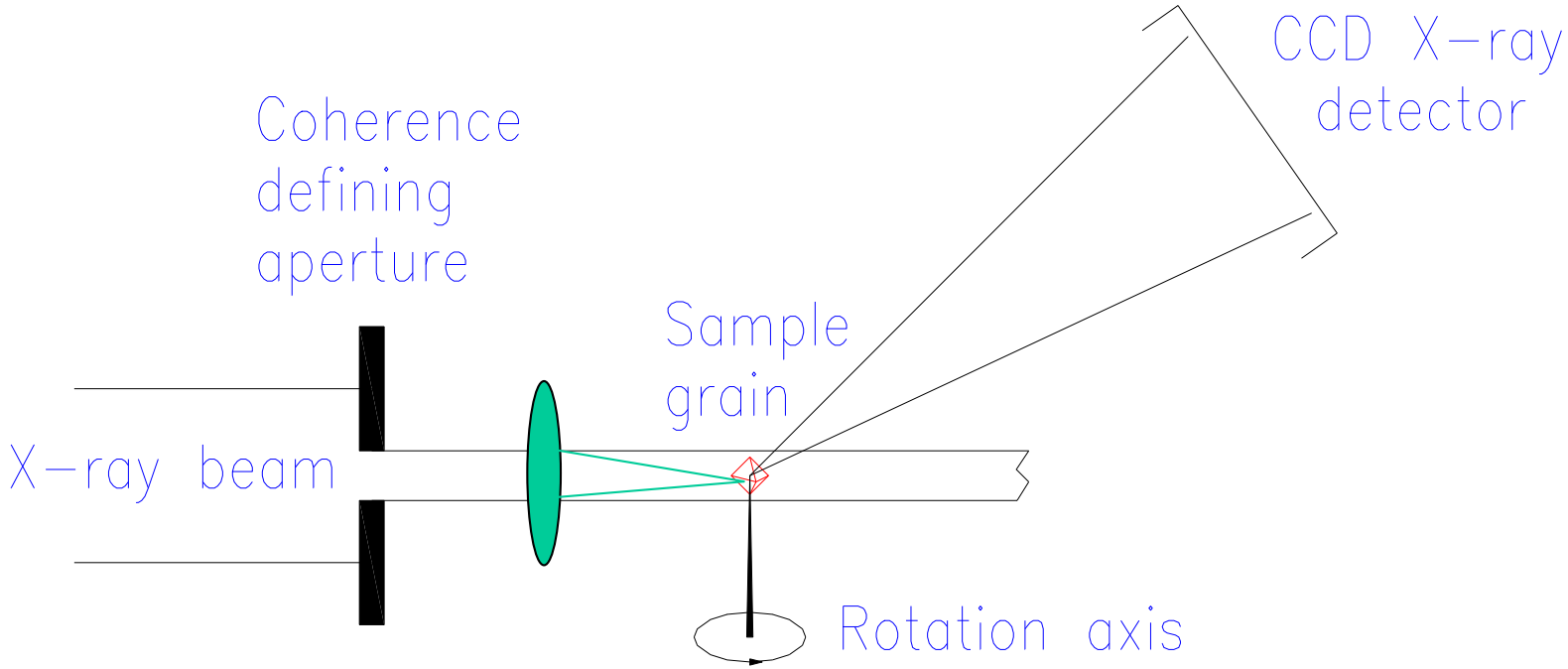
J. Wulff, "Structure and Property of Materials III" (1965)

~10μm

Cu



Lensless X-ray Microscope

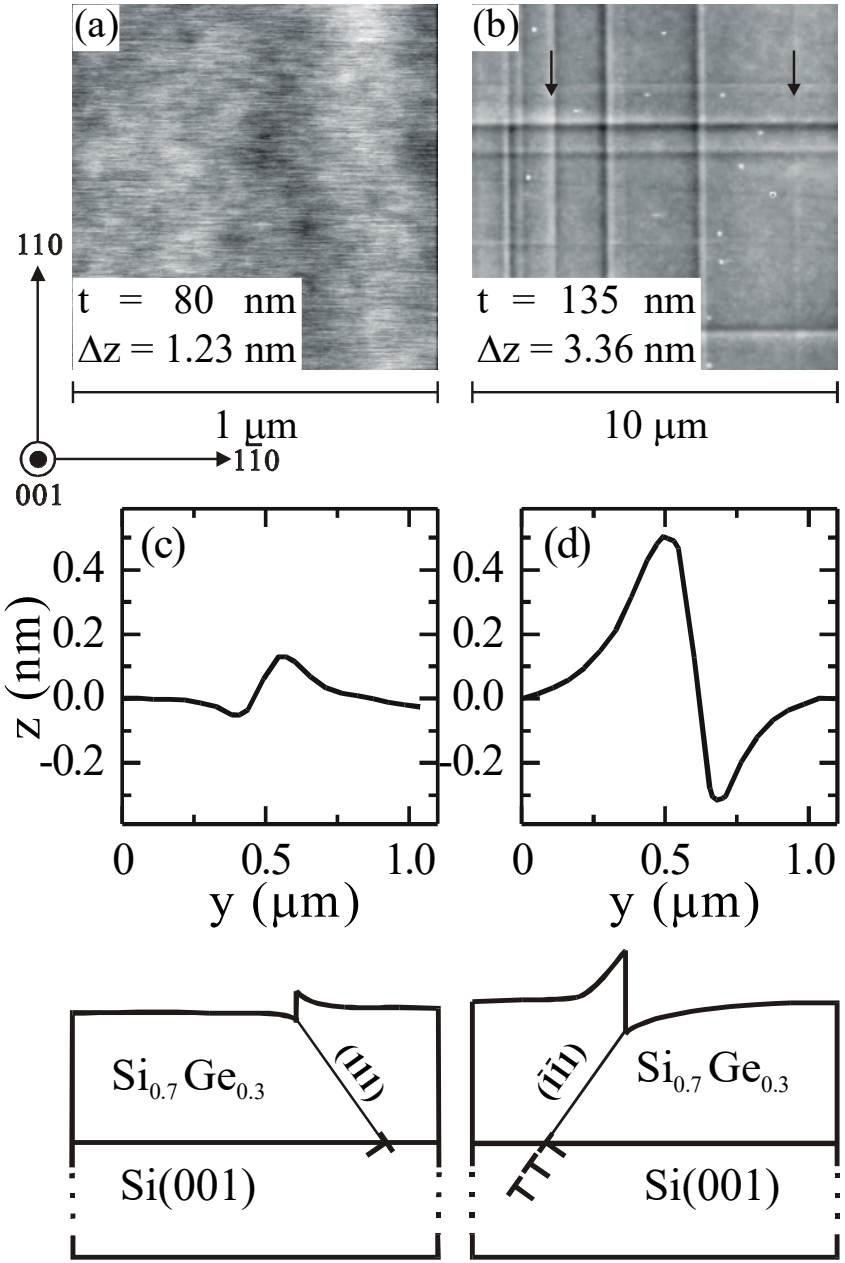


Low dislocation density GeSi films

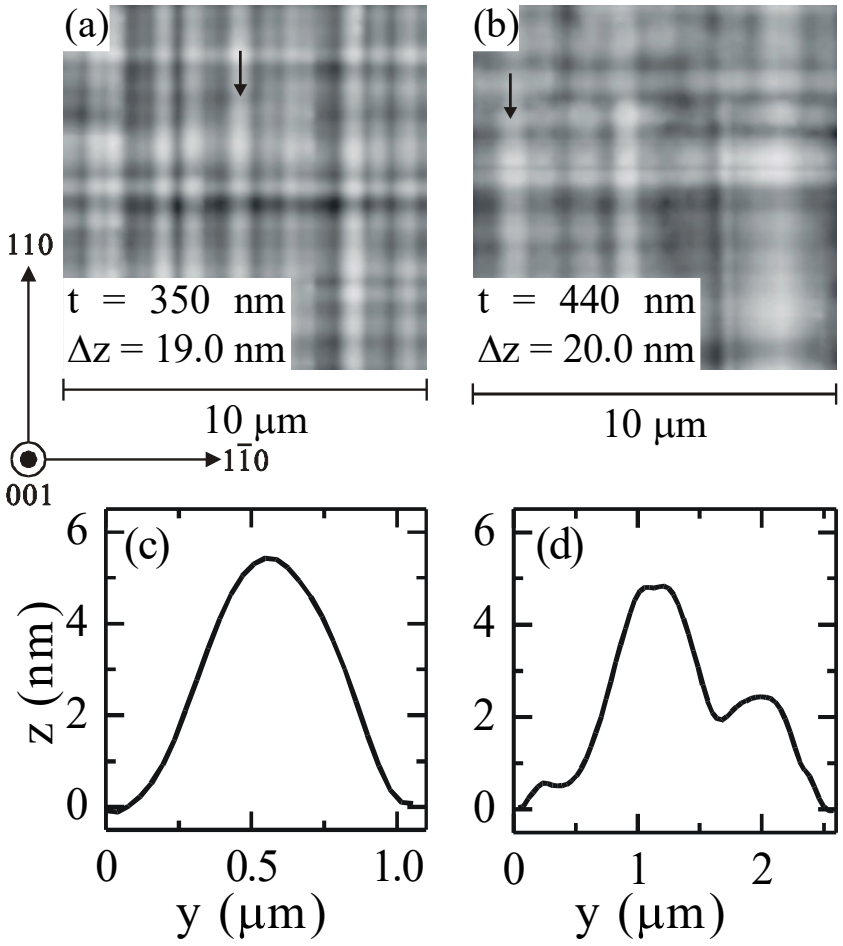
Thickness close to critical thickness

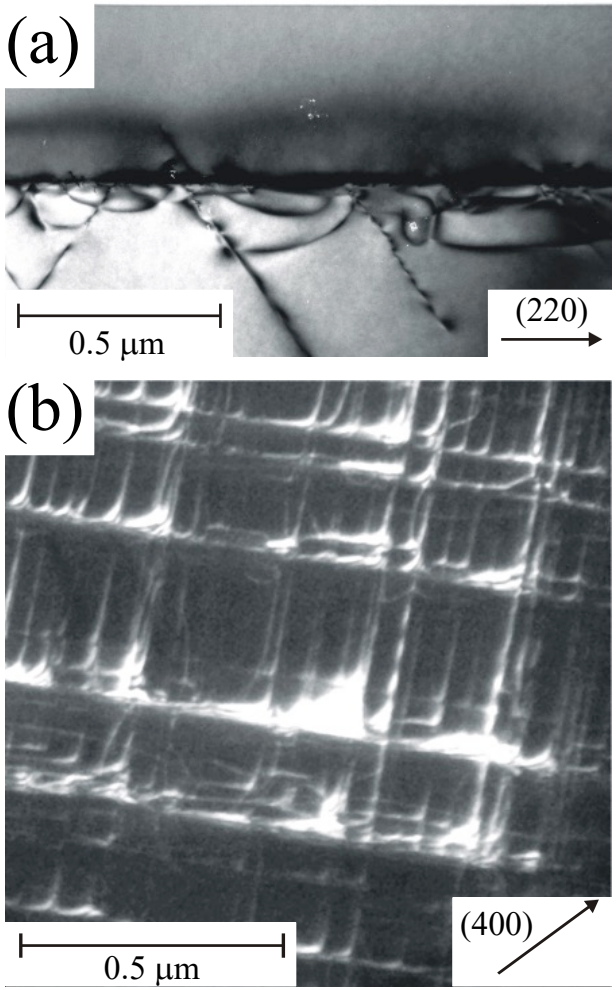
Dislocations aggregate at interface and glide to surface along {111}

T. Spila, UIUC Thesis



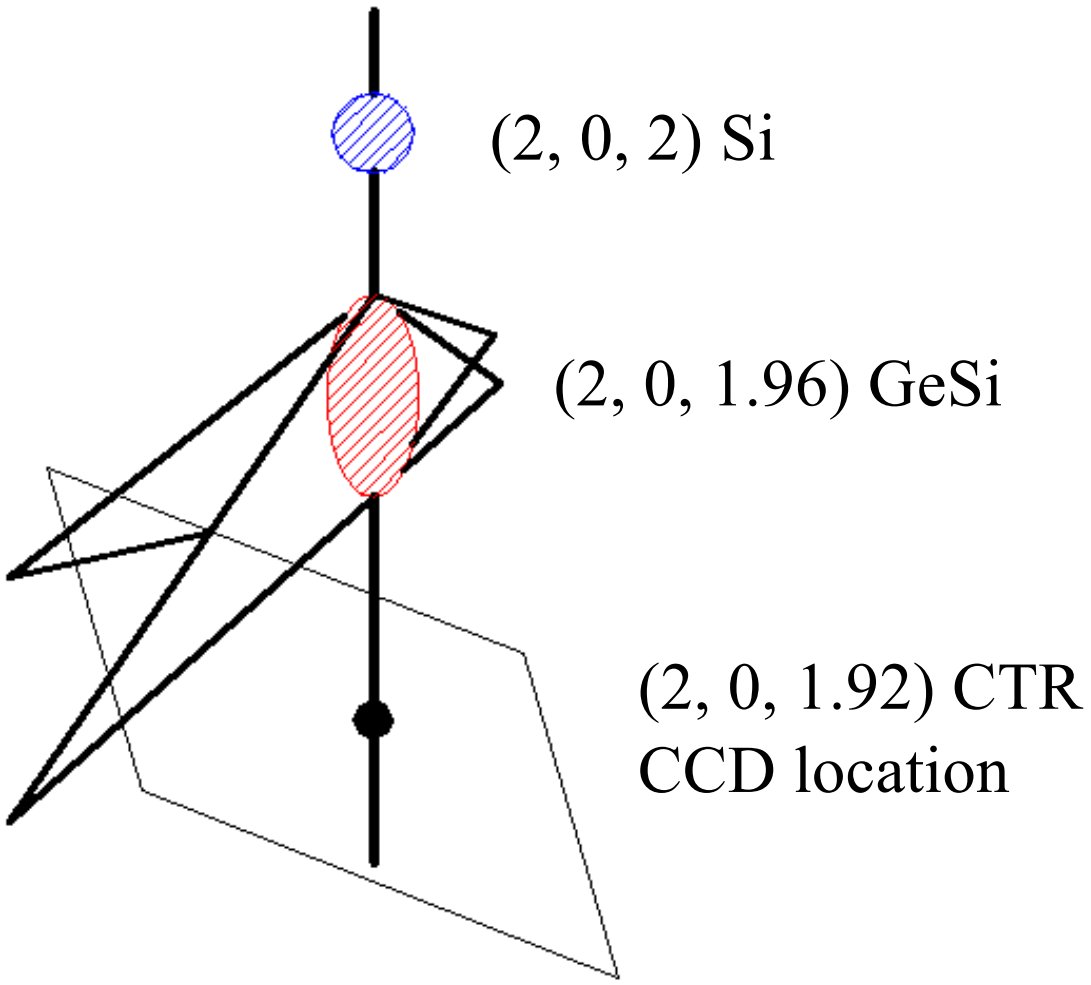
Higher Dislocation Density $Ge_{0.3}Si_{0.7}$





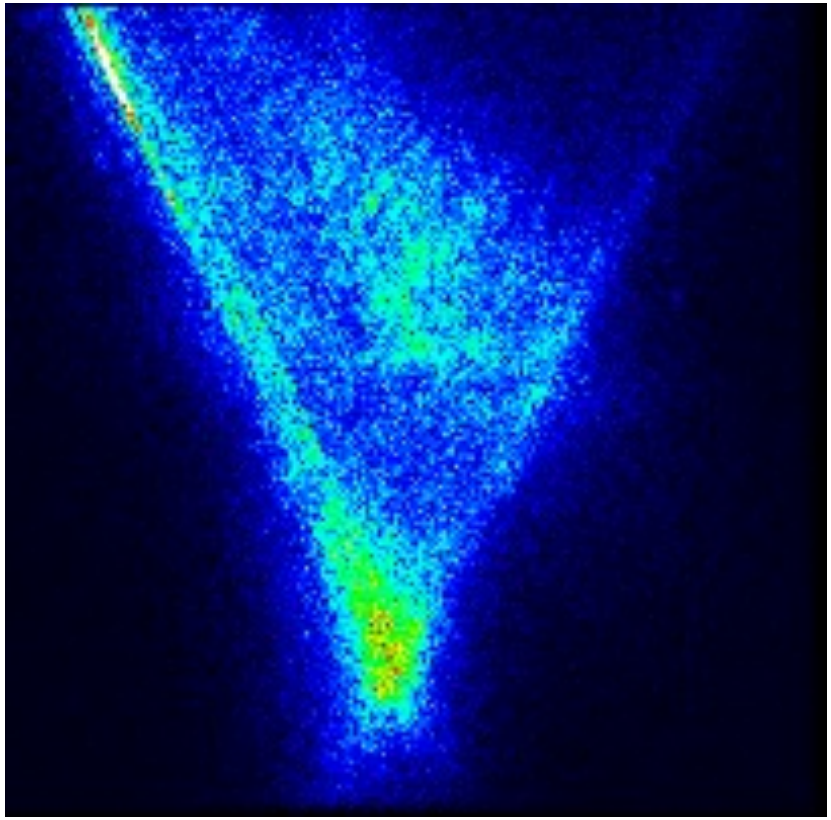
t=440nm

Dislocations in Reciprocal Space

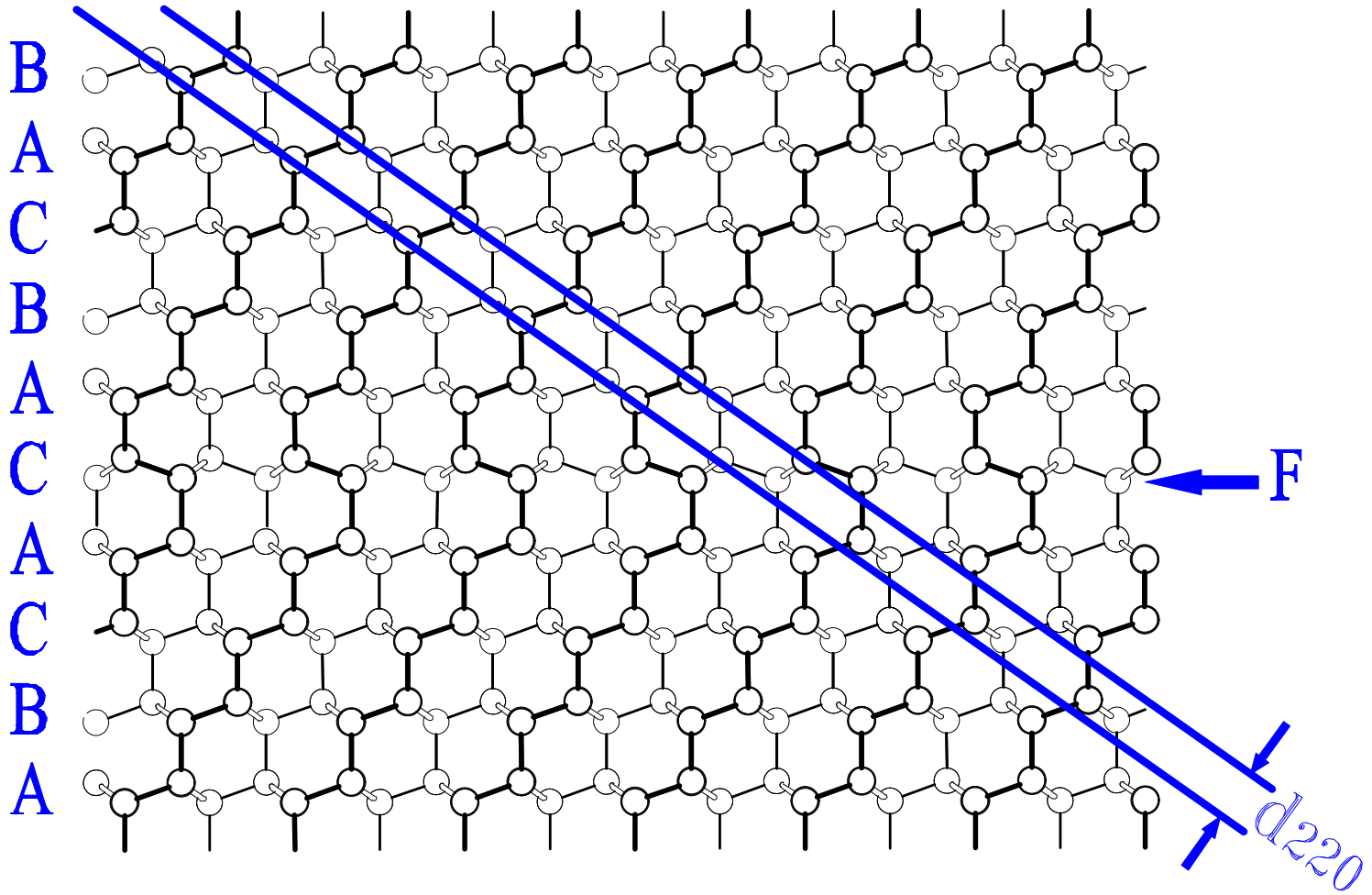


Use CCD and scan sample position

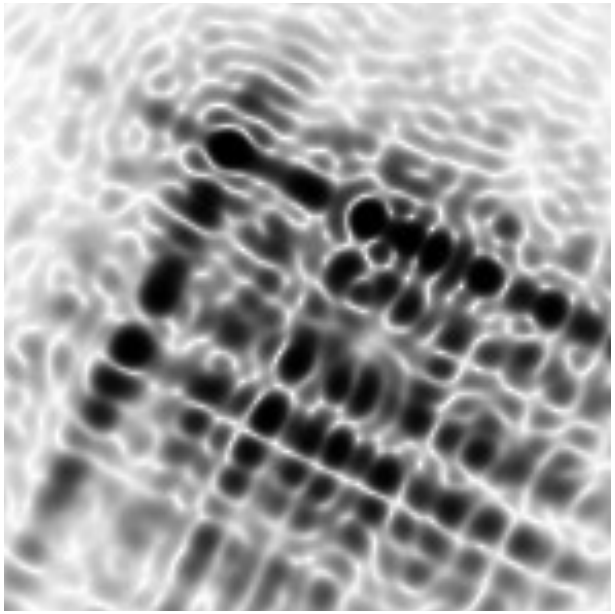
(2,0,1.92) 280nm thick $Ge_{0.3}Si_{0.7}$



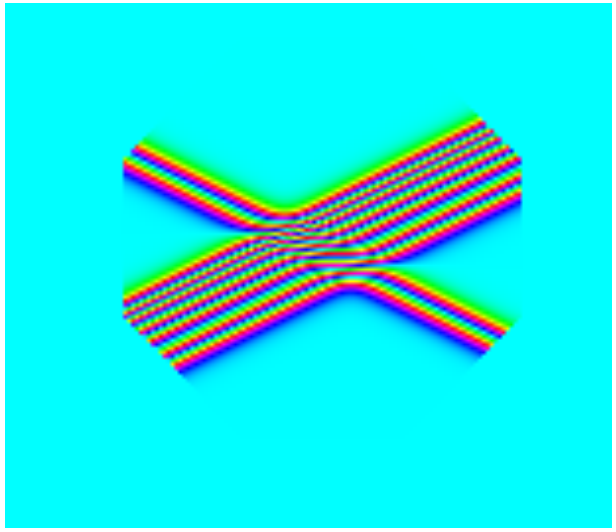
Deformation fault in Silicon

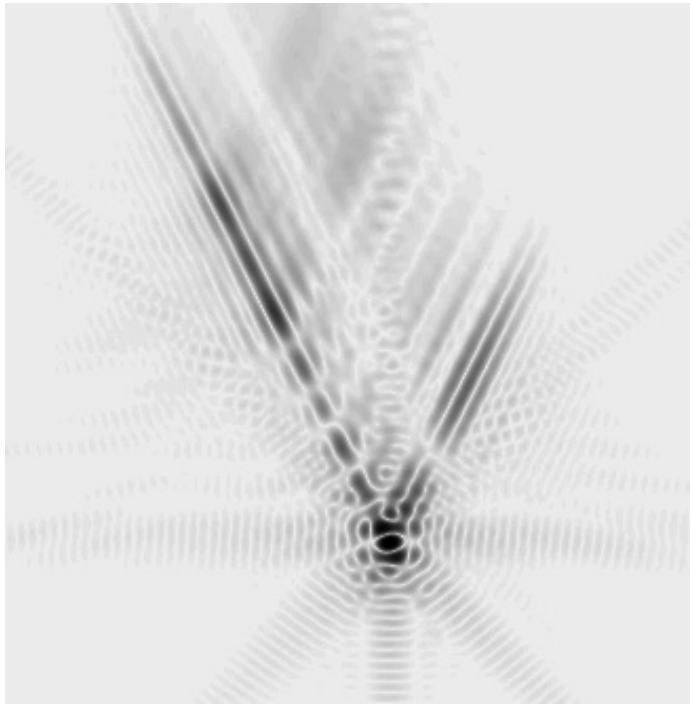


Dislocation Diffraction



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