Phasing of Nanocrystal Diffraction Patterns

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Student Presentation
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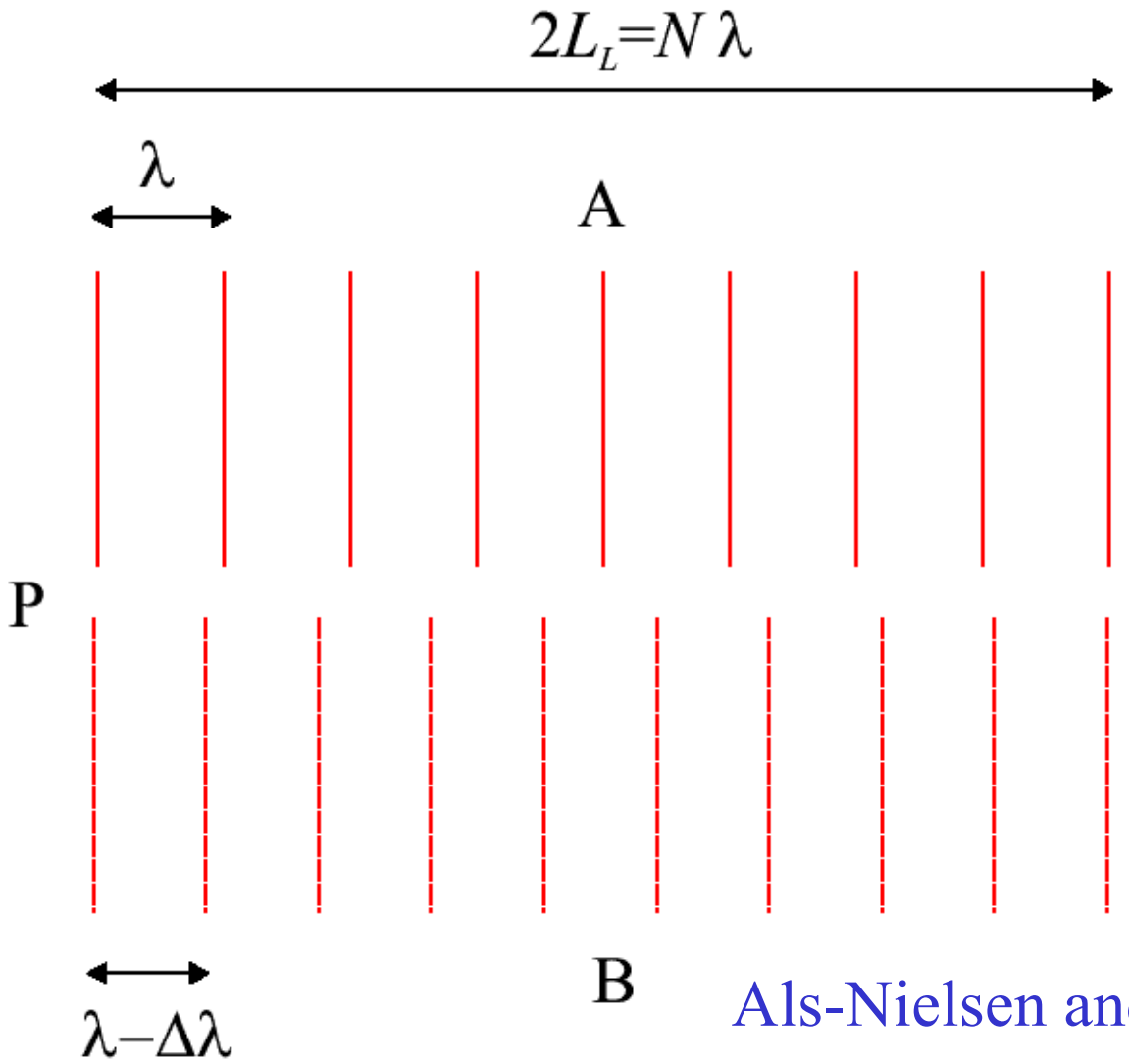
Outline

- Coherence in Diffraction
- CXD Beamline at APS
- How to Solve the Phase Problem
- Nanocrystal Shapes
- Use of Optics in CXD

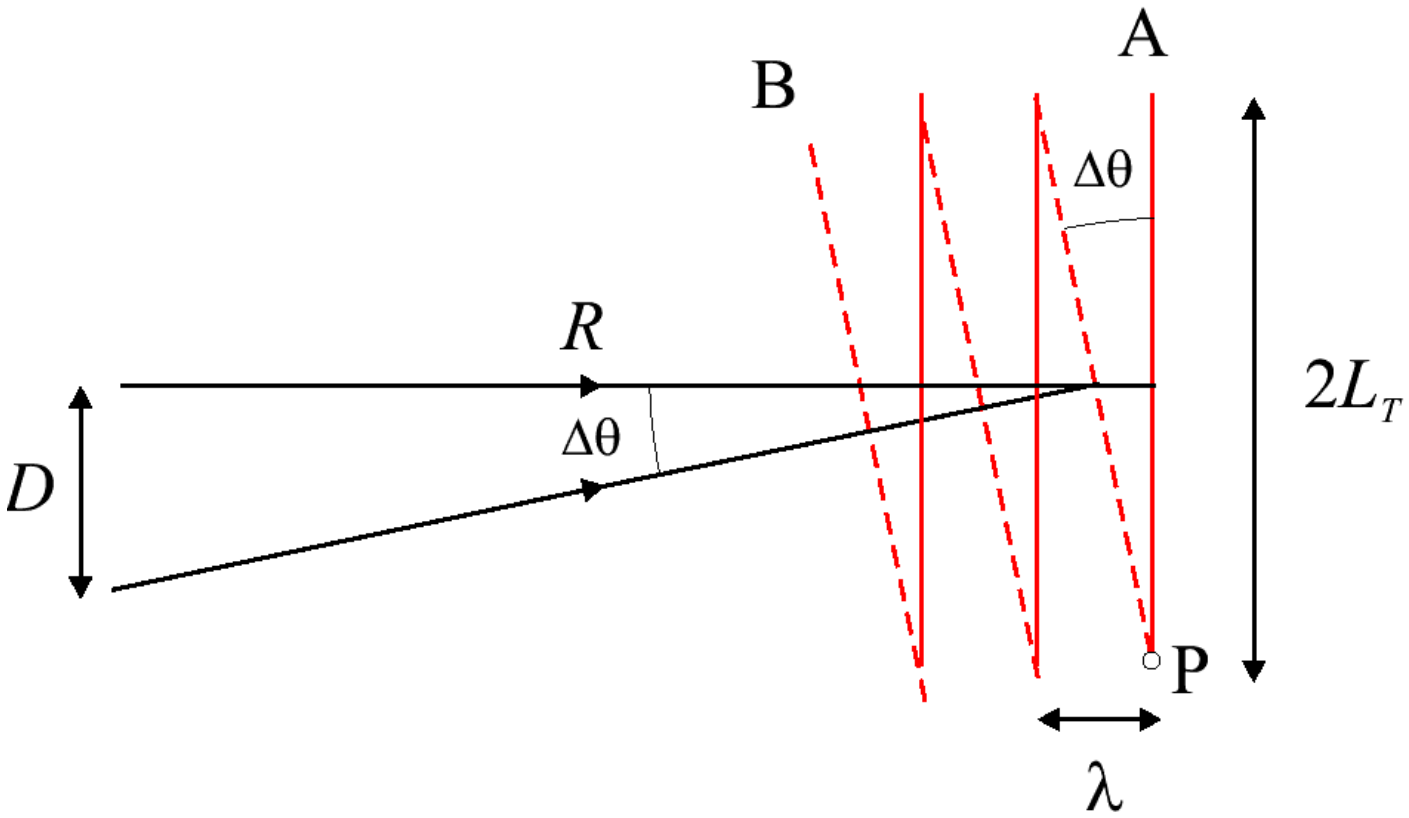
Longitudinal Coherence



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

Als-Nielsen and McMorrow (2001)

Lateral (Transverse) Coherence



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

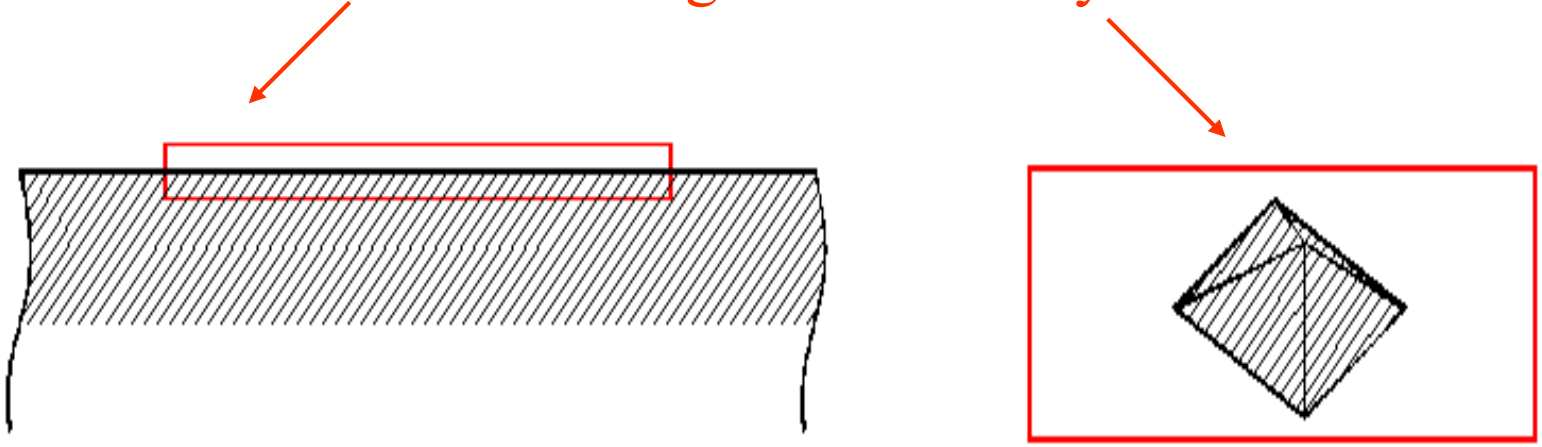
Als-Nielsen and McMorrow (2001)

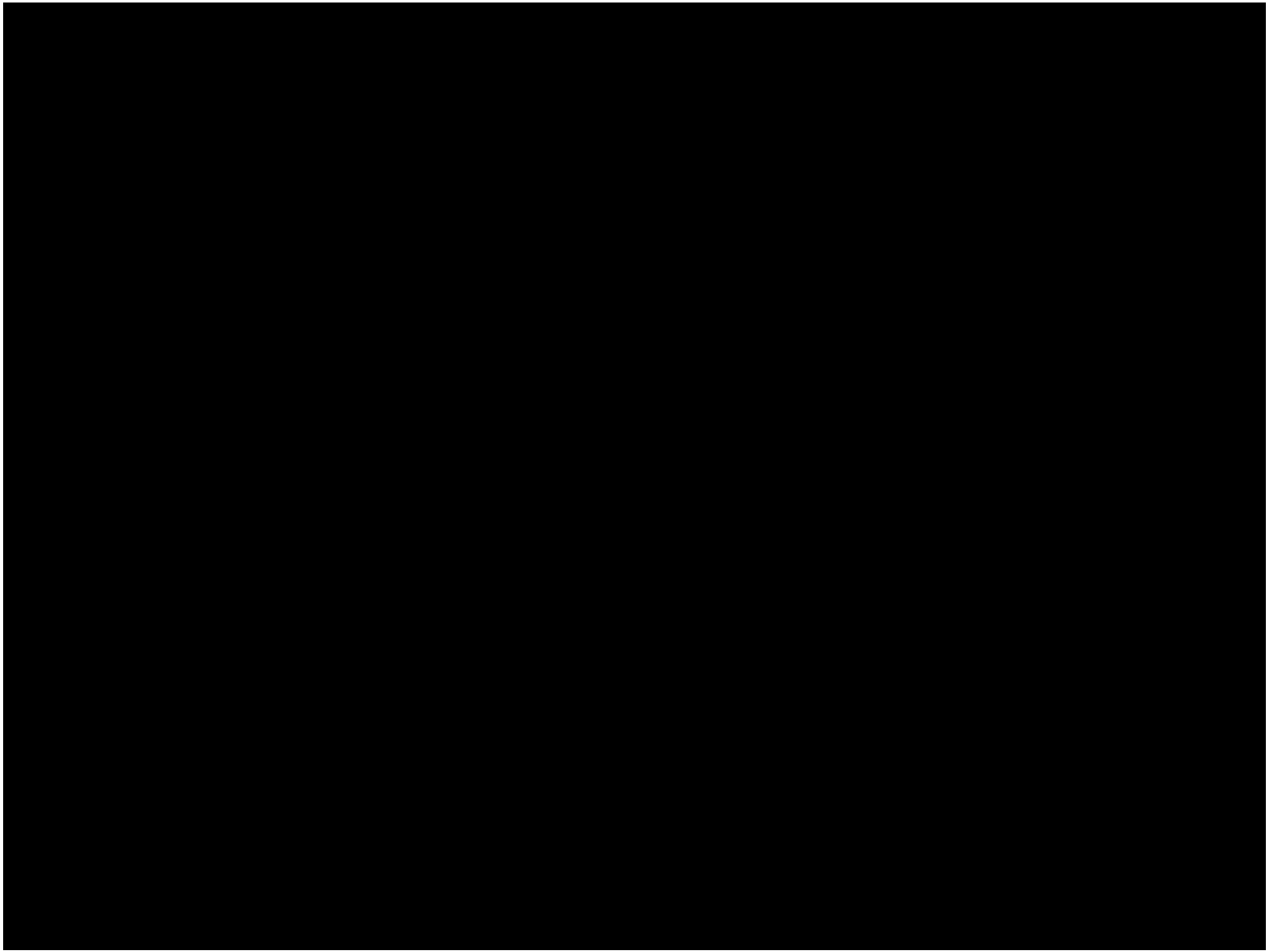
Coherence at the APS or ESRF

Typical of 3rd Generation (undulator) Synchrotron Source

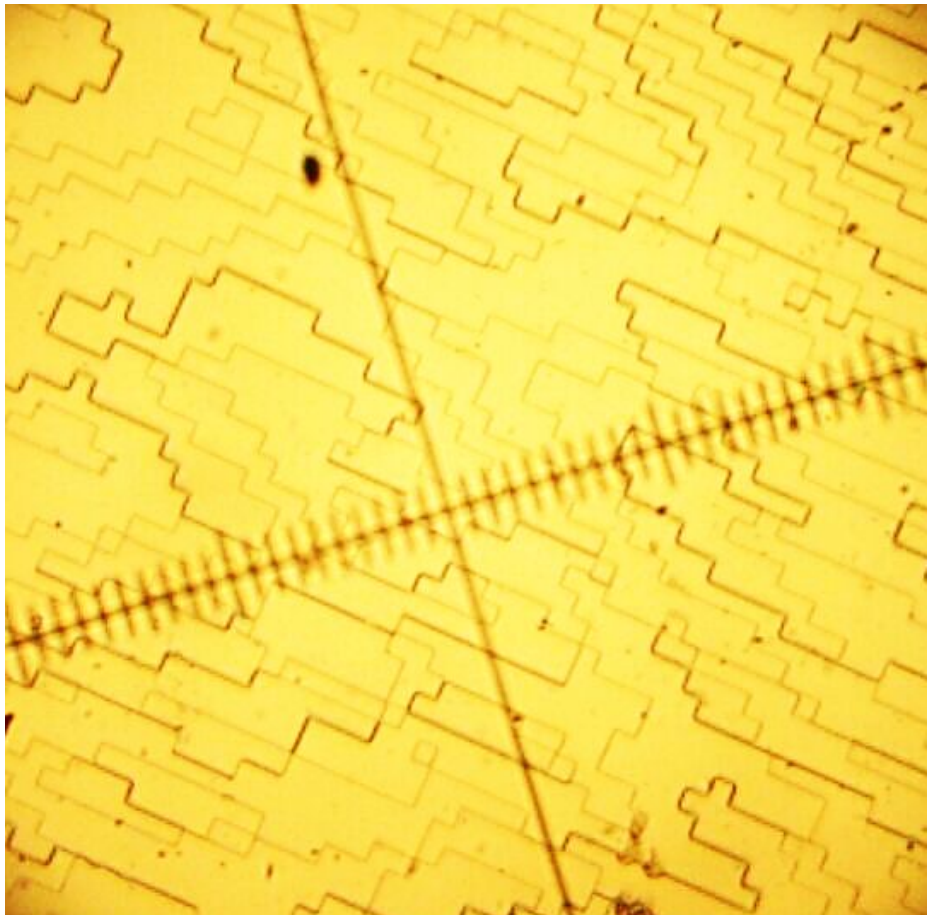
Coherence of	ξ_{VER}	ξ_{HORIZ}	ξ_{LONG}	Flux
Raw Undulator	35μm	9μm	0.004μm	2×10^{12}
Si(111) Monochromator	35μm	9μm	1μm	1×10^{10}
C(111) Monochromator	35μm	9μm	3μm	3×10^{9}

Coherent region defined by slits

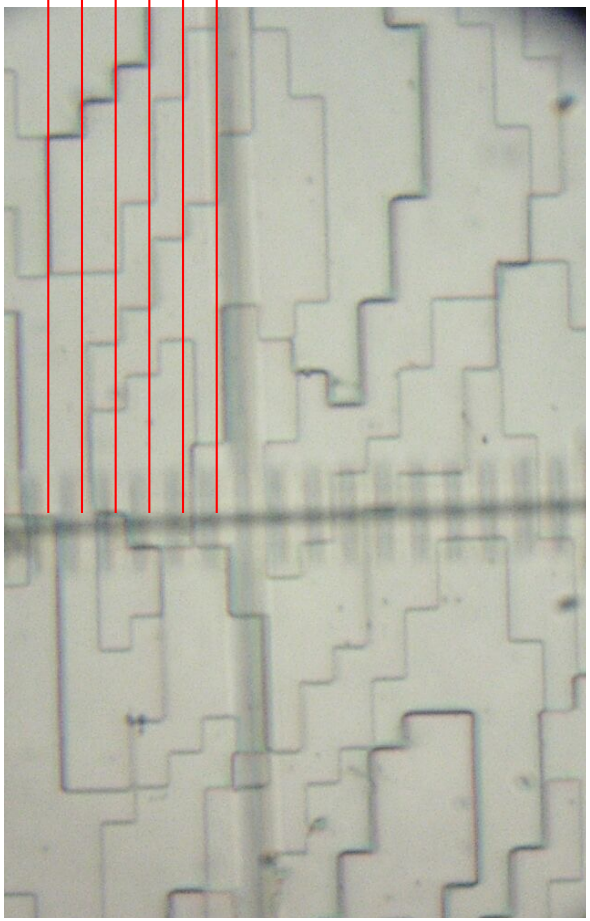


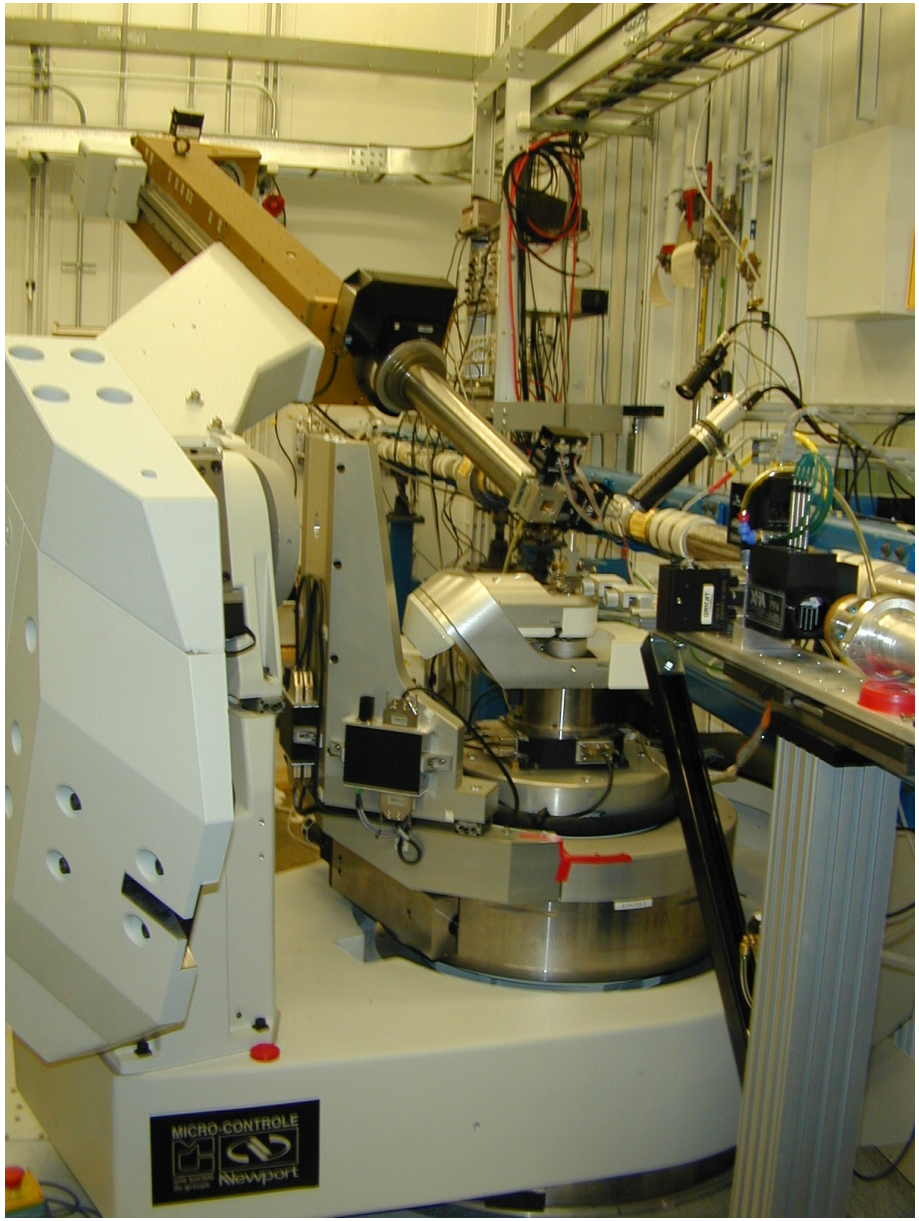


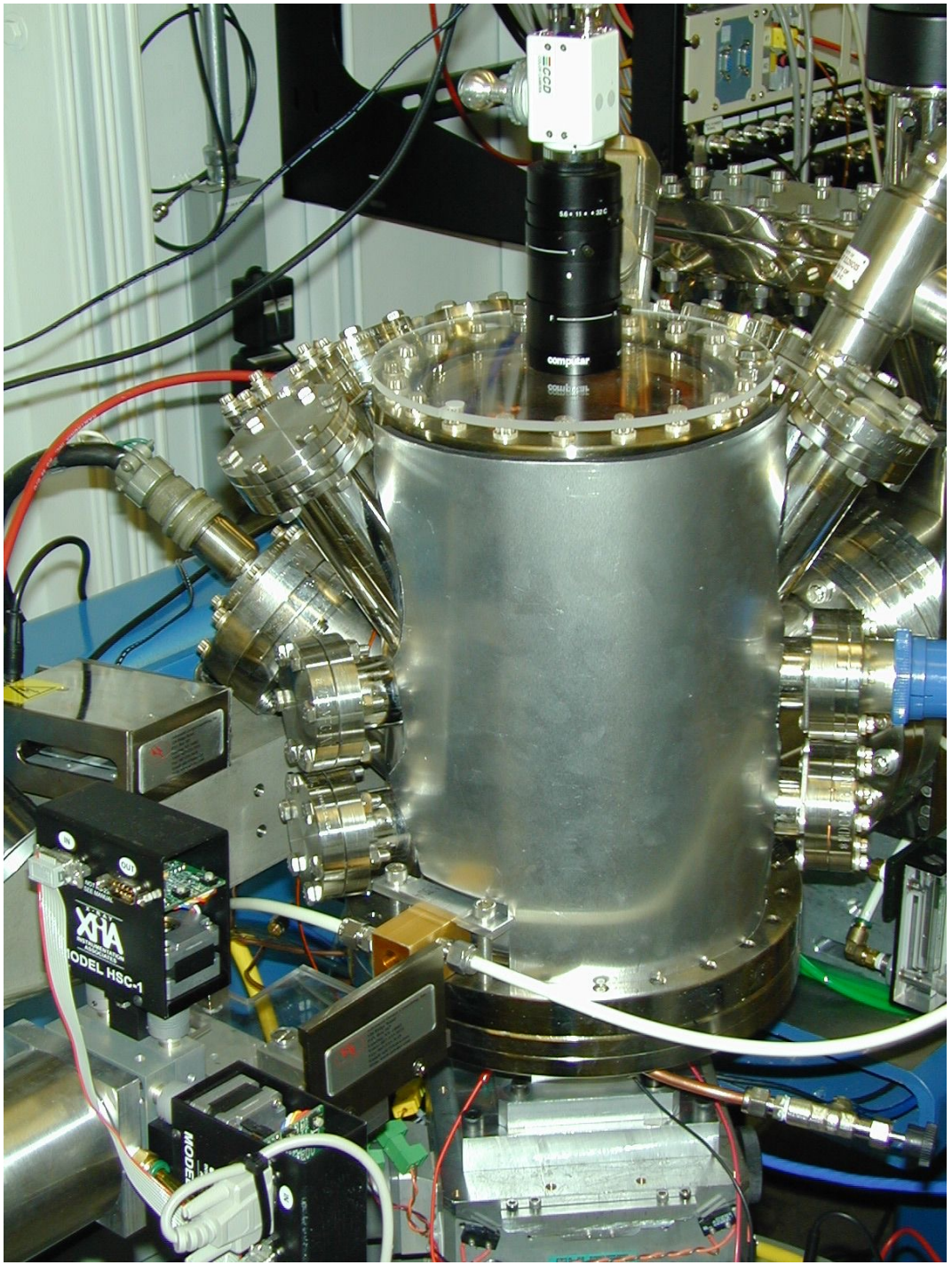
Microscope Images of Gratings

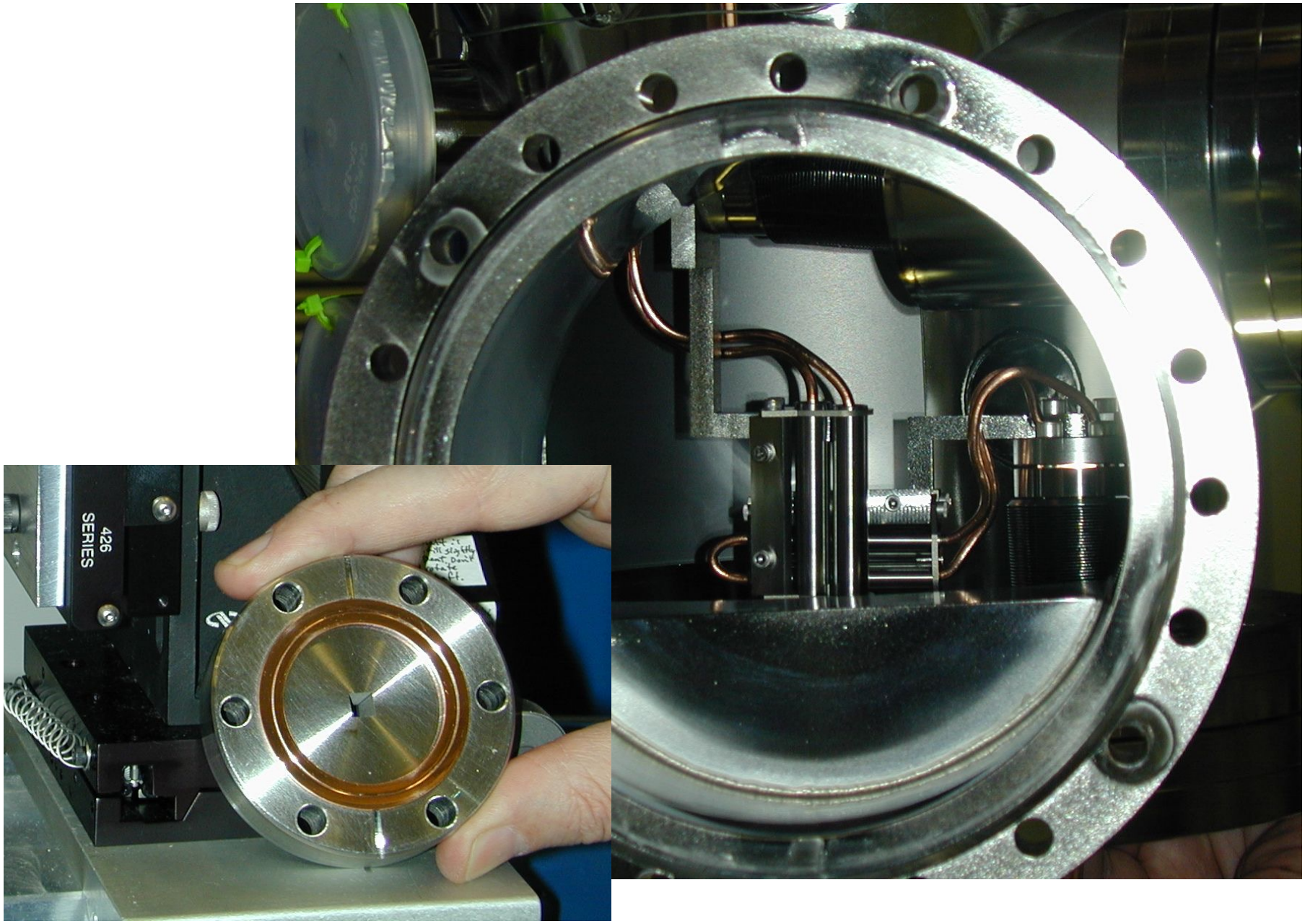


5μm grid lines

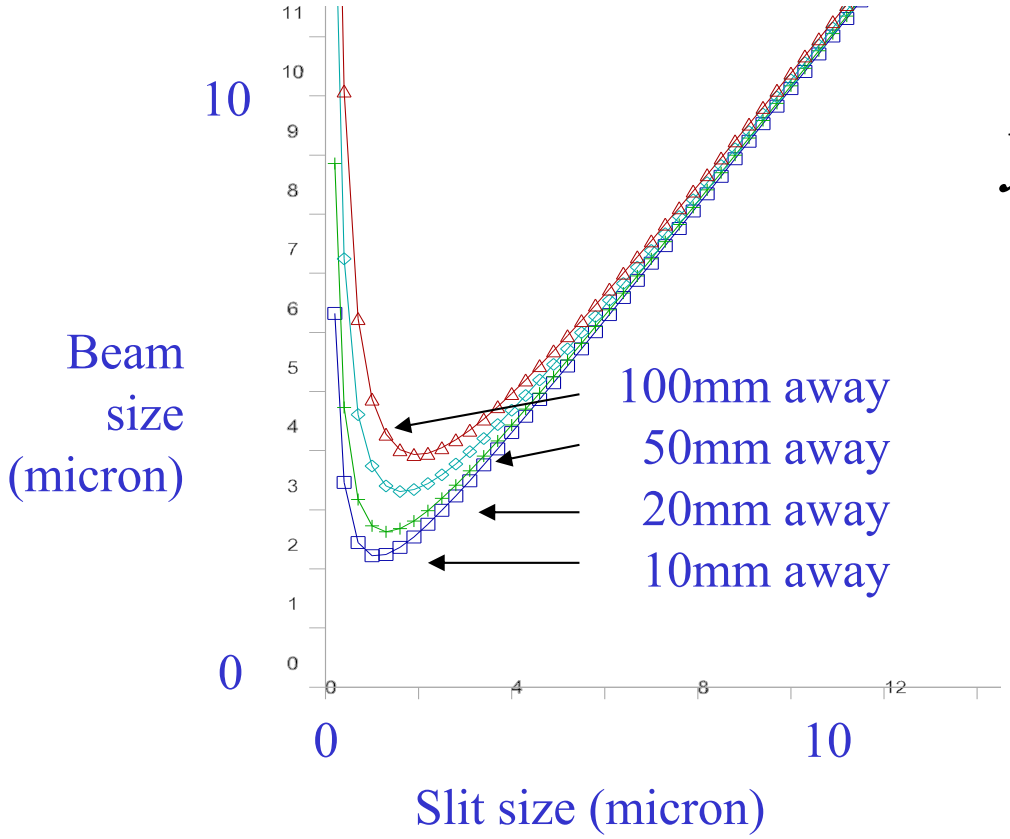



MICRO-CONTROLE
Newport

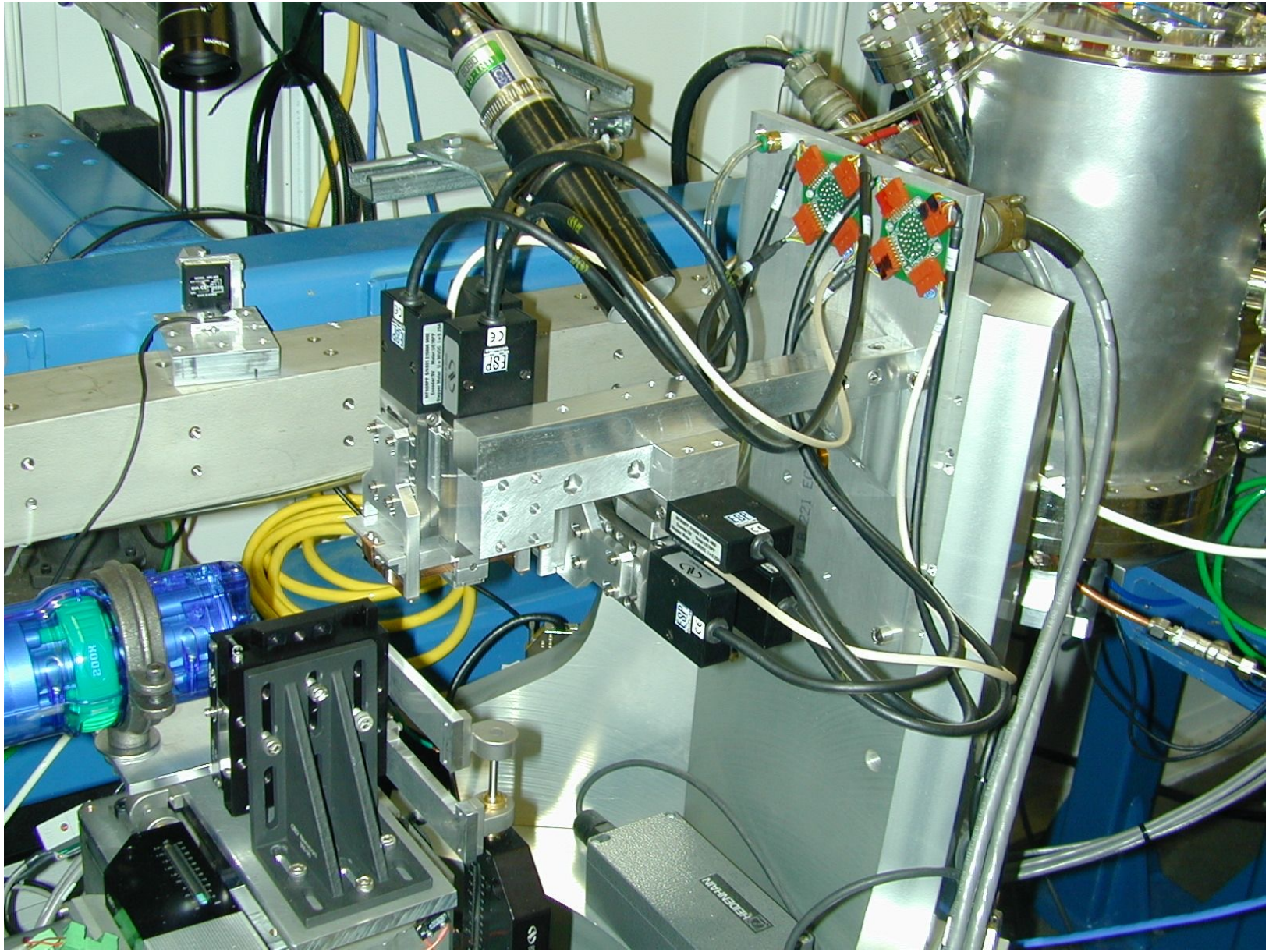

computar
MODEL HSC-1


426
SERIES

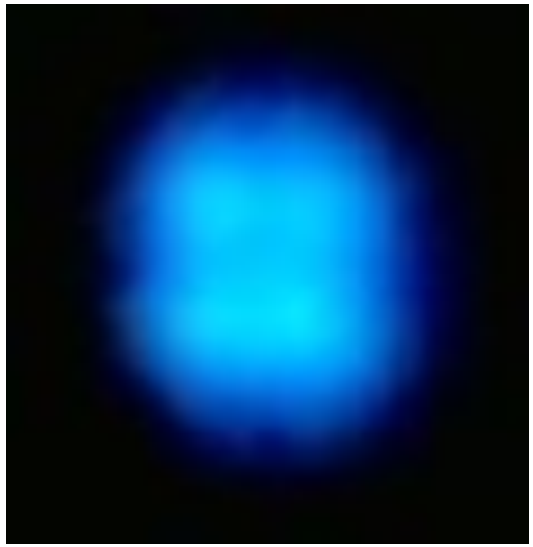
Smallest Beam using Slits (9keV)

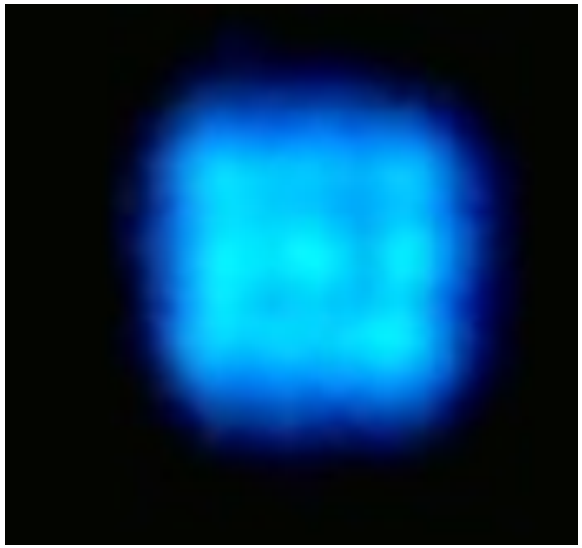


$$y(x) = x + \frac{\lambda d}{x}$$

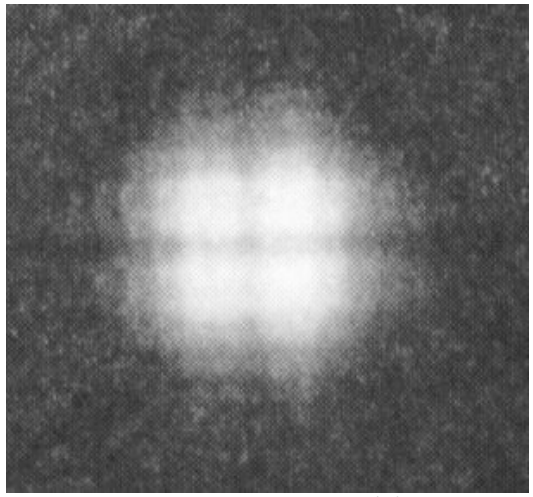


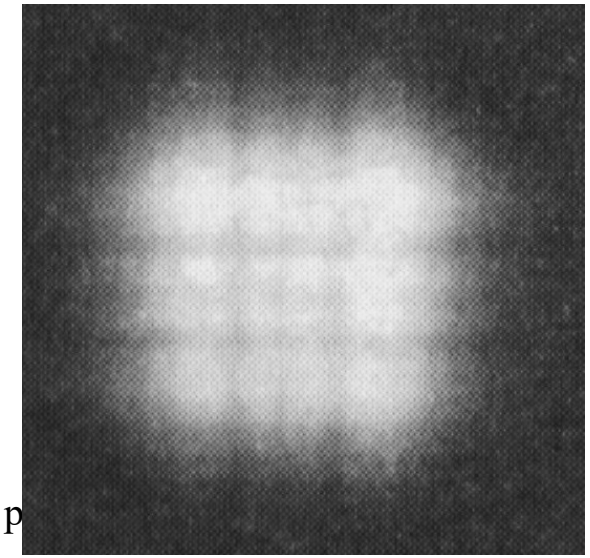
Fresnel Diffraction when $d^2 \sim \lambda D$





X-ray beam defined by RB slits

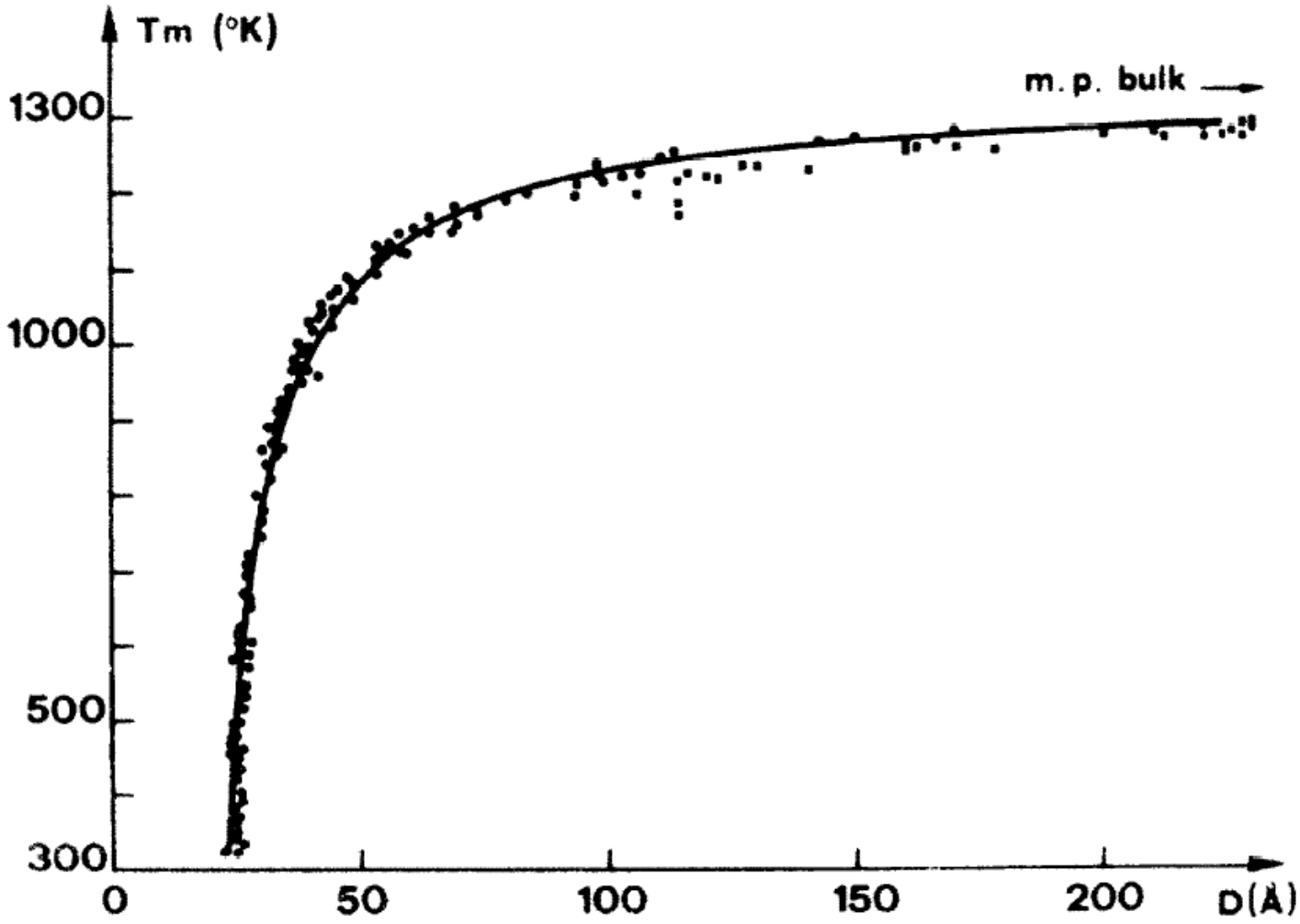




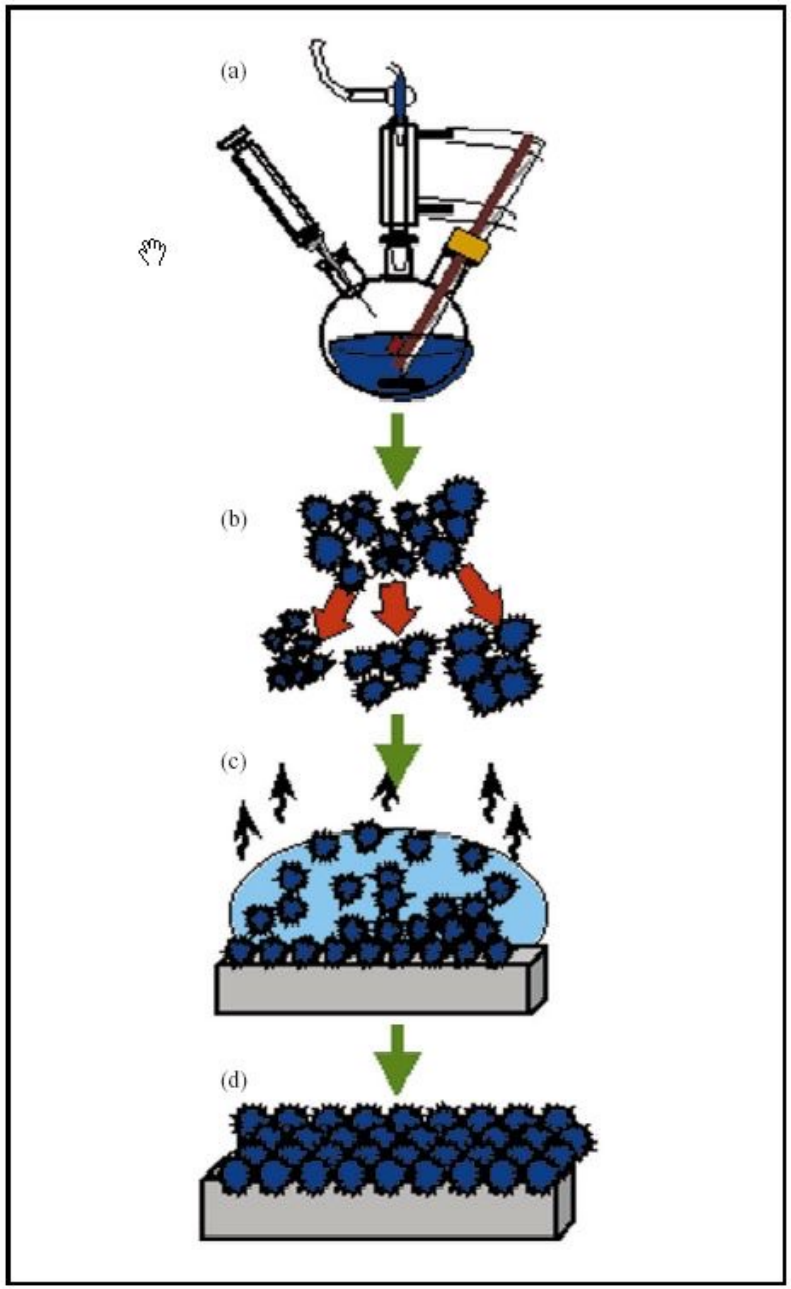
Visible Fresnel diffraction from Hecht "Optics"

Size-dependent Melting of Au Particles

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

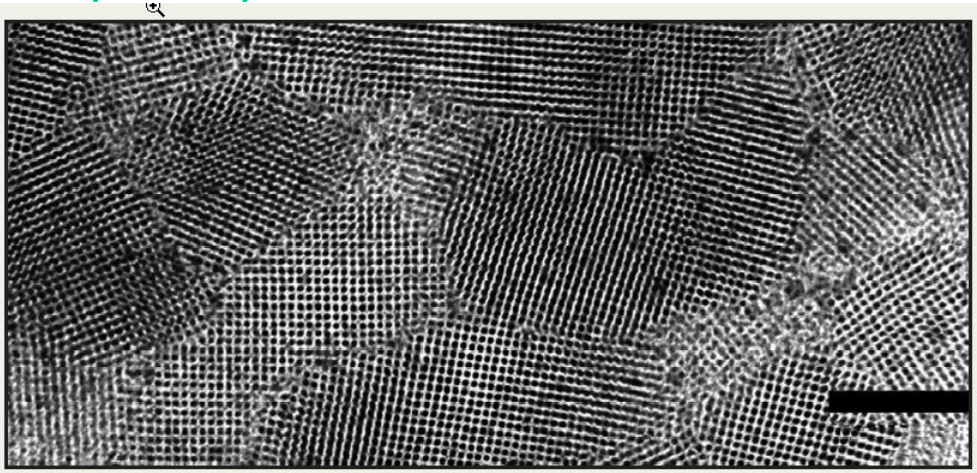


Chemical Synthesis of Nanocrystals



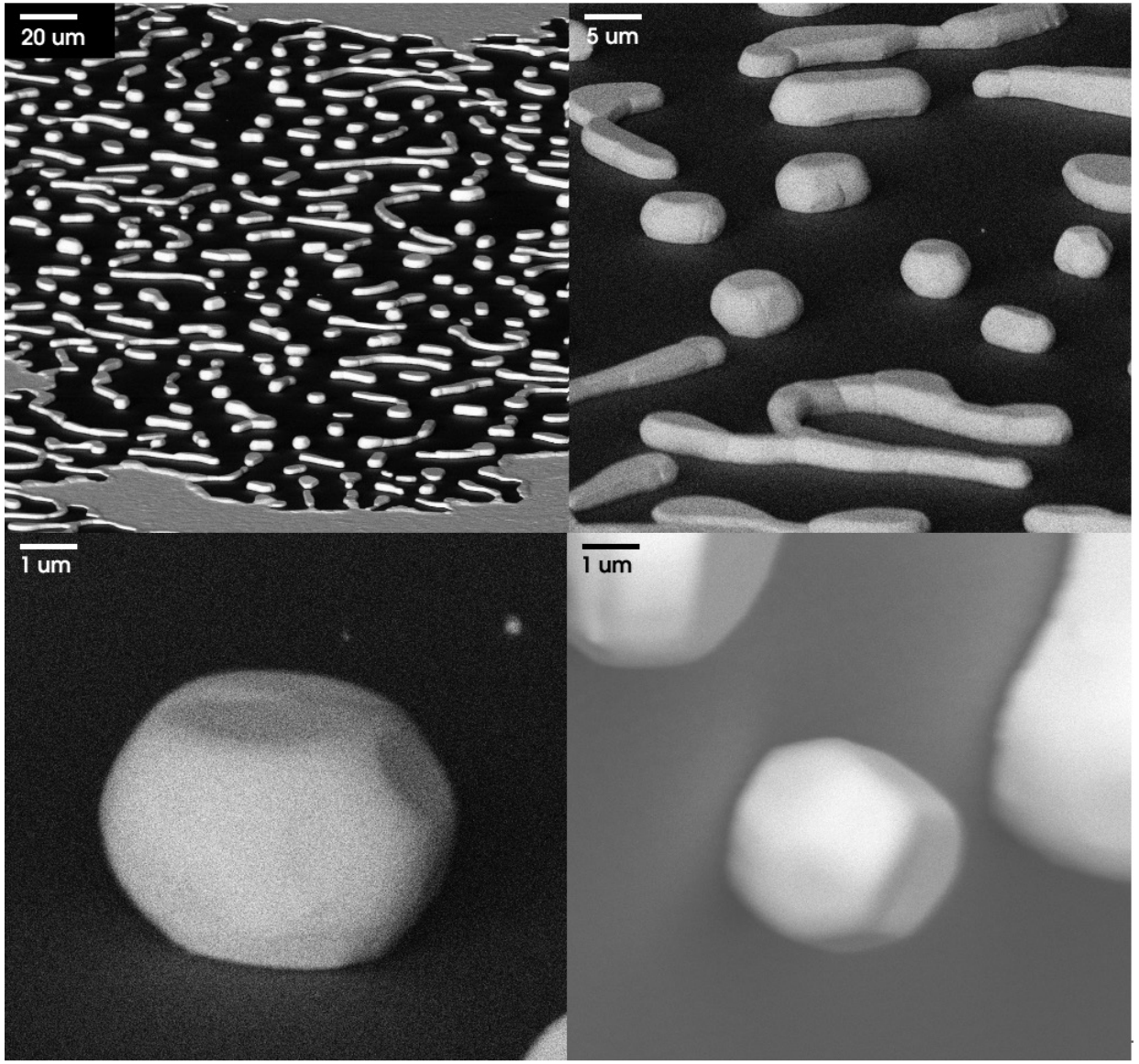
- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

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

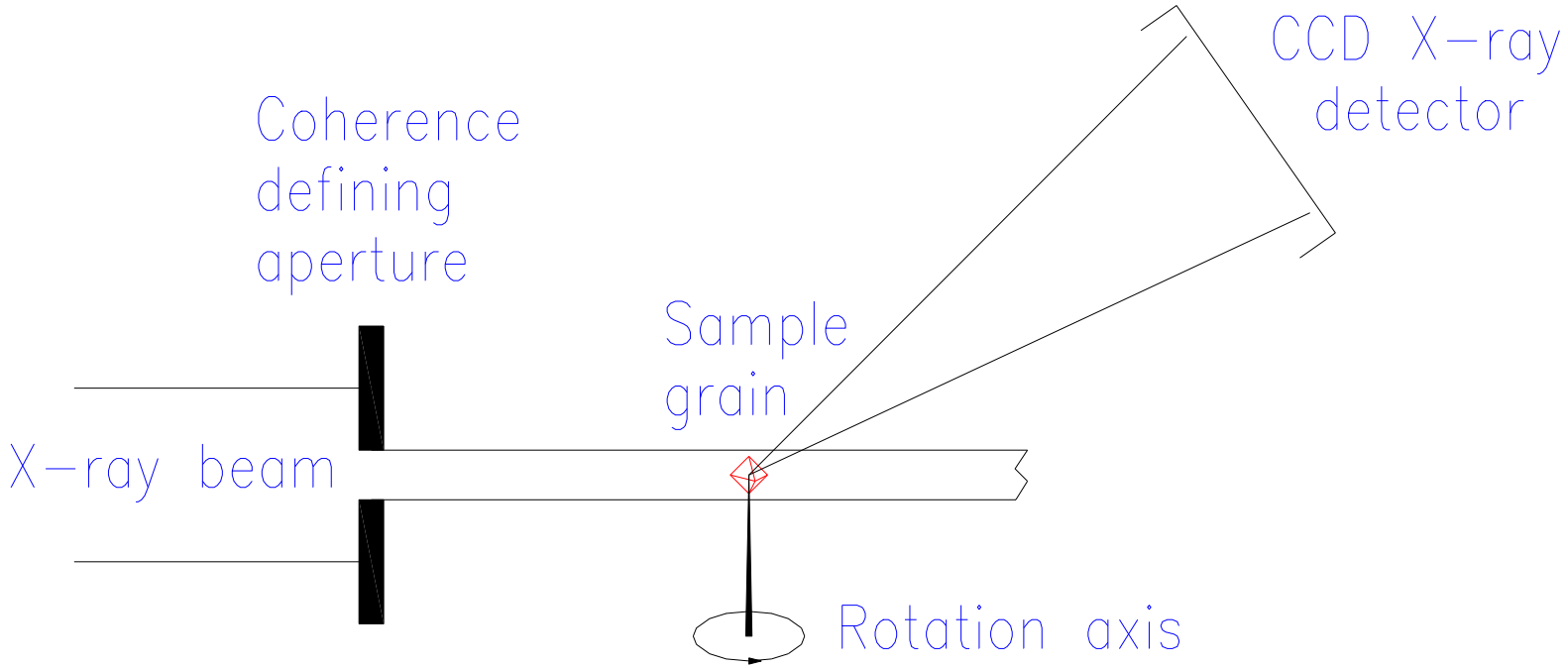


SEMS

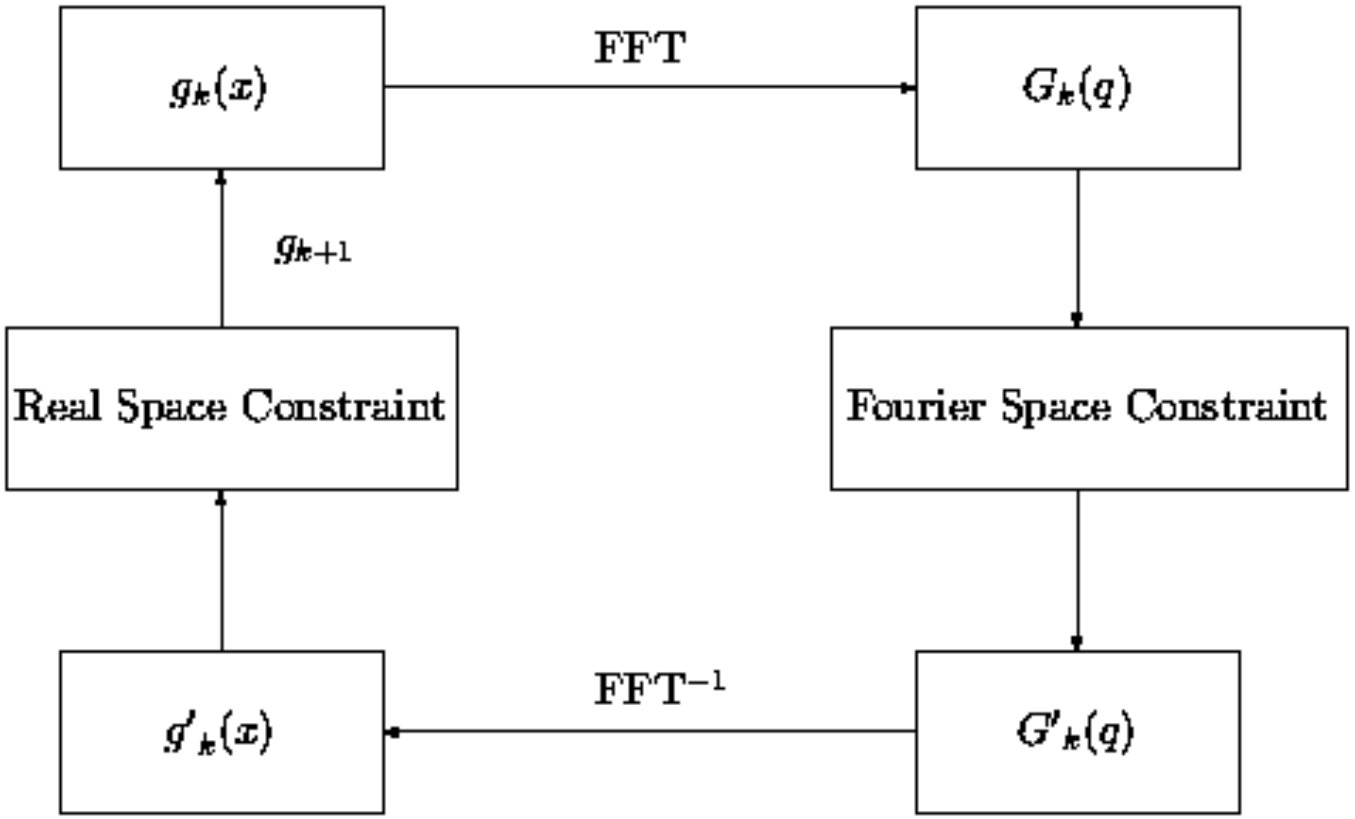
- Au blanket film
- Quartz substrate
- Annealed at 950°C for 70 hrs.



Lensless X-ray Microscope

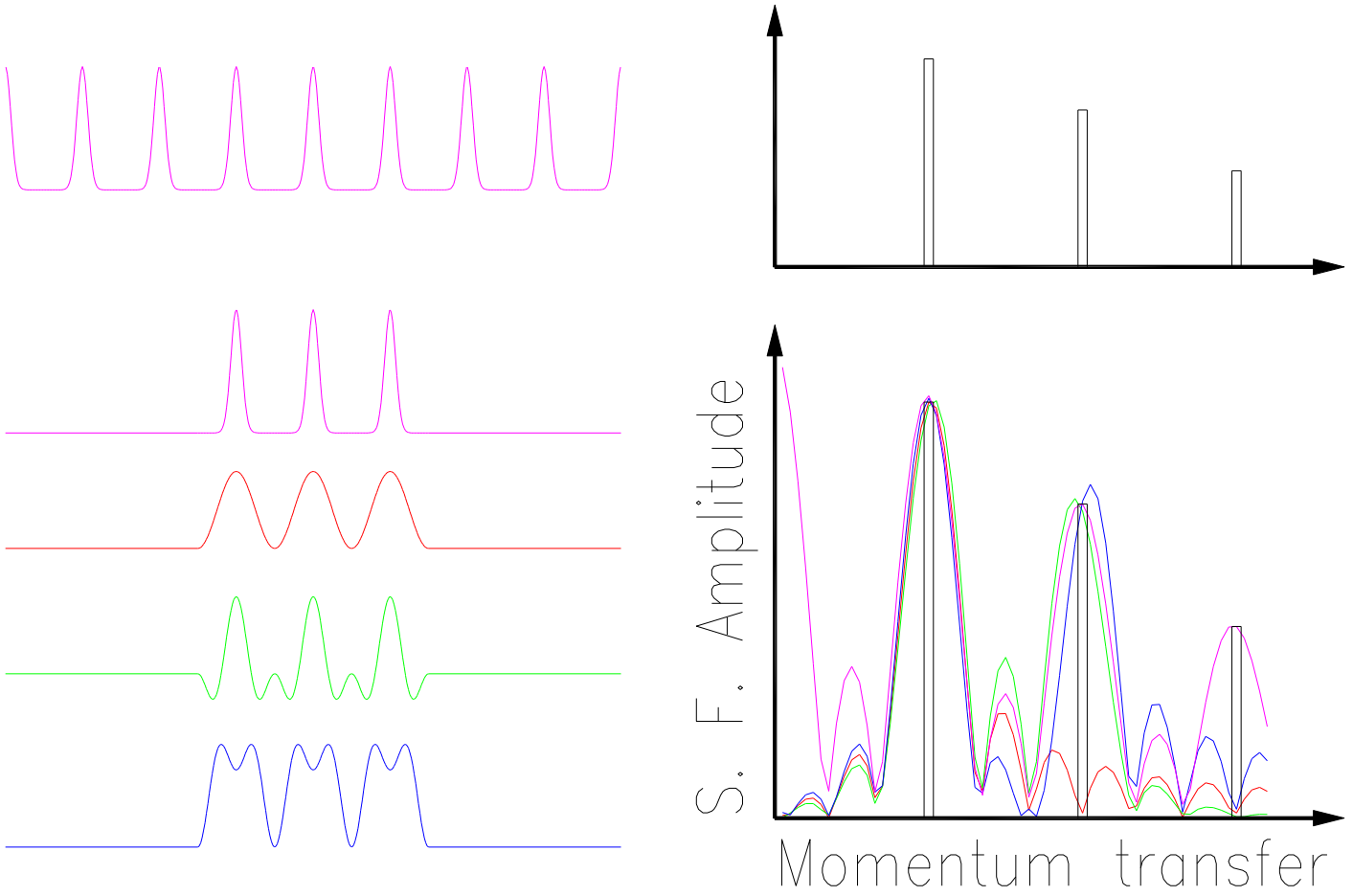


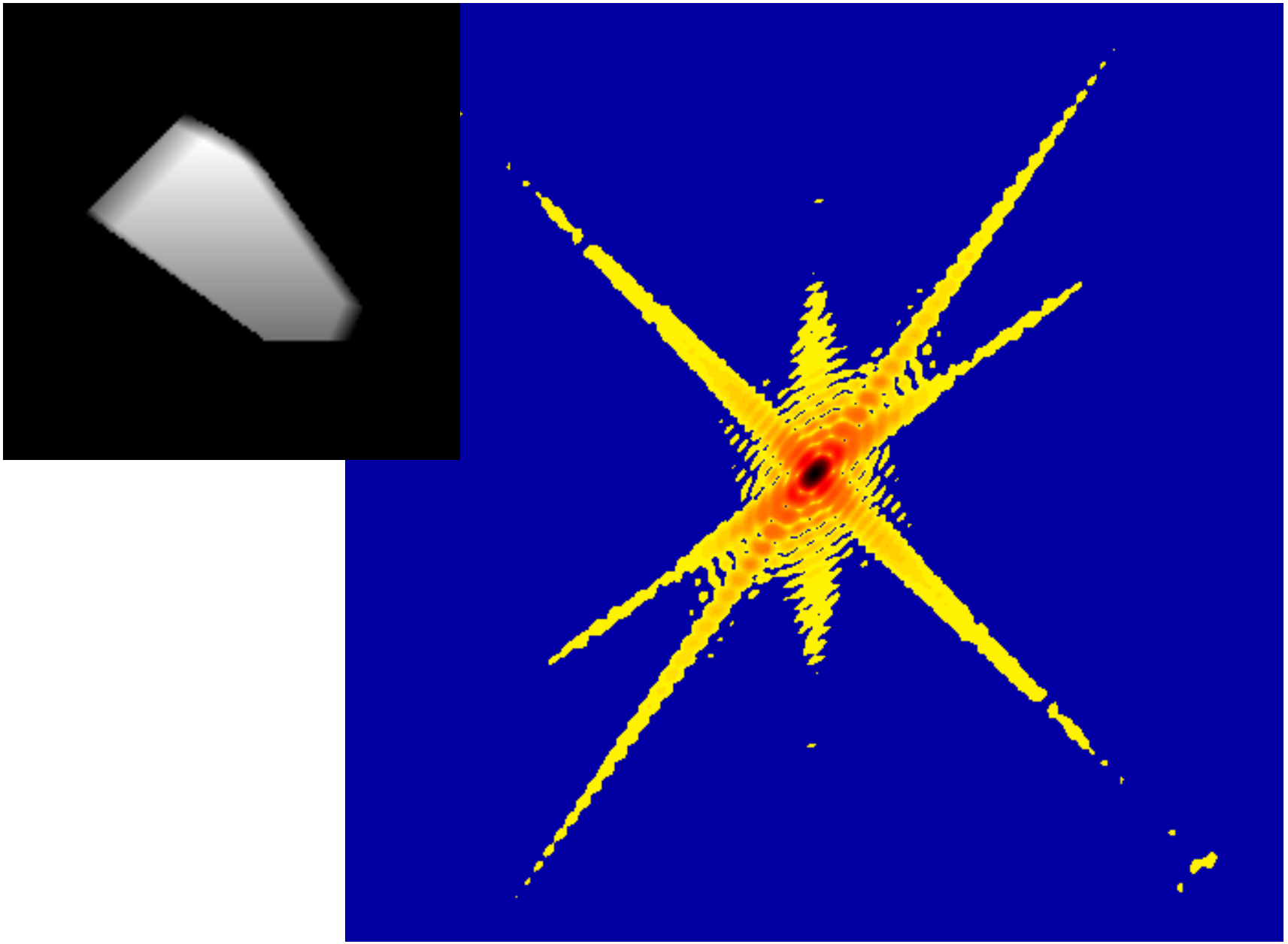
Generic "Error Reduction" method



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

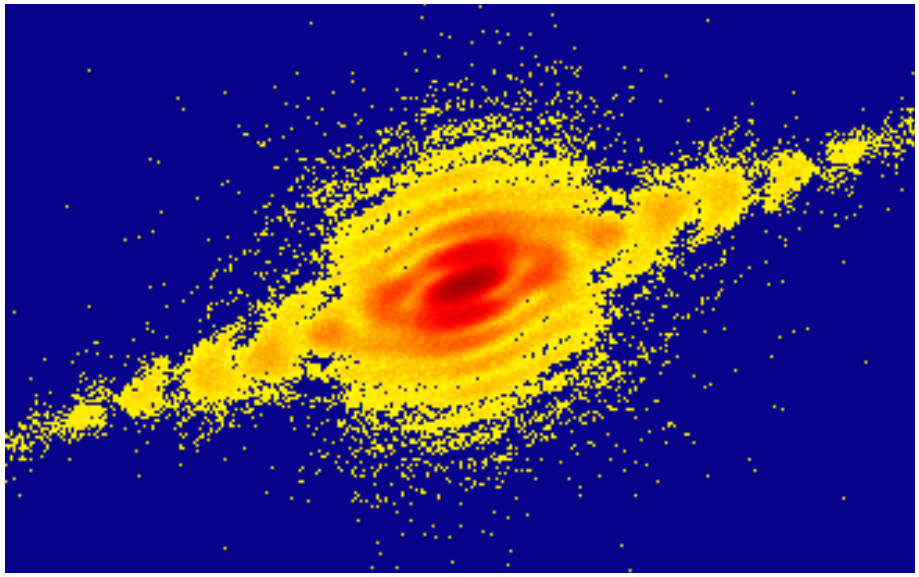
Phase Problem: Finite-size Effect

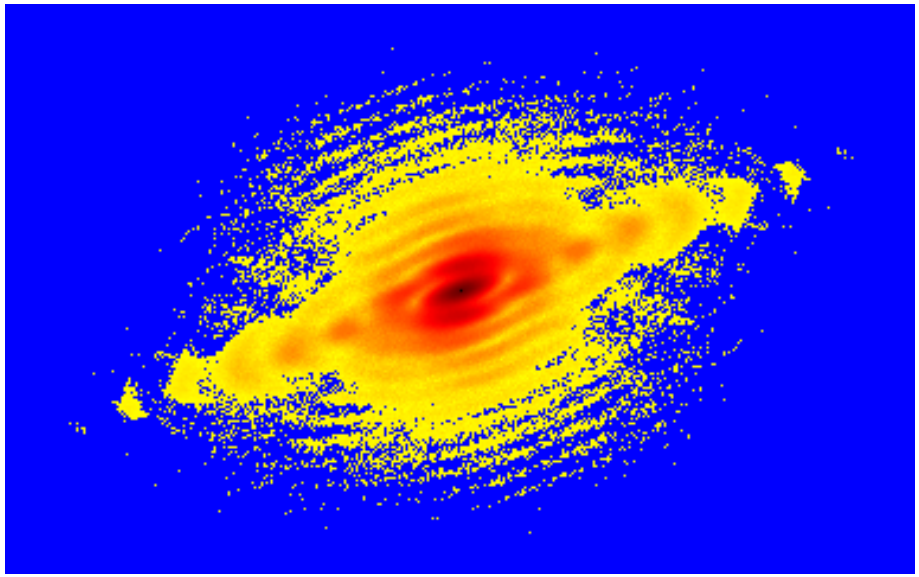


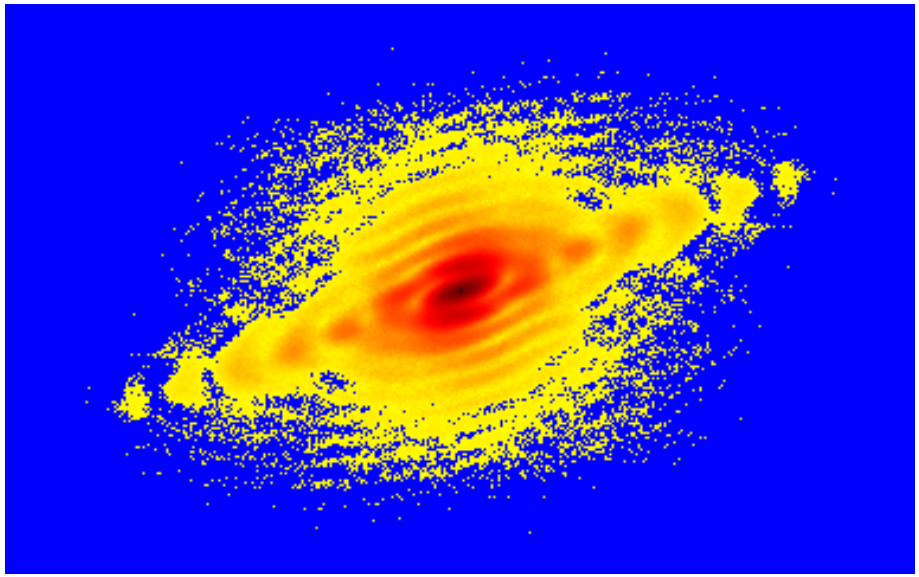


Symmetrized Data and two best fits

Chisq=0.0005

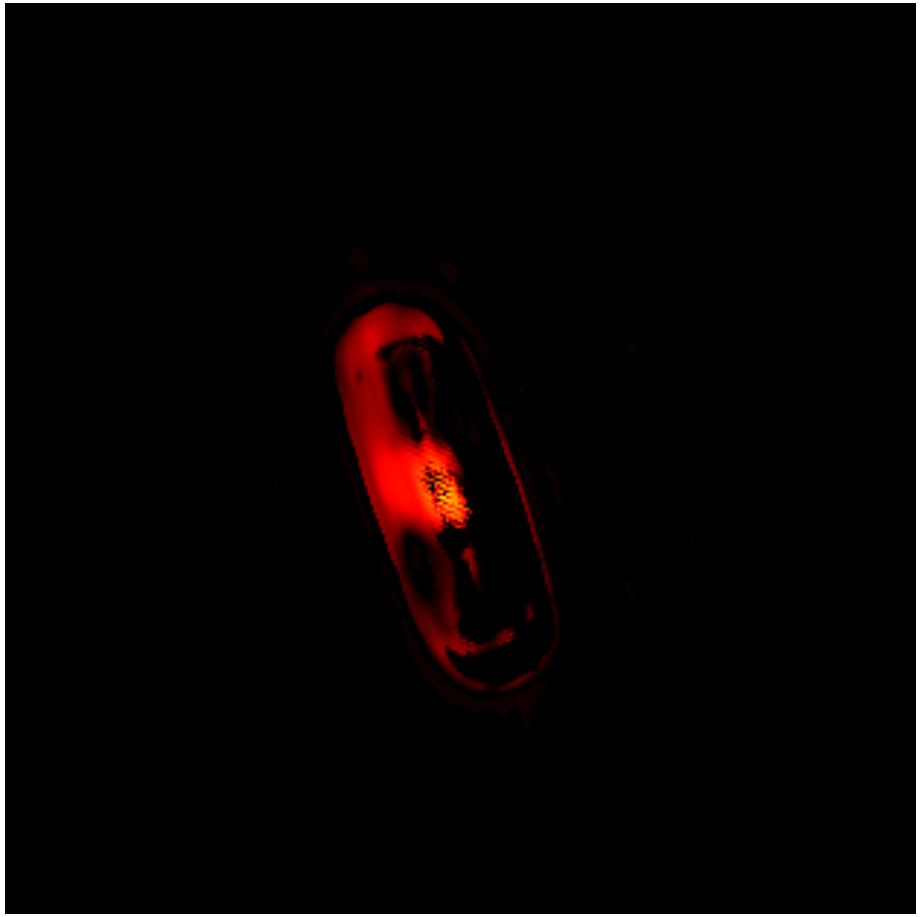


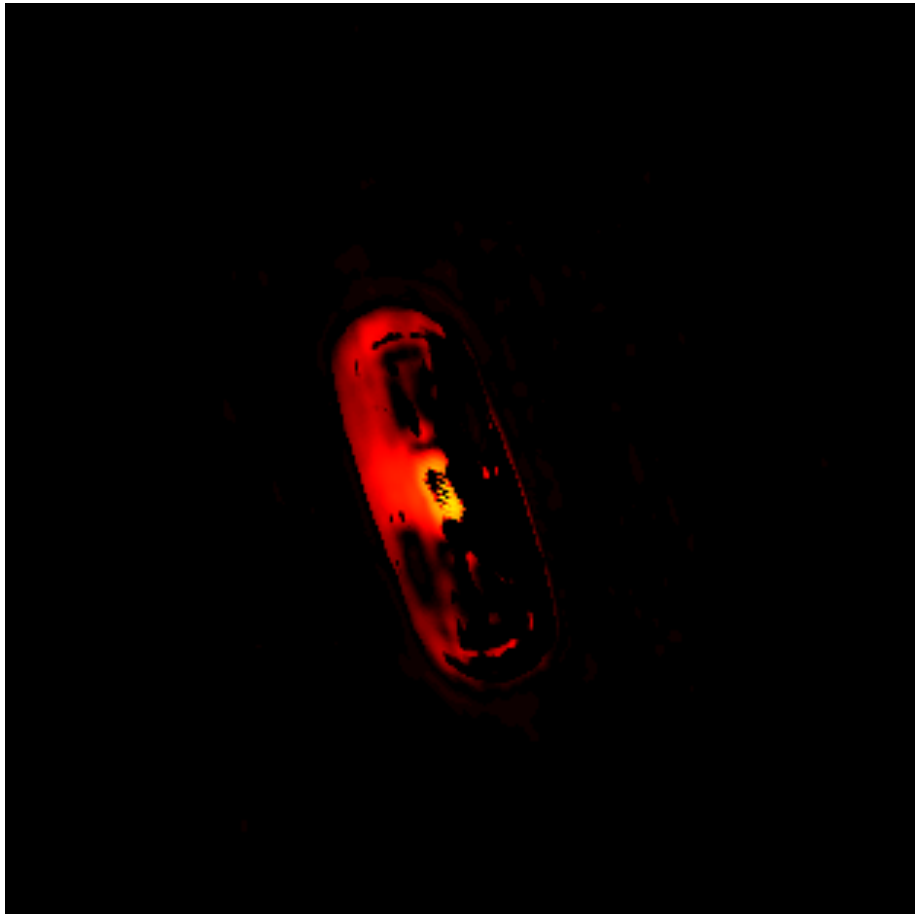




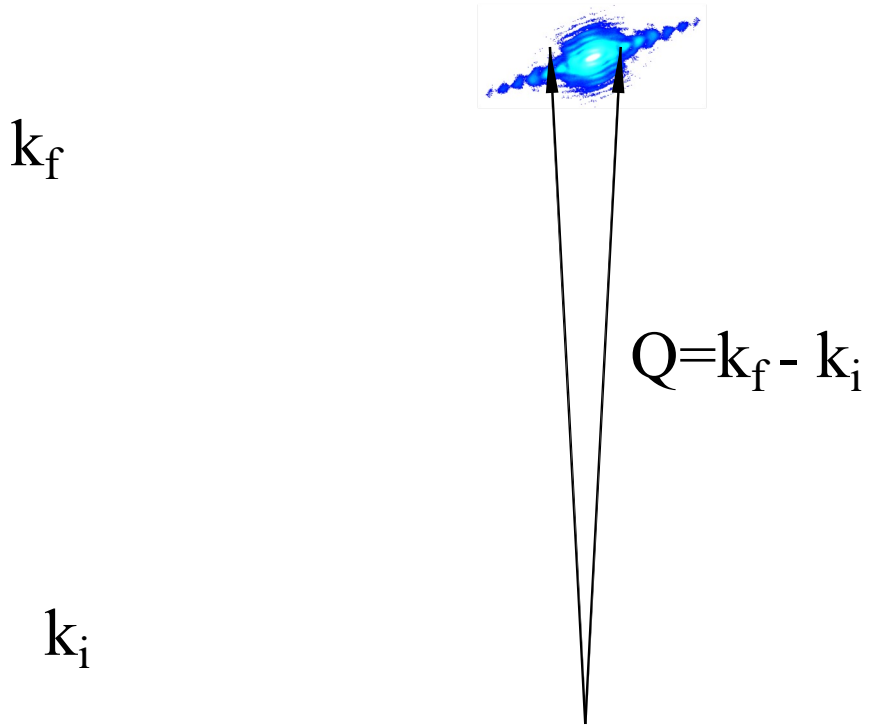
2D Reconstructions

chisquare = 0.0005

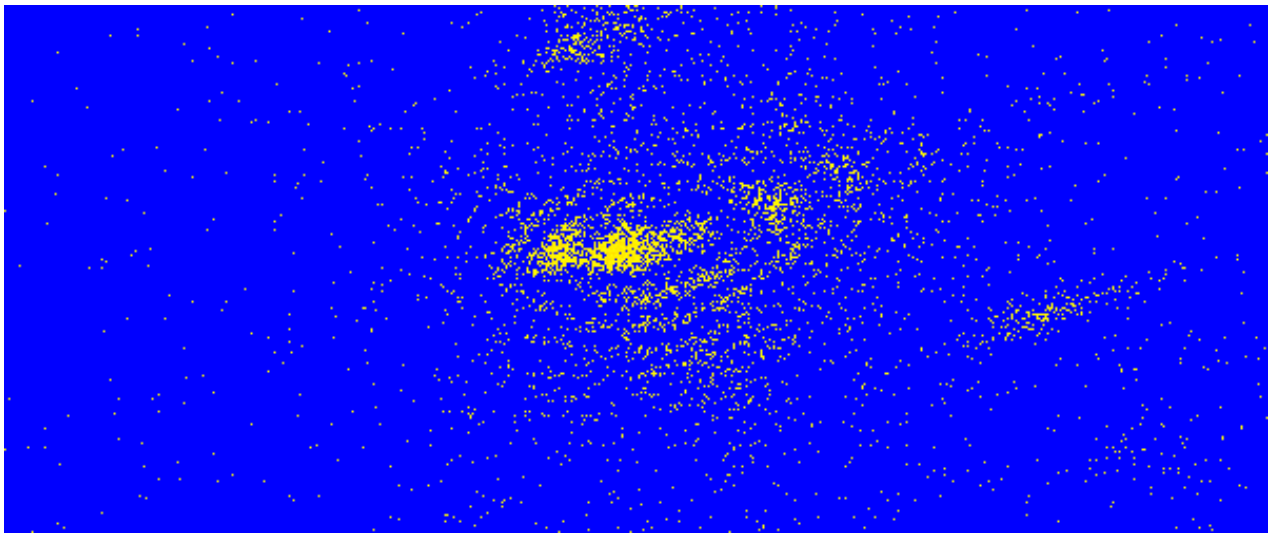


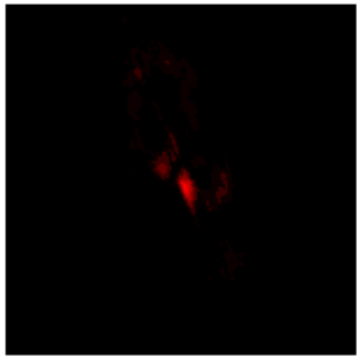
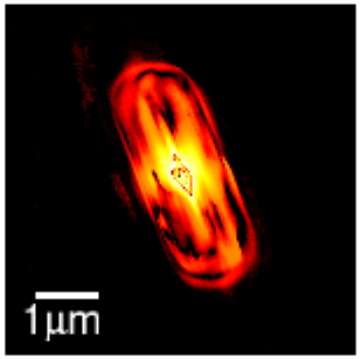


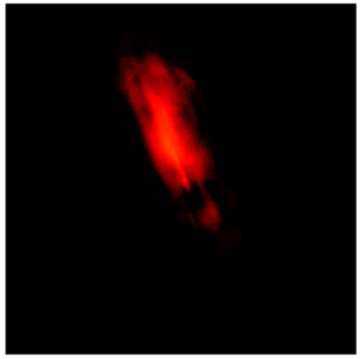
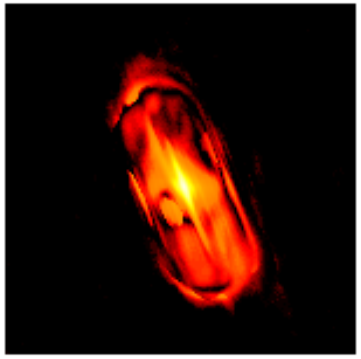
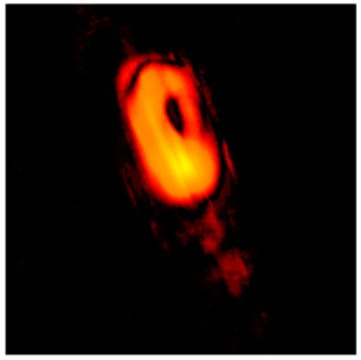
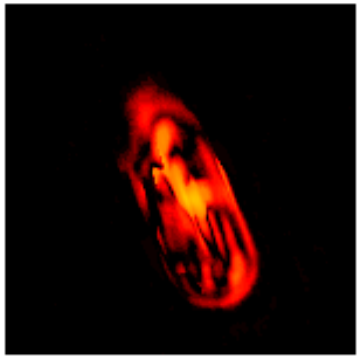
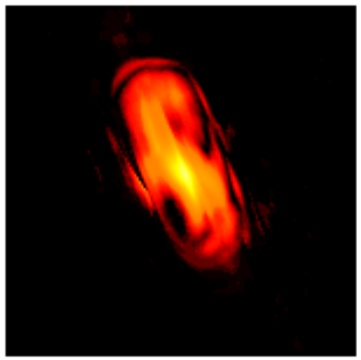
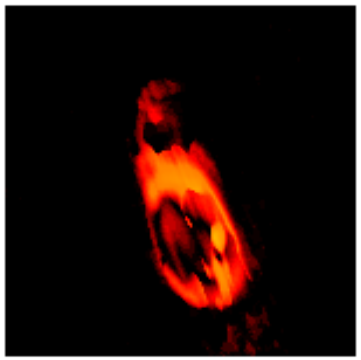
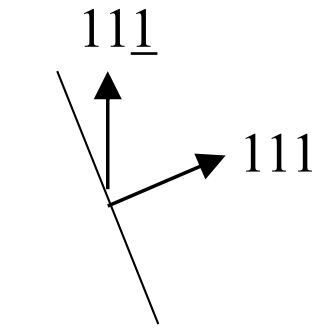
3D Diffraction Method

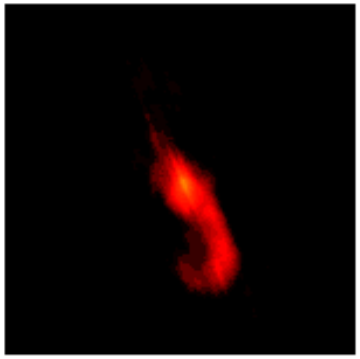
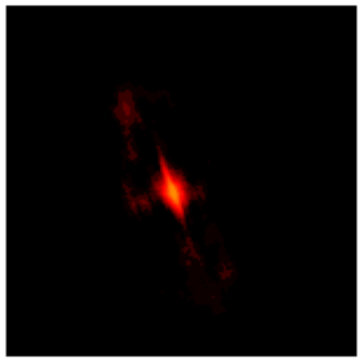


3D Diffraction Data
1 micron Au crystal

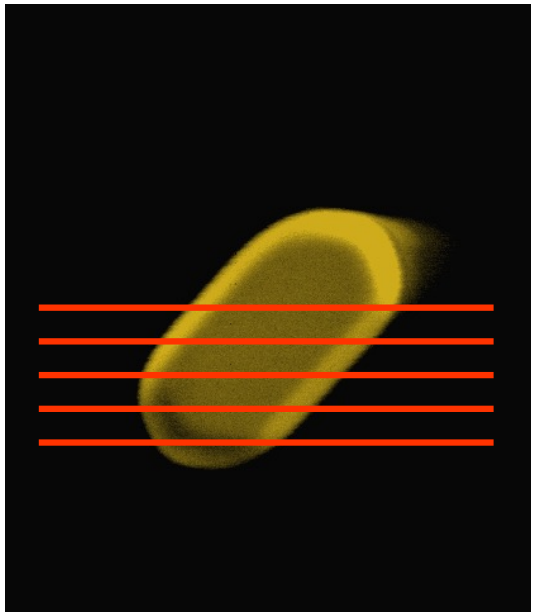


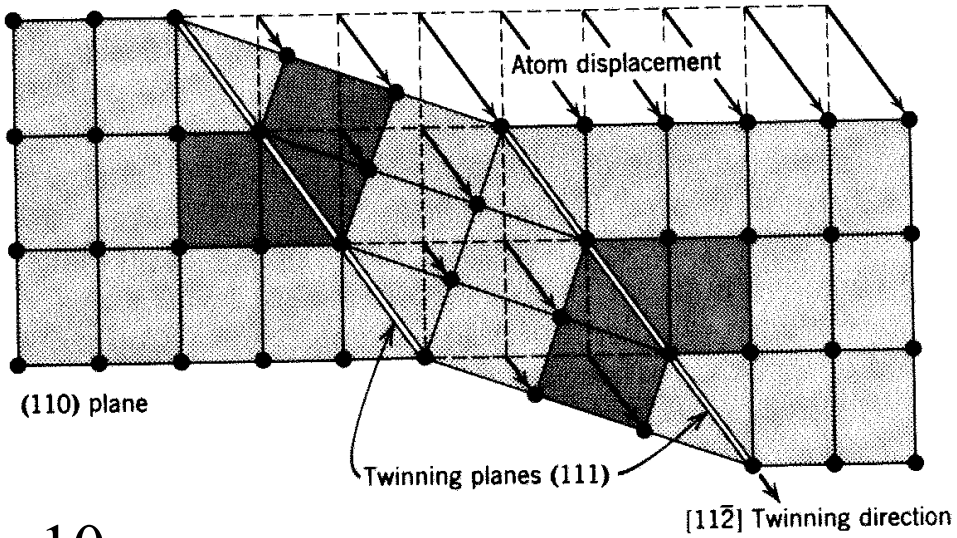



Slices through plan view SEM:



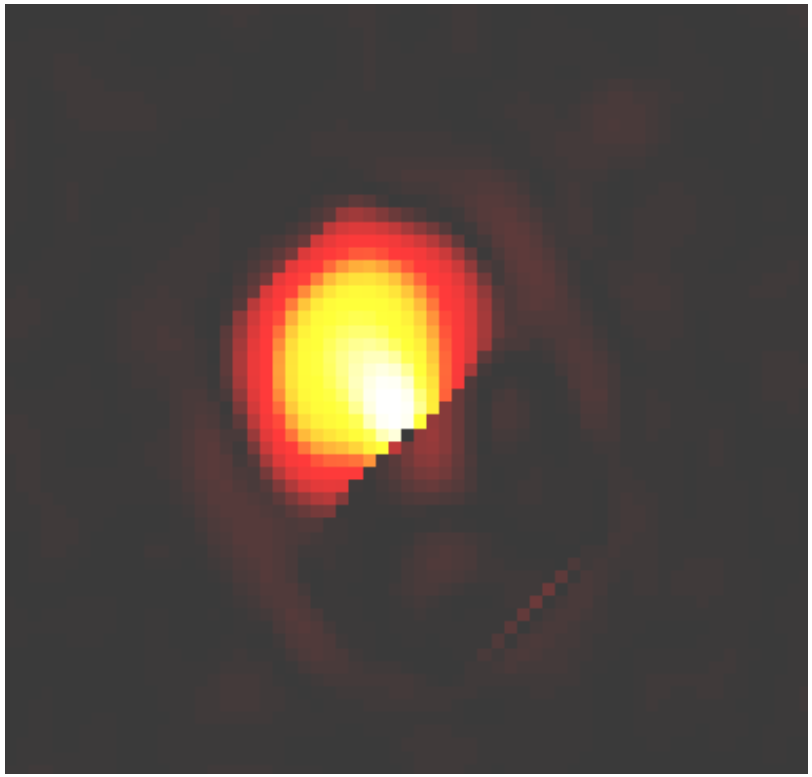
Twinning in deformed FCC metals

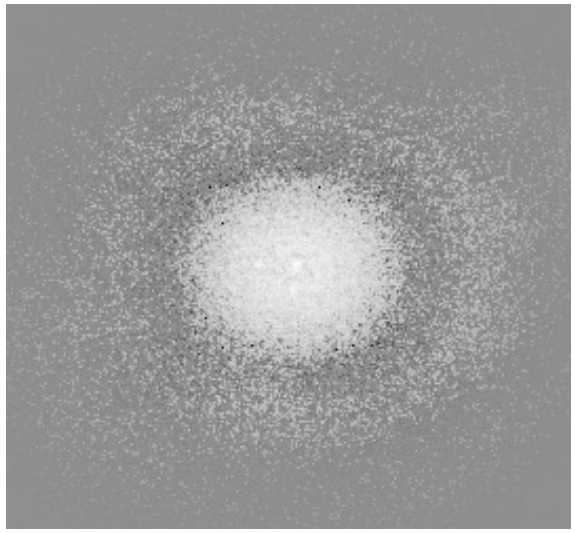
J. Wulff, "Structure and Property of Materials III" (1965)

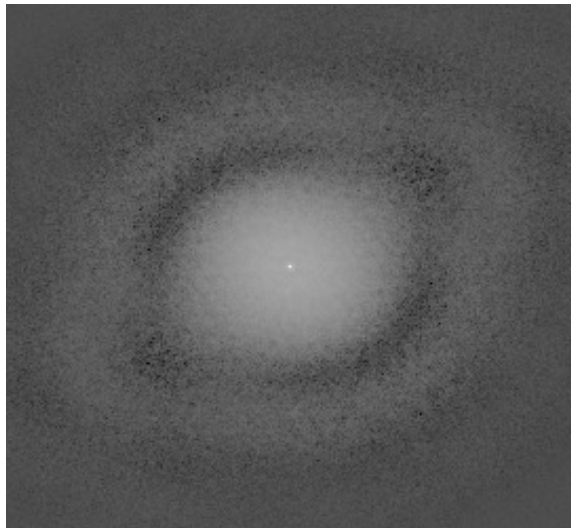


~10μm
Cu

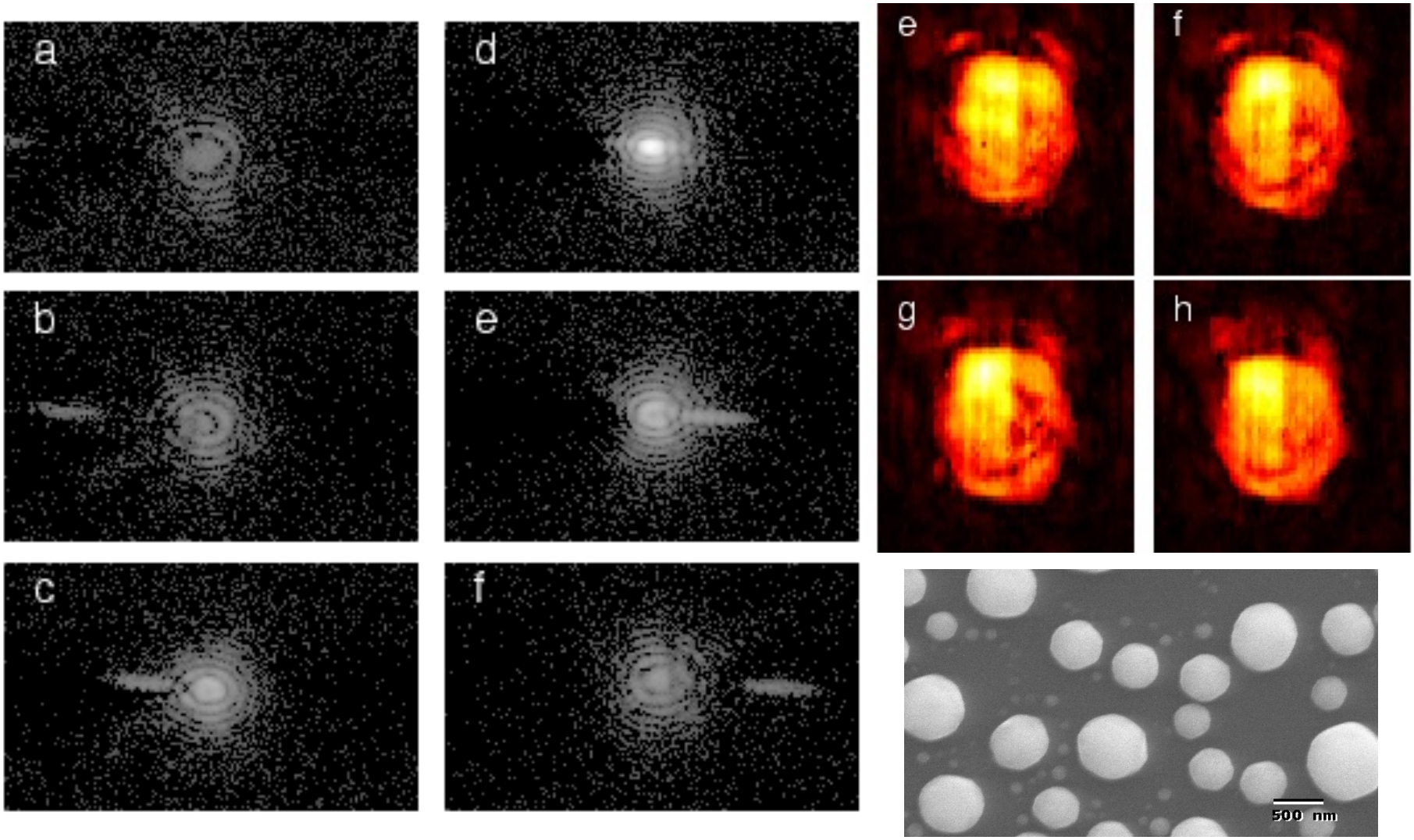
Reconstruction of Pb Nanocrystal



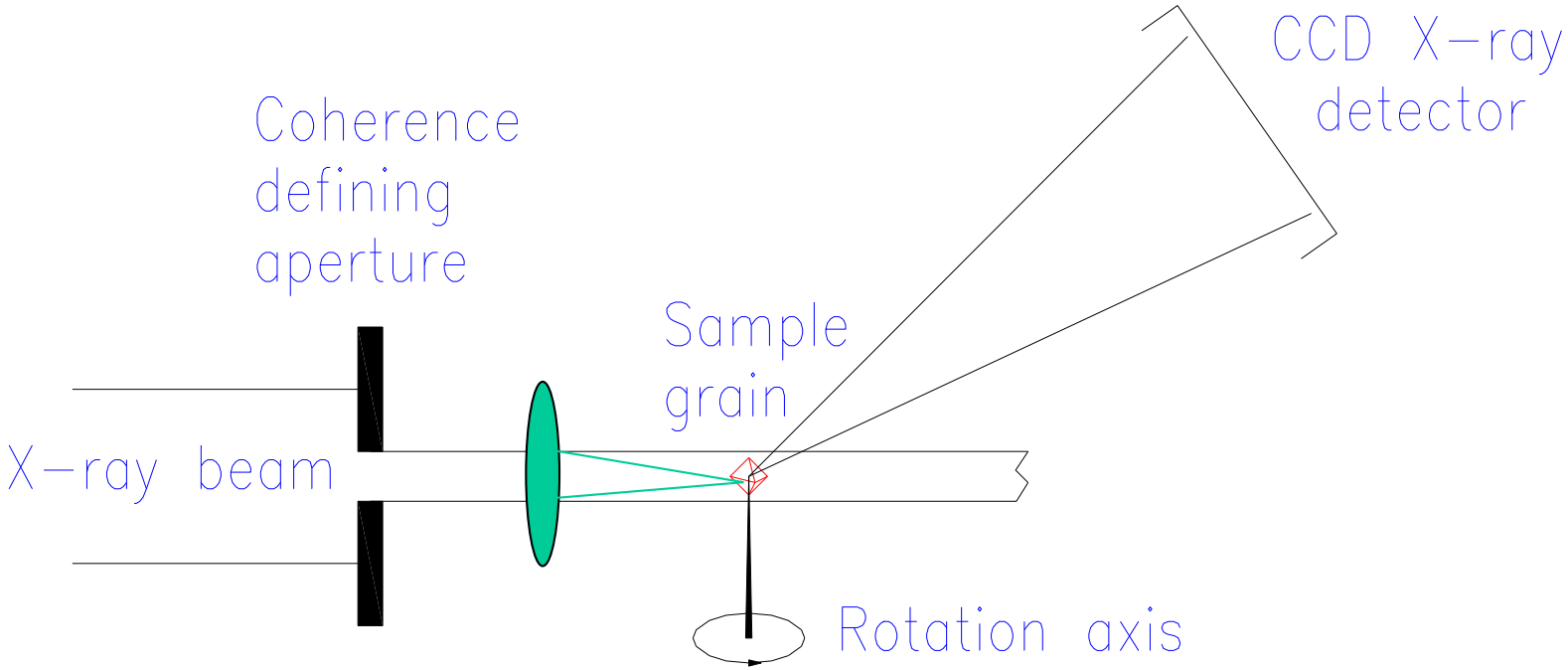




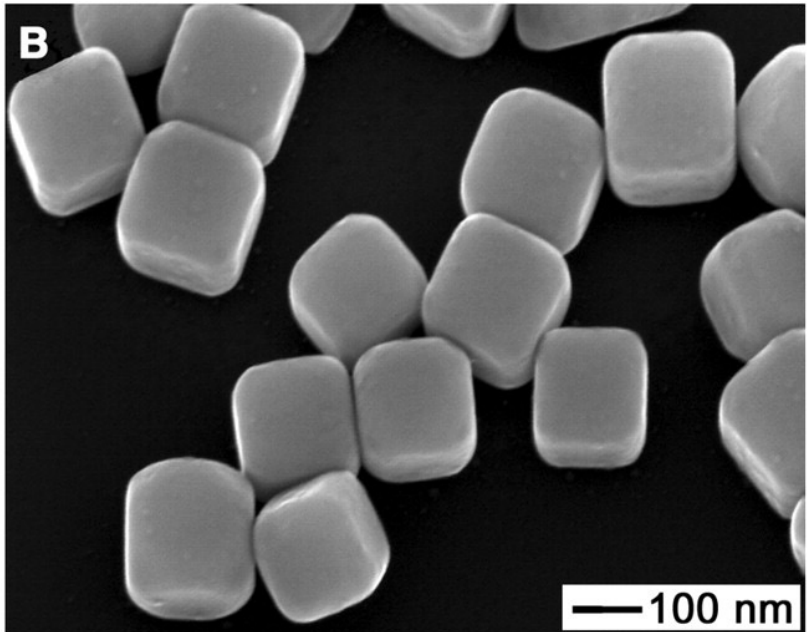
3D reconstruction of Pb nanocrystals

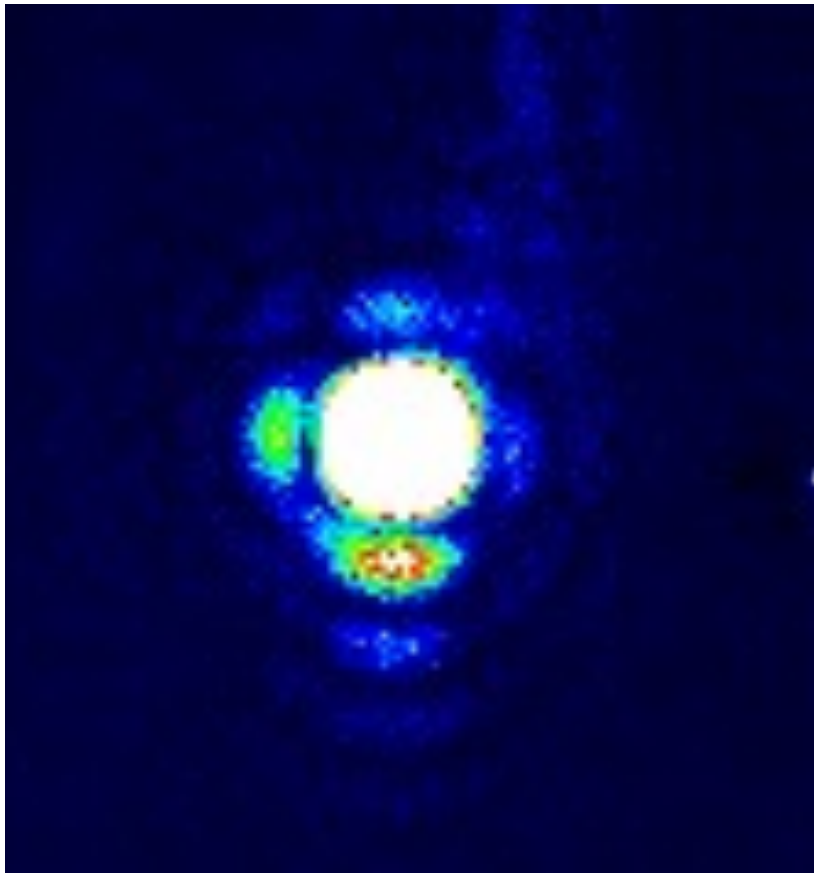


Lensless X-ray Microscope



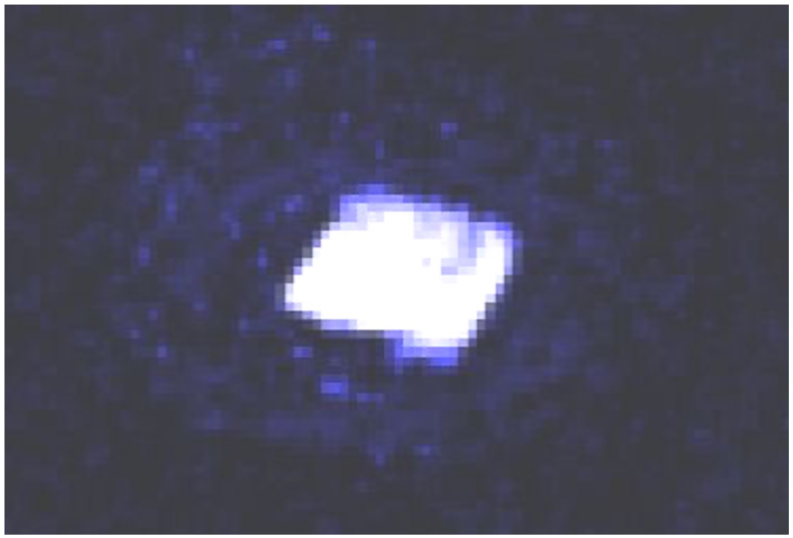
Chemically Synthesized Silver Nanocubes



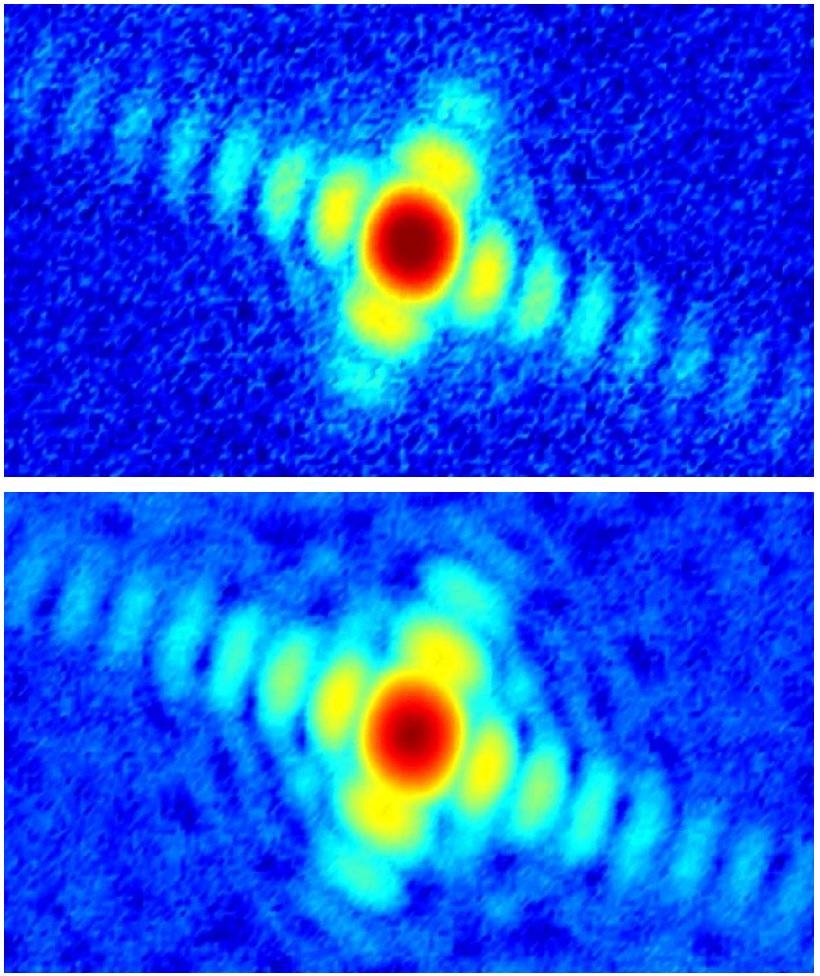


Yugang Sun and Younan Xia,
Science 298 2177 (2003)

Reconstruction of Ag Nanocrystal

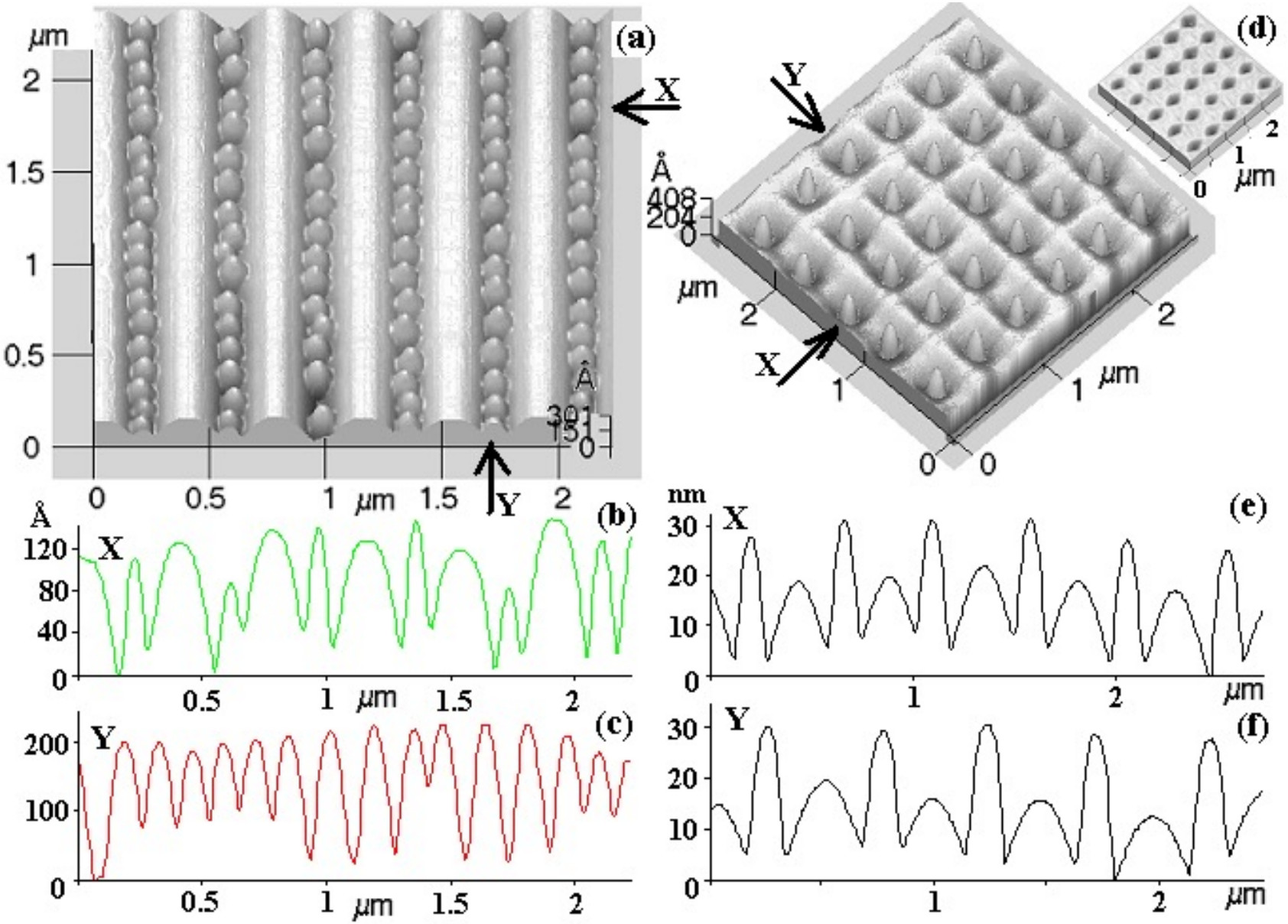


200nm



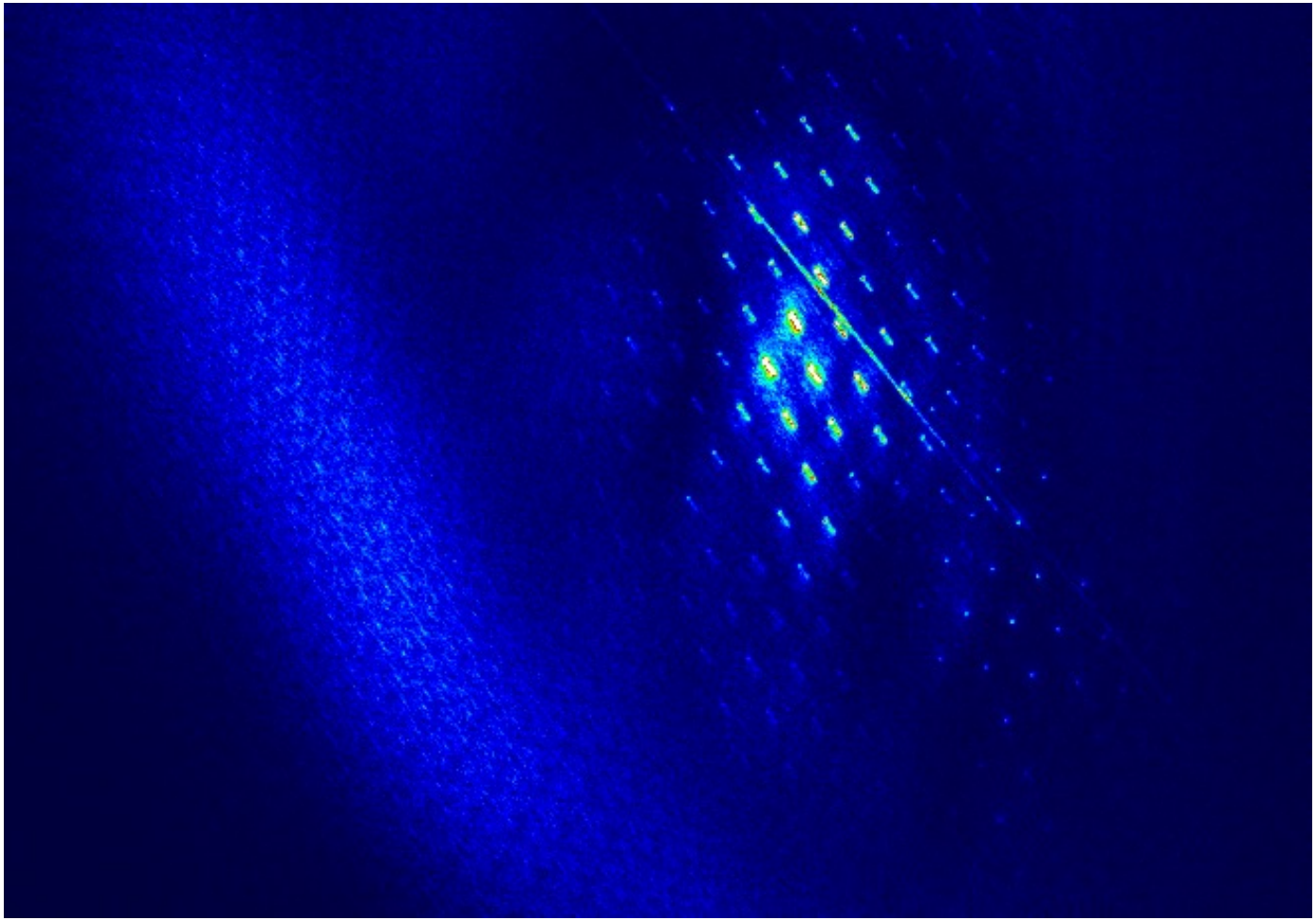
1D and 2D Quantum Dot Arrays

Zhenyang Zhong, G. Bauer, Johannes Kepler Universität Linz

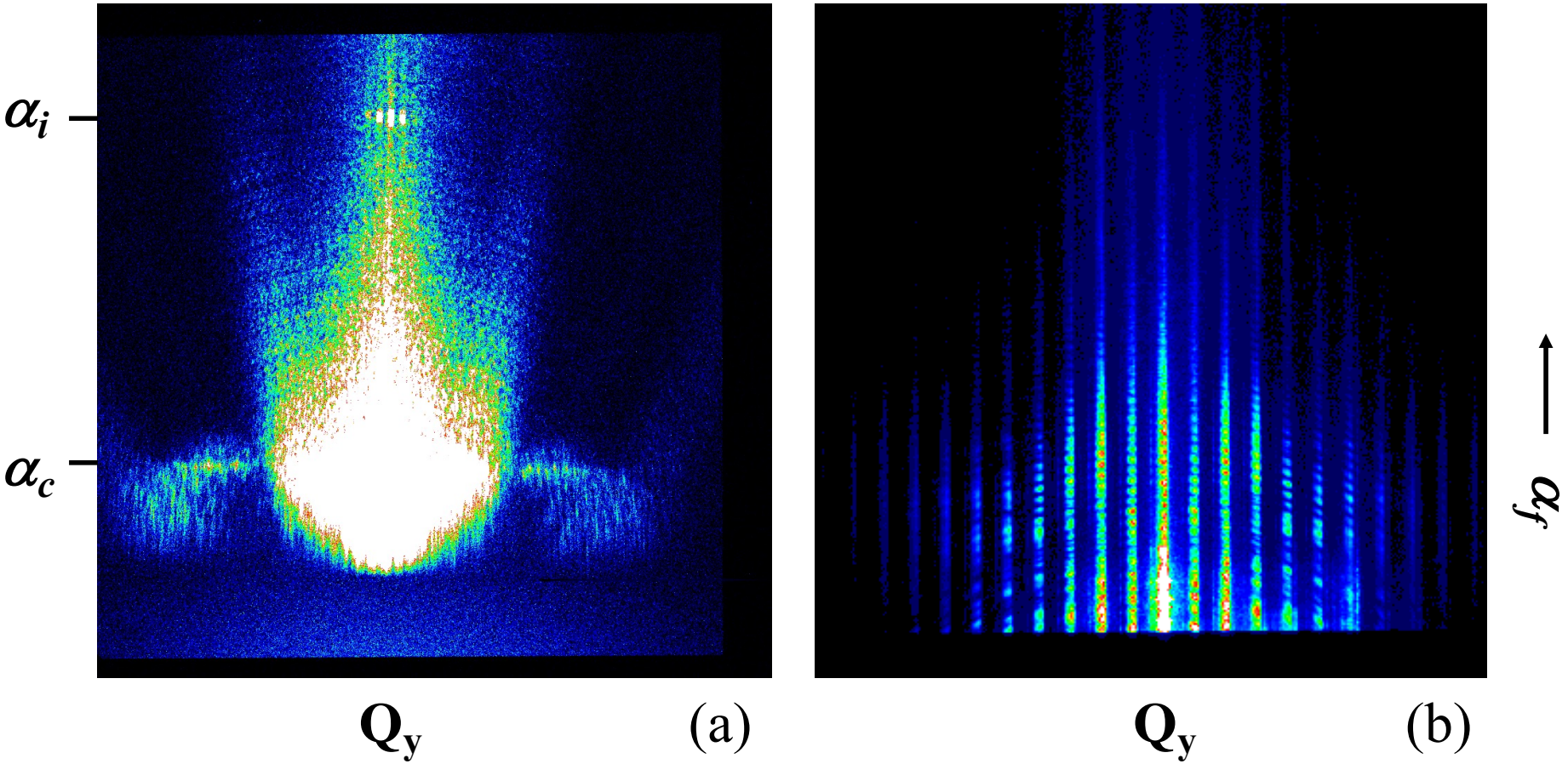


202 Diffraction from Ge QD array

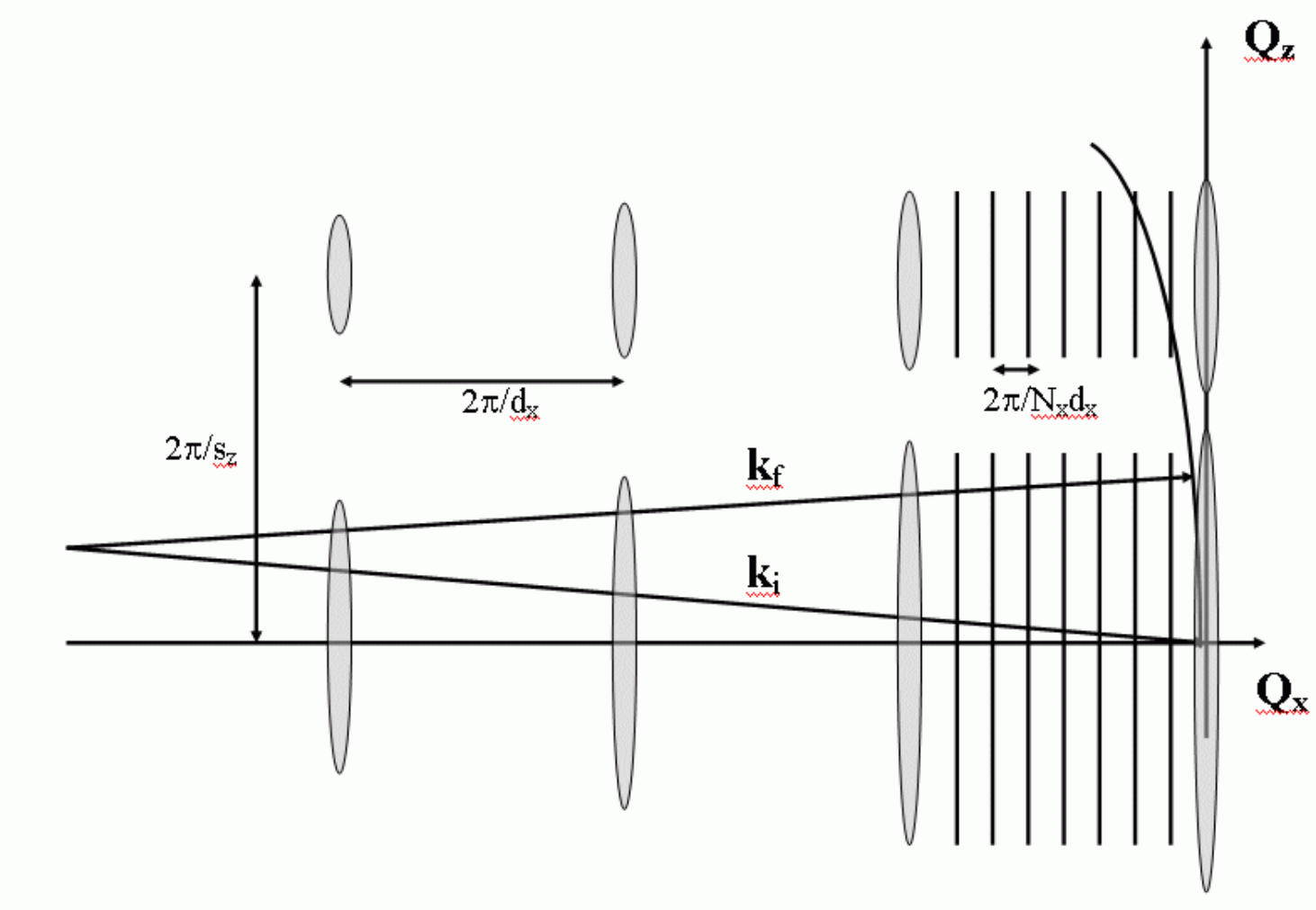
with G. Bauer, Z. Zhong and T. H. Metzger



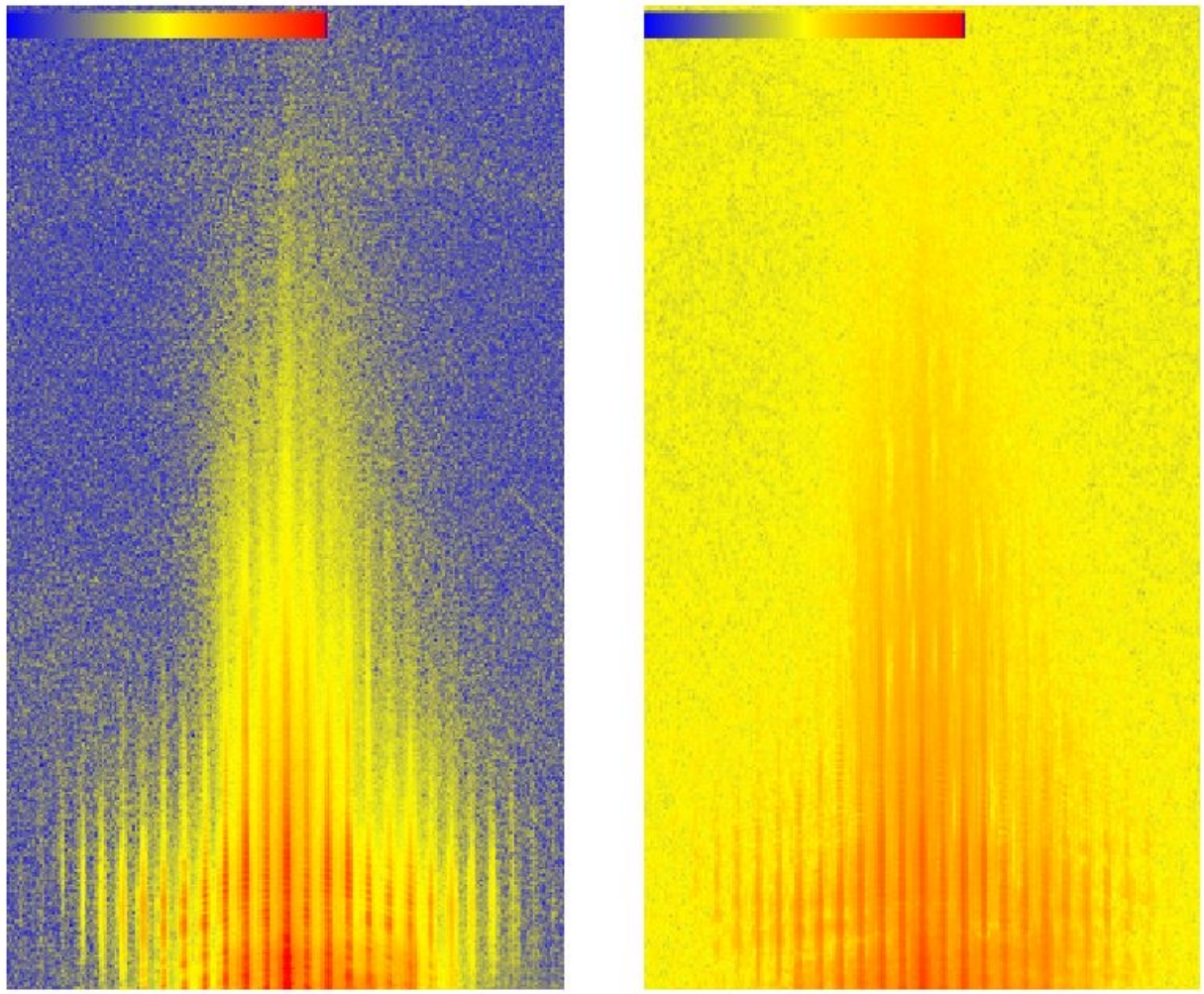
Yoneda and GISAXS geometries



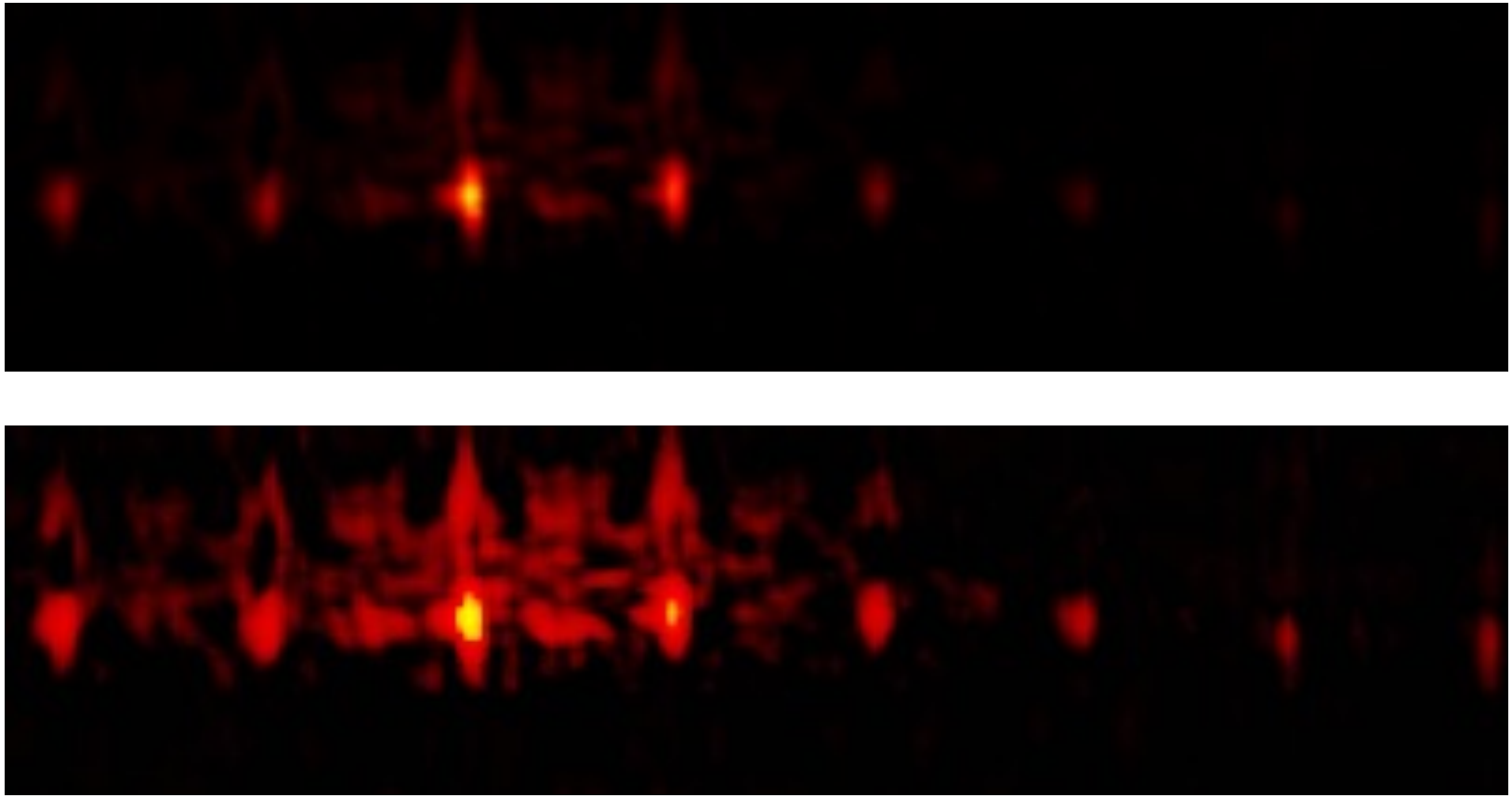
Modulations along Q_Z



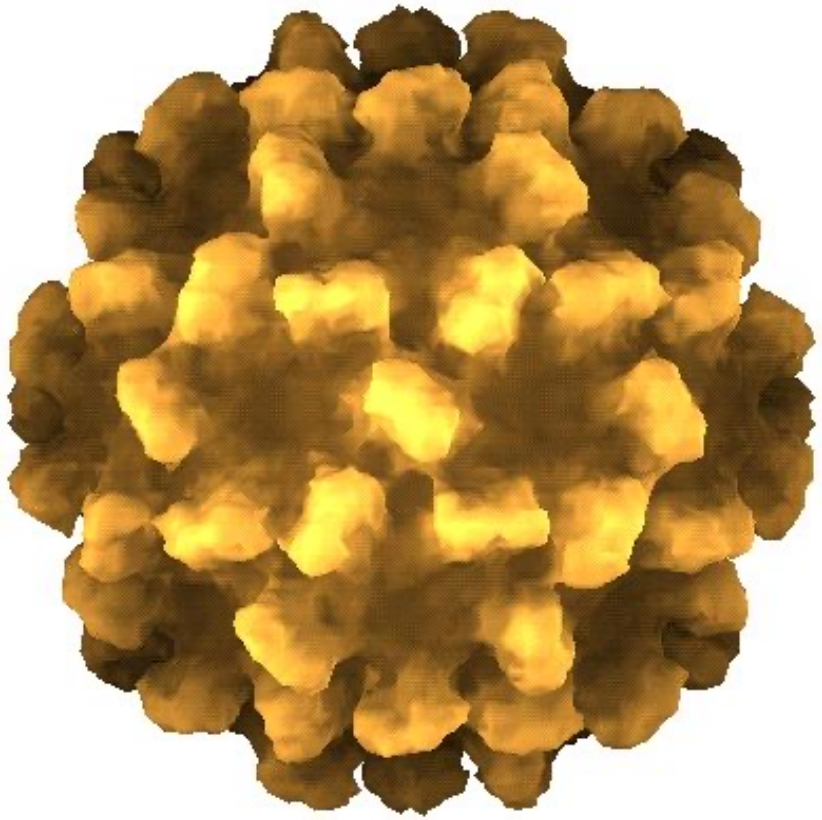
Data and Best Fit (Ivan)



Reconstructed Images (Ivan)



Tomato Bushy Stunt Virus
1980



Conclusions and Outlook

- Inversion of CXD demonstrated
- Internal structure of Au Nanocrystals
- Preservation of coherence upon focussing
- Dislocations, Quantum Dots all possible now
- Single molecules one day