Coherent Beams in the Nano Word

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NSLS Users Meeting
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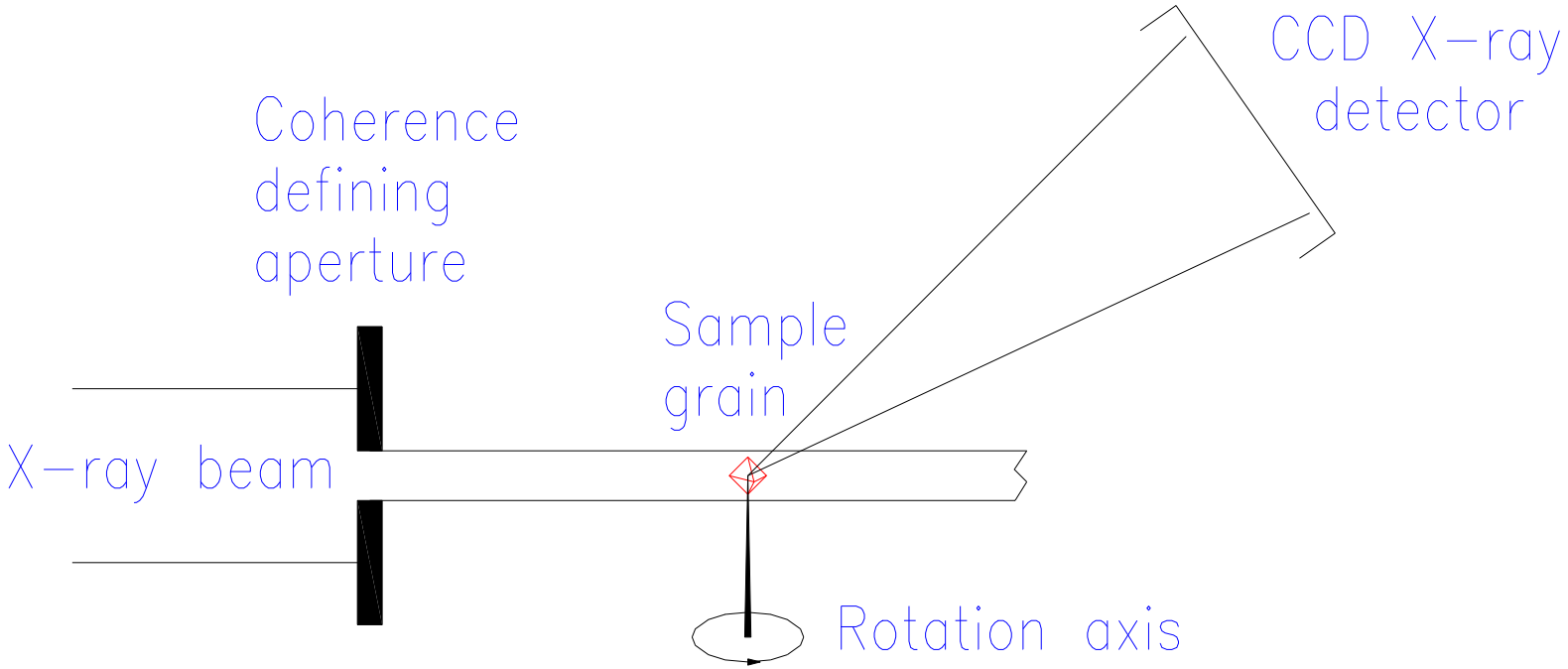
Outline

- Coherence in Diffraction
- The Phase Problem
- Nanocrystal Shapes
- Future Applications
  - Smaller Nanocrystals
  - Dislocation Structure
  - Single-Molecule Imaging with XFEL

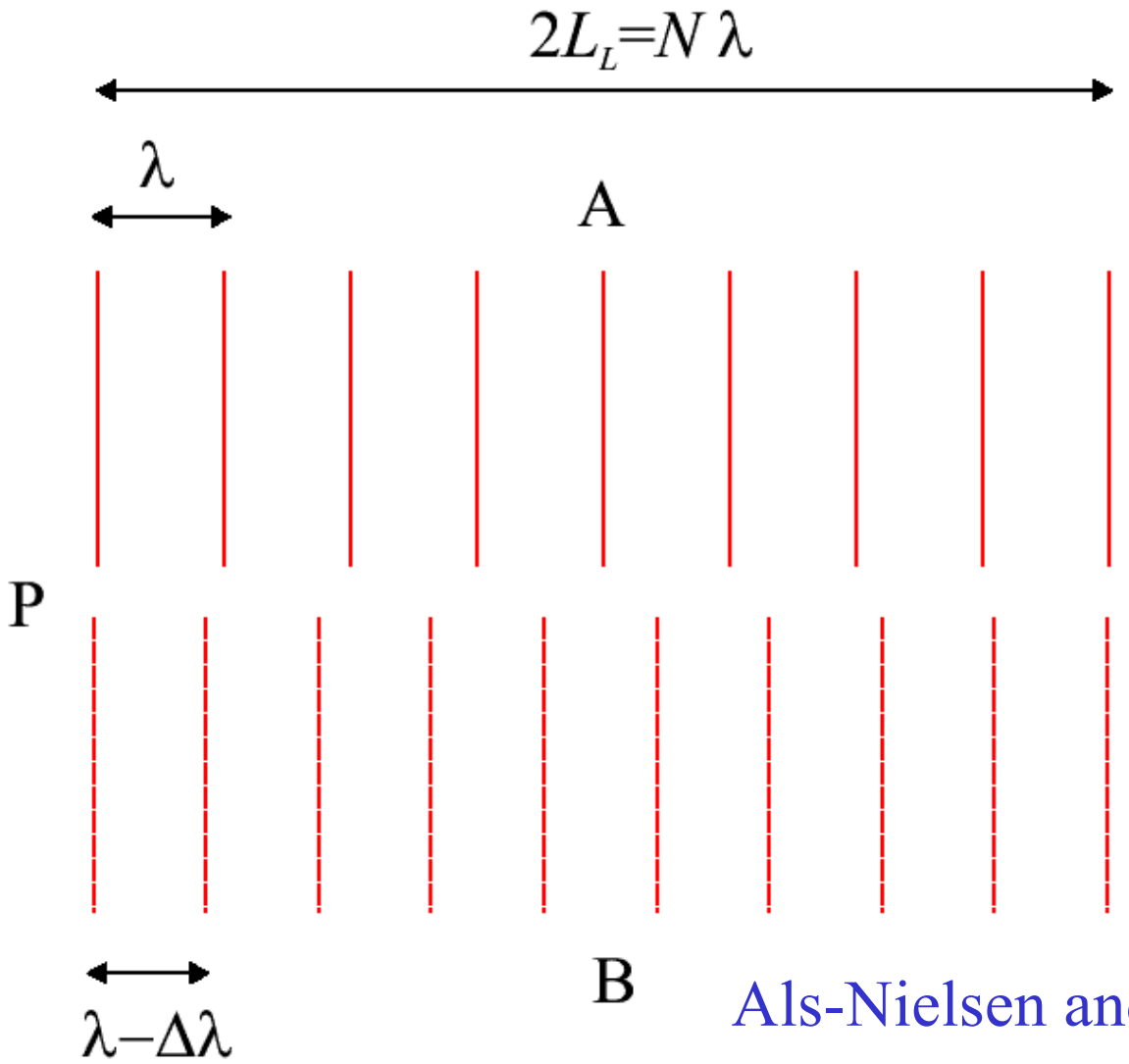
Goals of Coherent Diffraction

- Thermodynamic fluctuations
  - No ensemble average in CXD
- Probe of structure on nm scale
  - 1D, 2D and 3D
  - non-periodic object gives continuous F(**q**)
- Oversampling (in reciprocal space) permits solution of the phase problem

Lensless X-ray Microscope
based on diffraction from crystal lattice



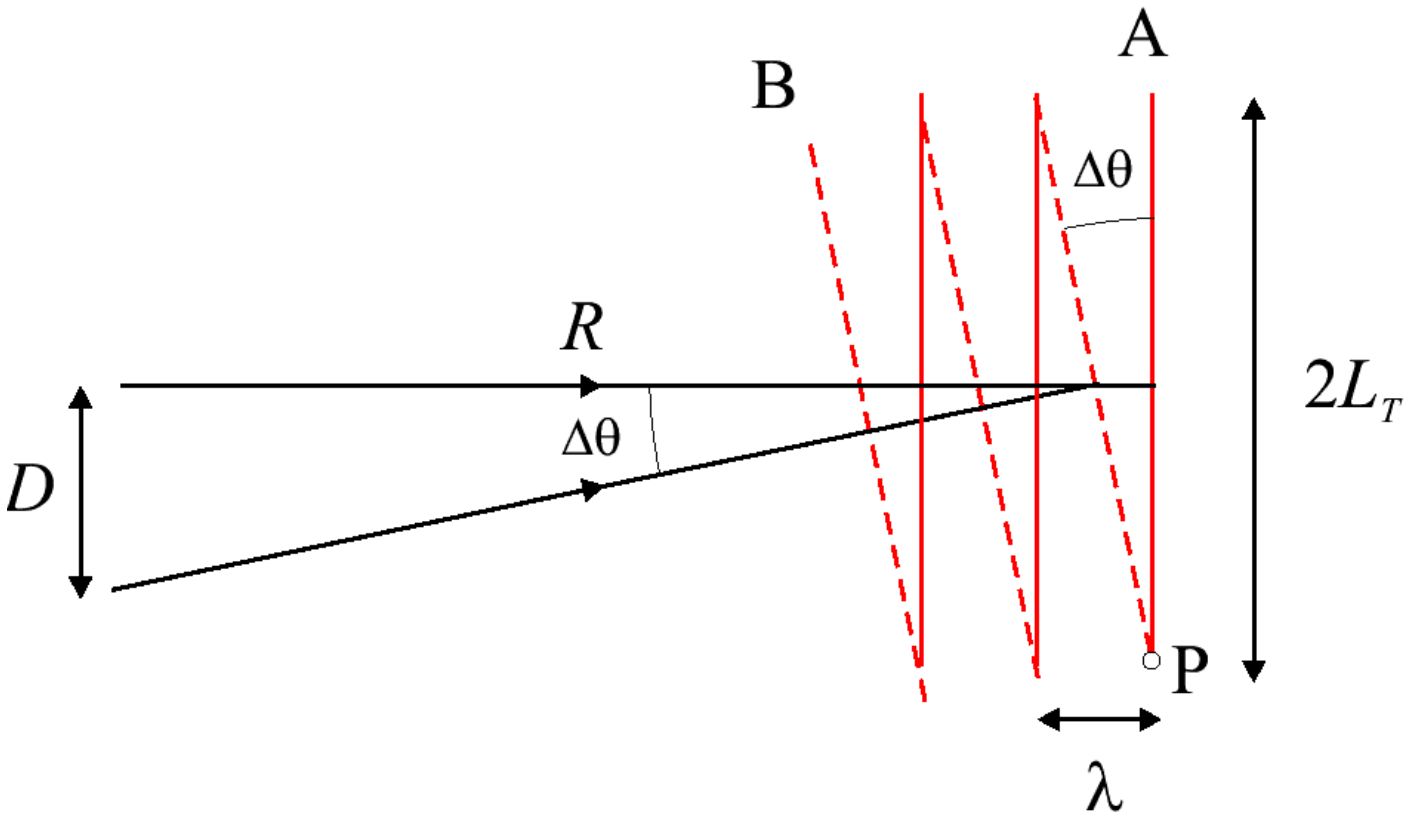
Longitudinal Coherence



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

Als-Nielsen and McMorrow (2001)

Lateral (Transverse) Coherence



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

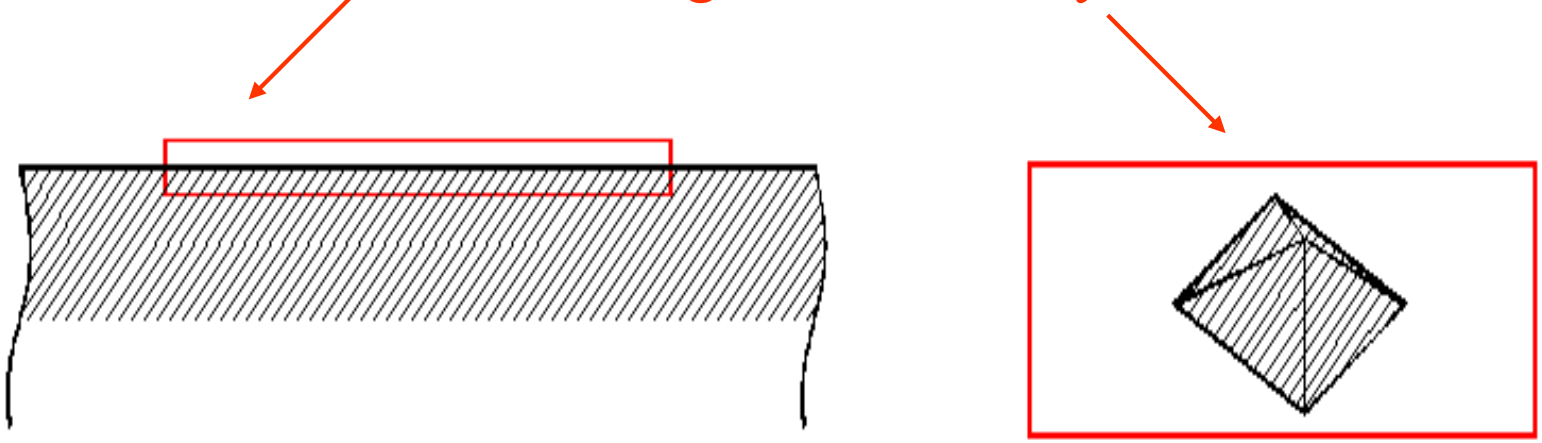
Als-Nielsen and McMorrow (2001)

Coherence at the APS

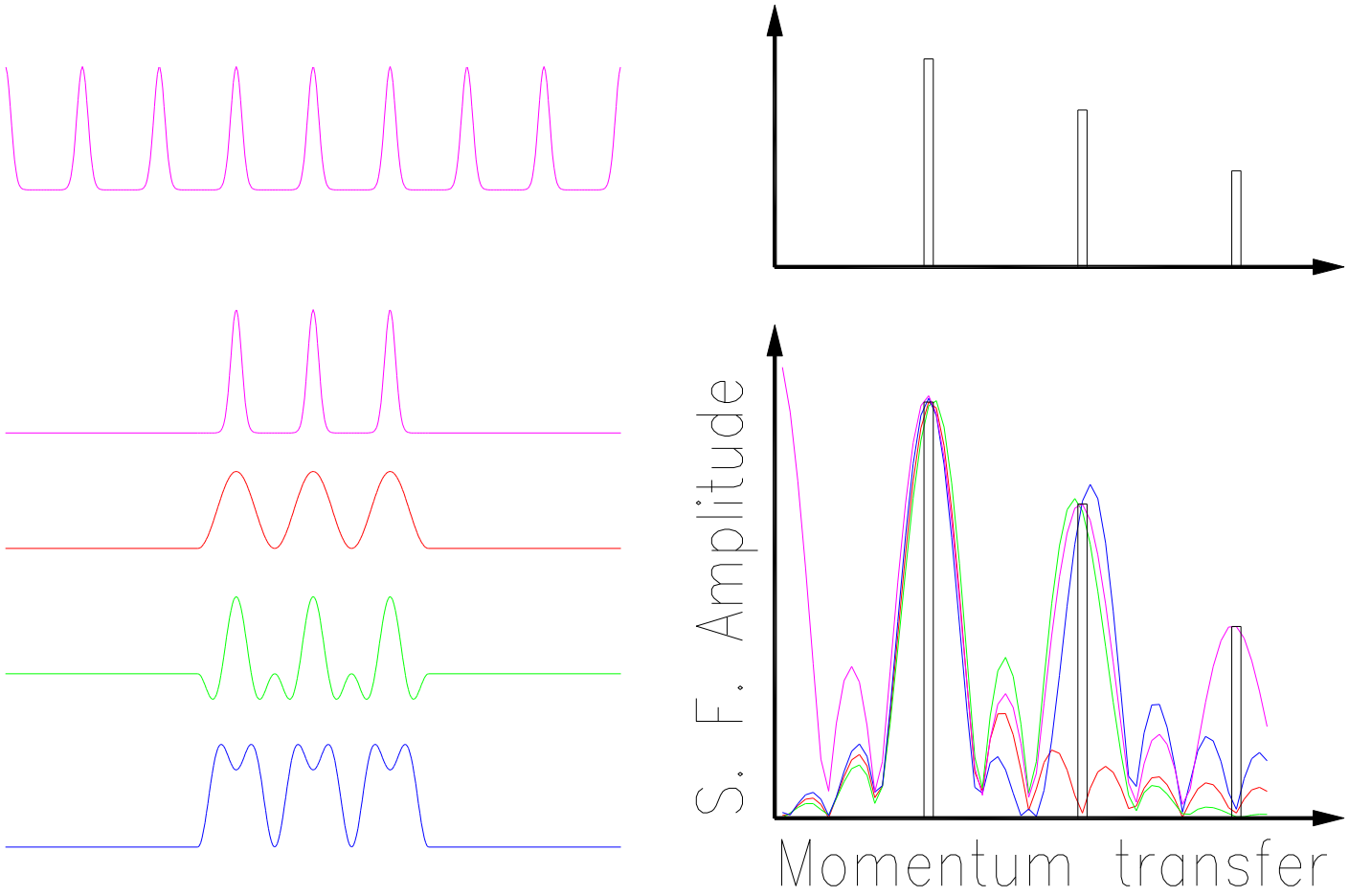
Typical 3rd Generation (undulator) Synchrotron Source
"New Ring" coherence and flux at 8keV will be similar

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}

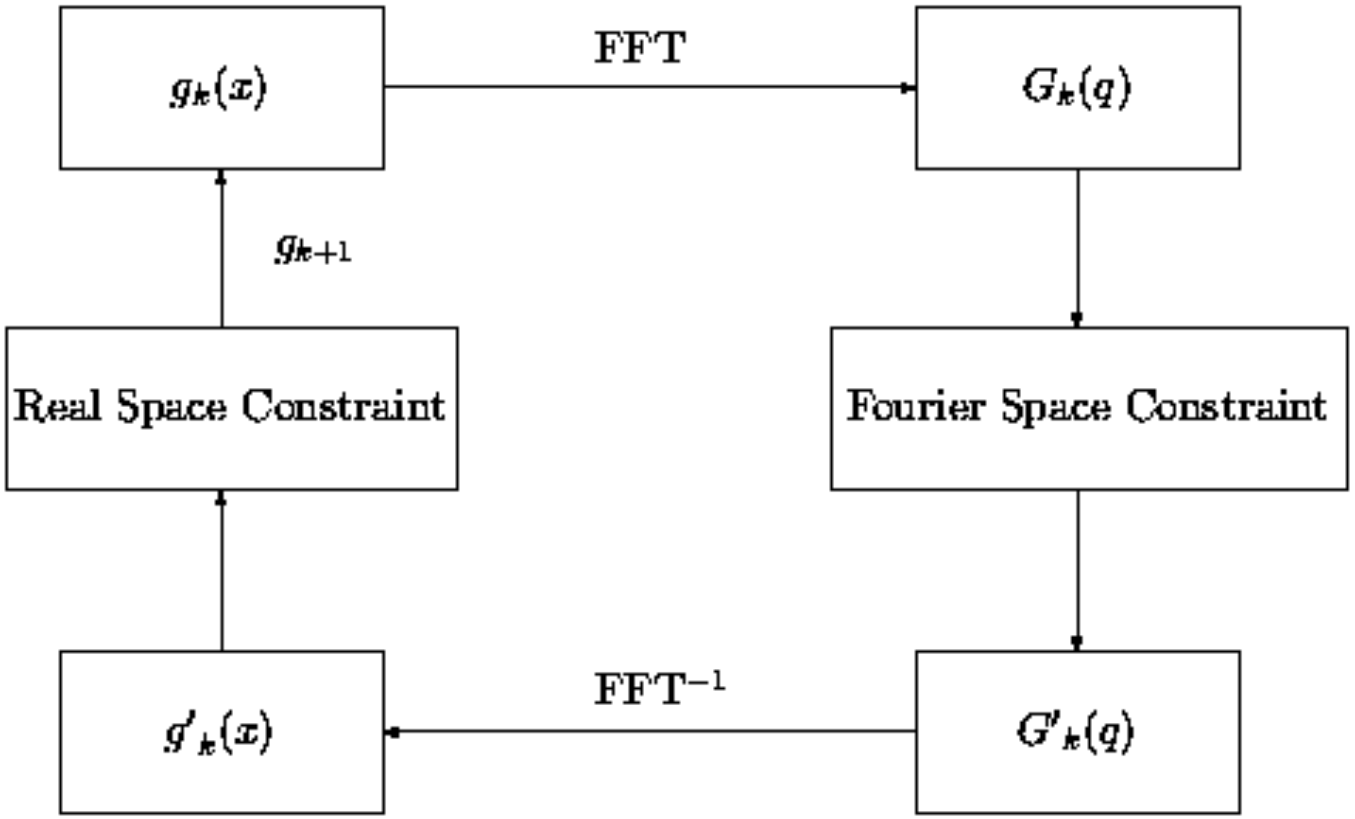
Coherent region defined by slits



Phase Problem: Finite-size Effect



Generic "Error Reduction" method

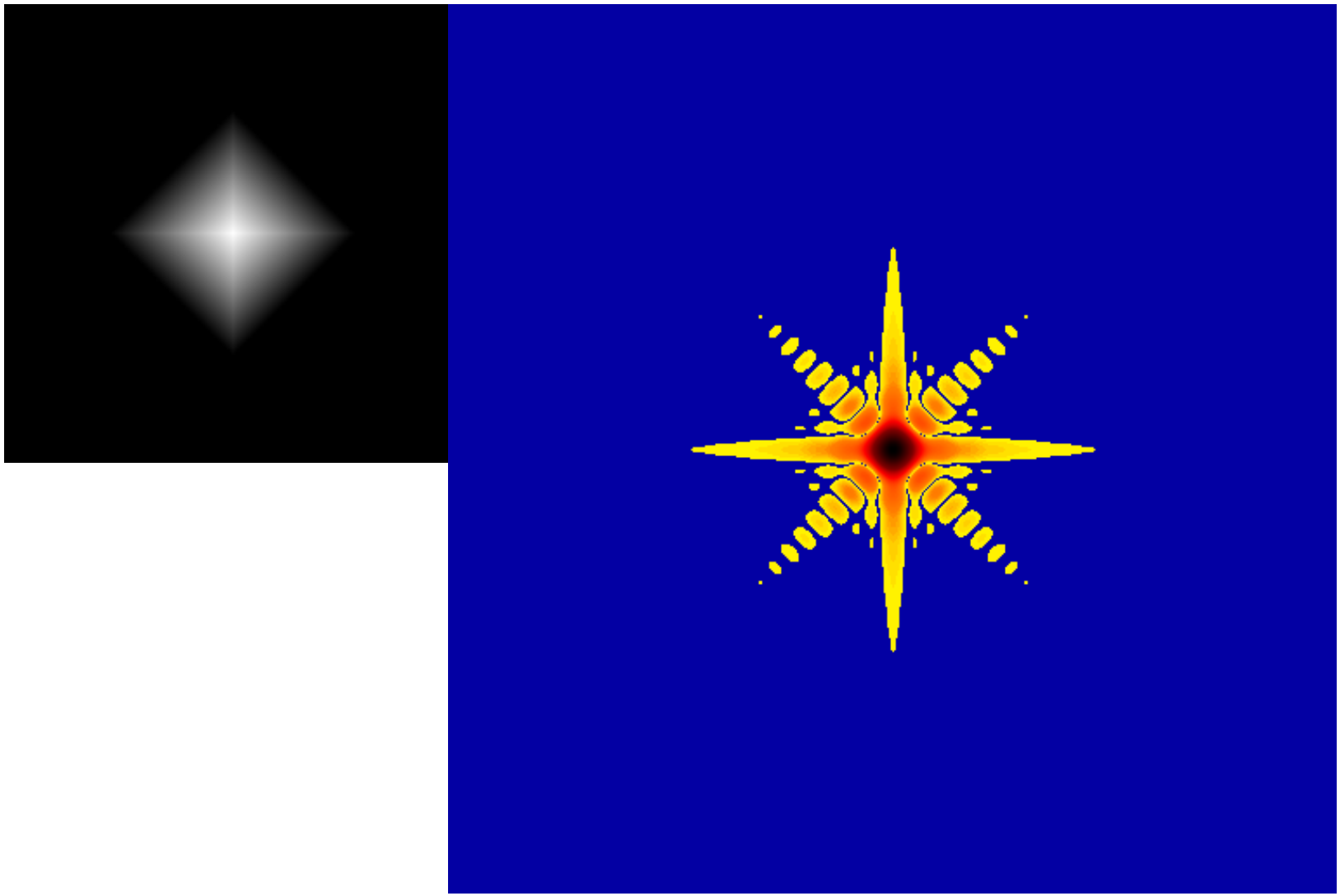


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

Real-space Constraints in Crystallograhy

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

- 'Positivity' constraint (Sayre)
- Finite support, molecular envelope
- Solvent flattening
- Molecular replacement
- Non-crystallographic symmetry
- Non-uniqueness is 'pathologically rare' (d>1)



Diffraction as a Surface Integral

Die äußere Form der Kristalle in ihrem Einfluß auf die Interferenzerscheinungen an Raumgittern

Von M. v. Laue

Annalen der Physik [5] 26 55 (1936)

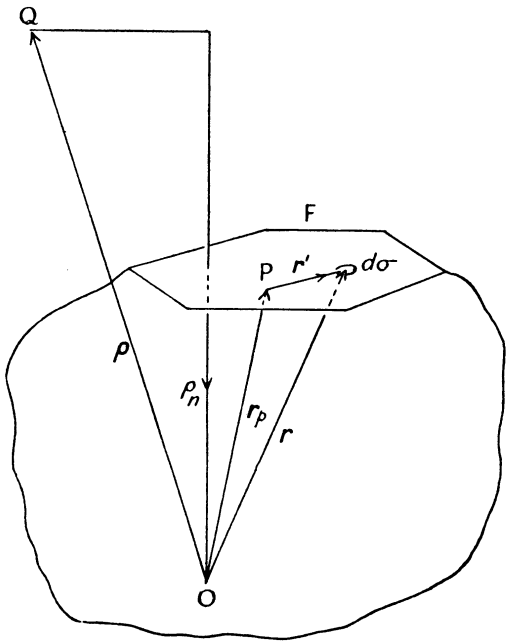
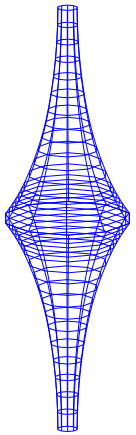
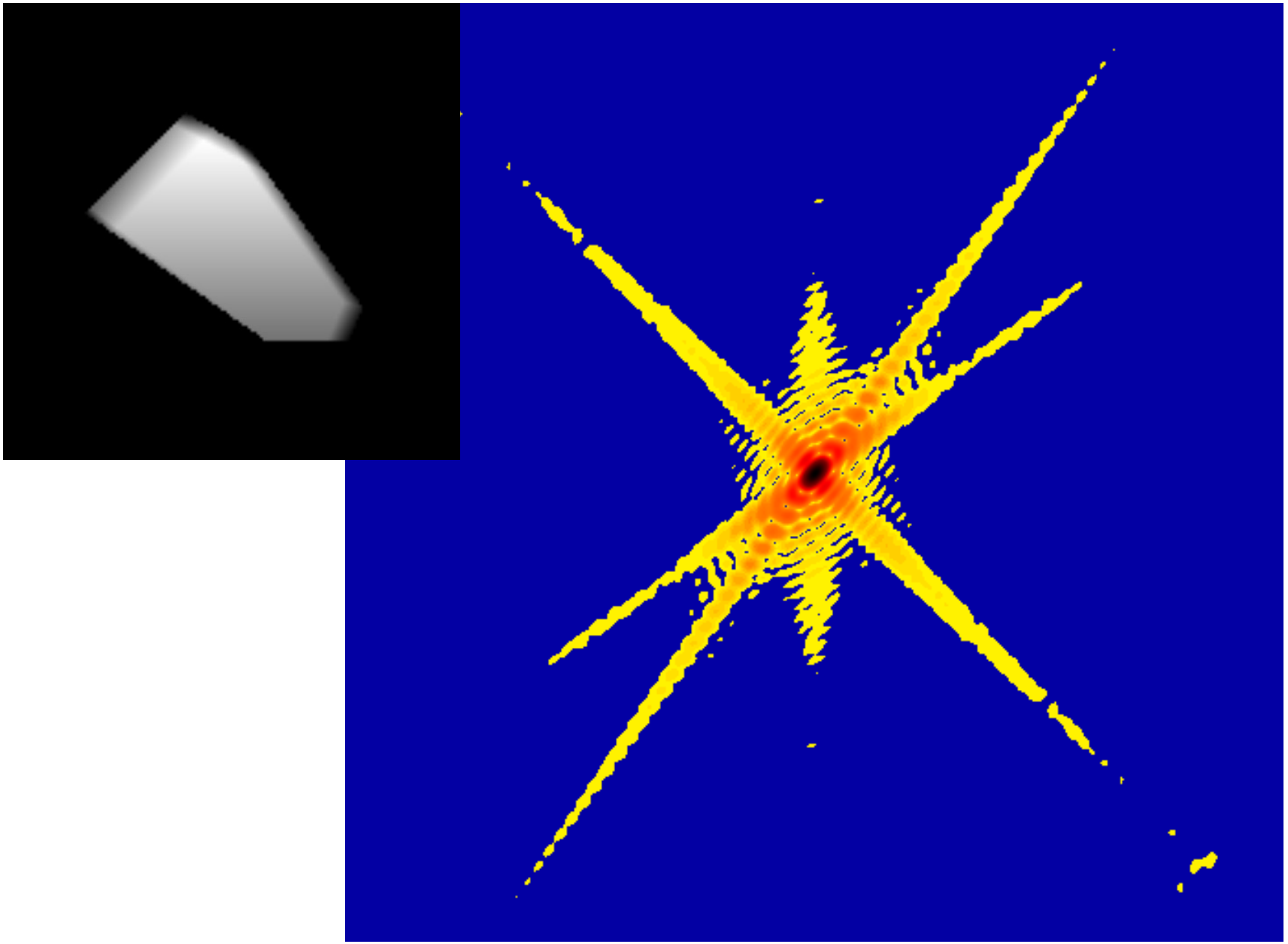


FIG. 200

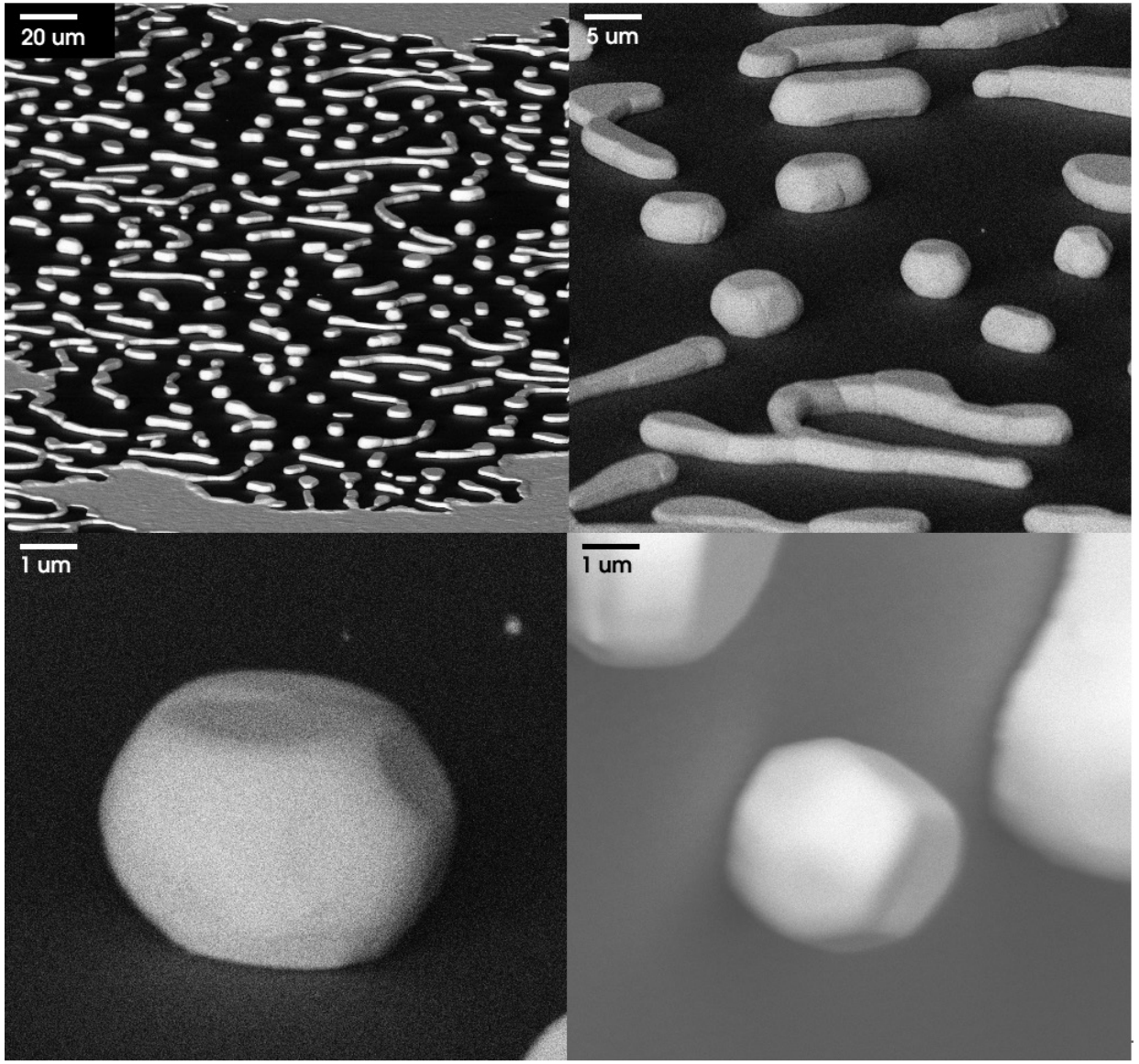


"Stacheln"

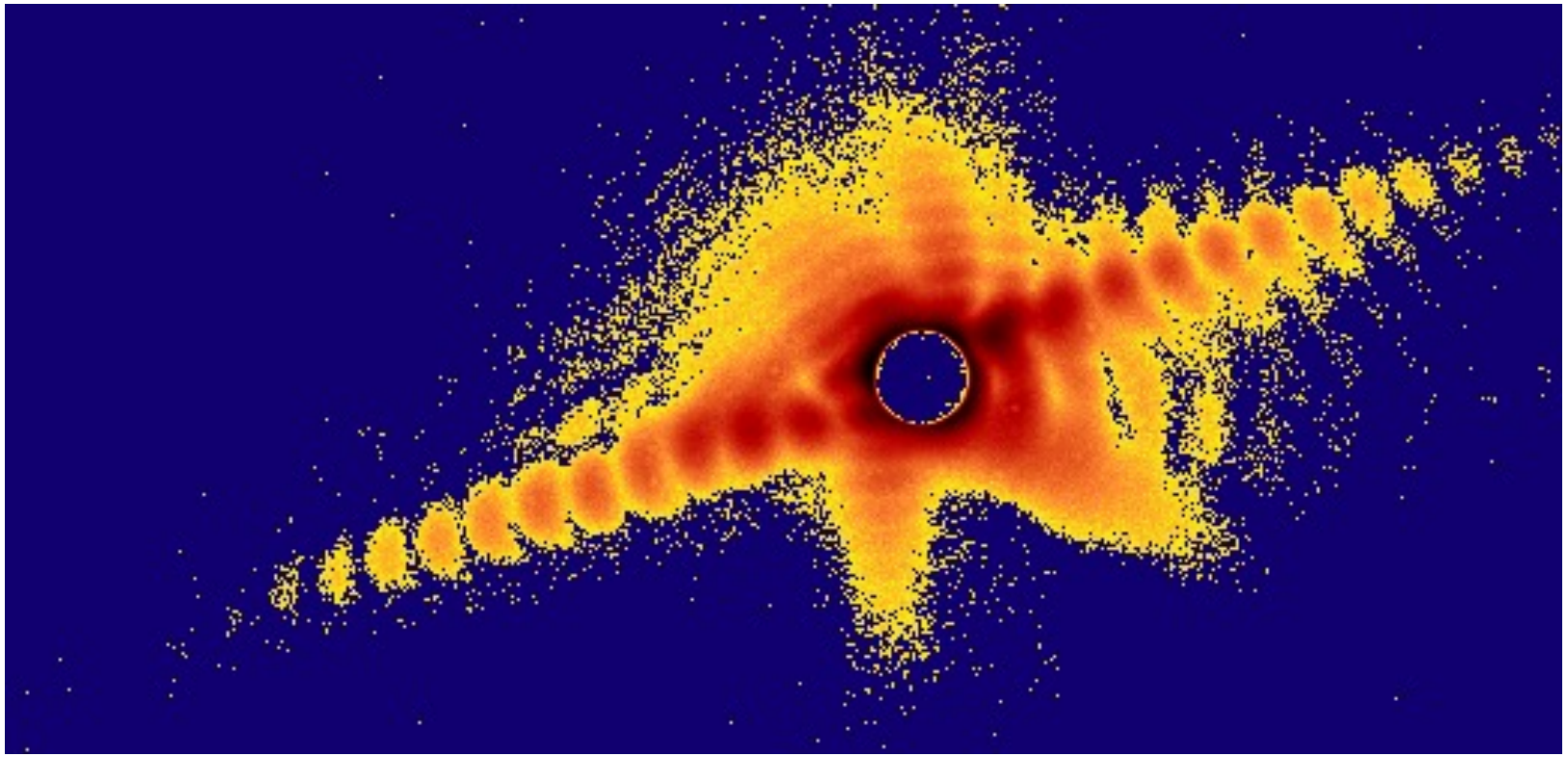


SEMS

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

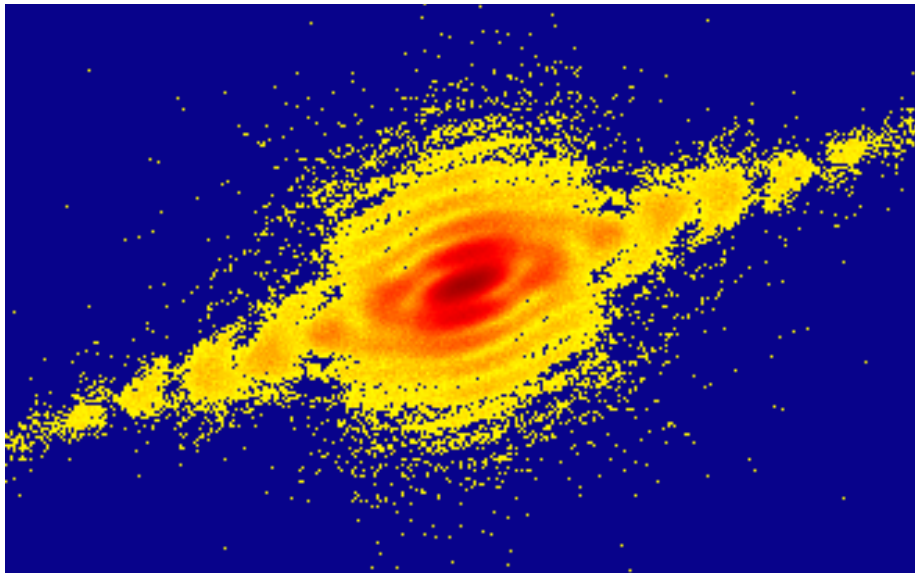


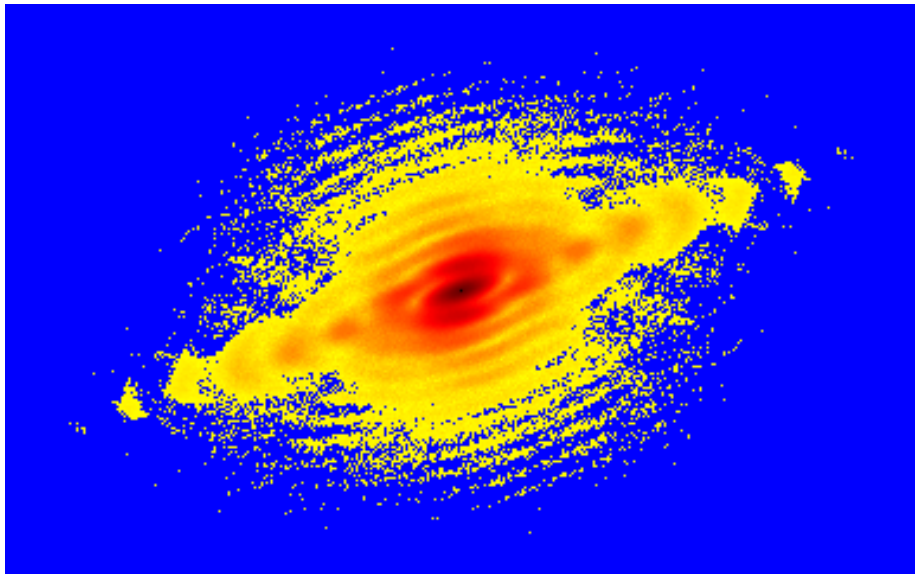
Micron-sized gold crystal: (111) Bragg reflection

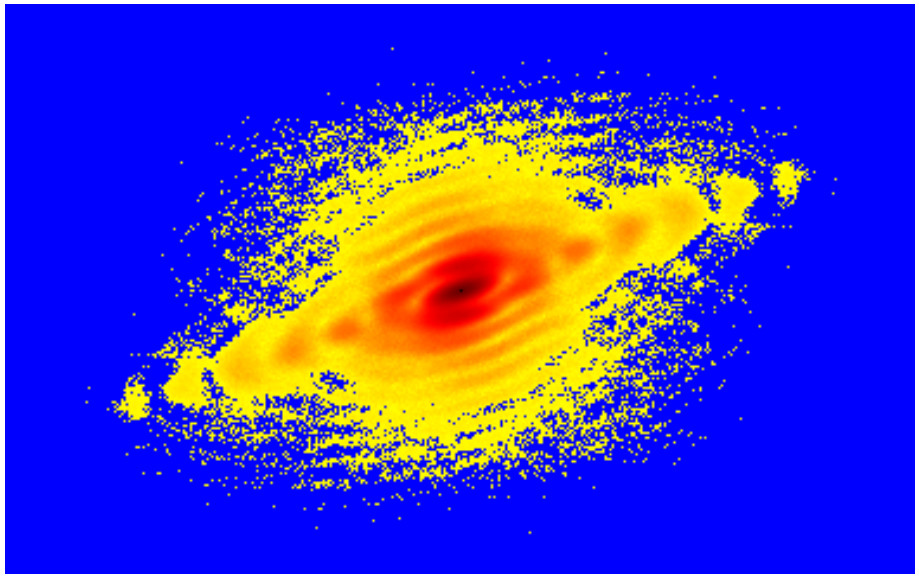


Symmetrized Data and two best fits

Chisq=0.0005

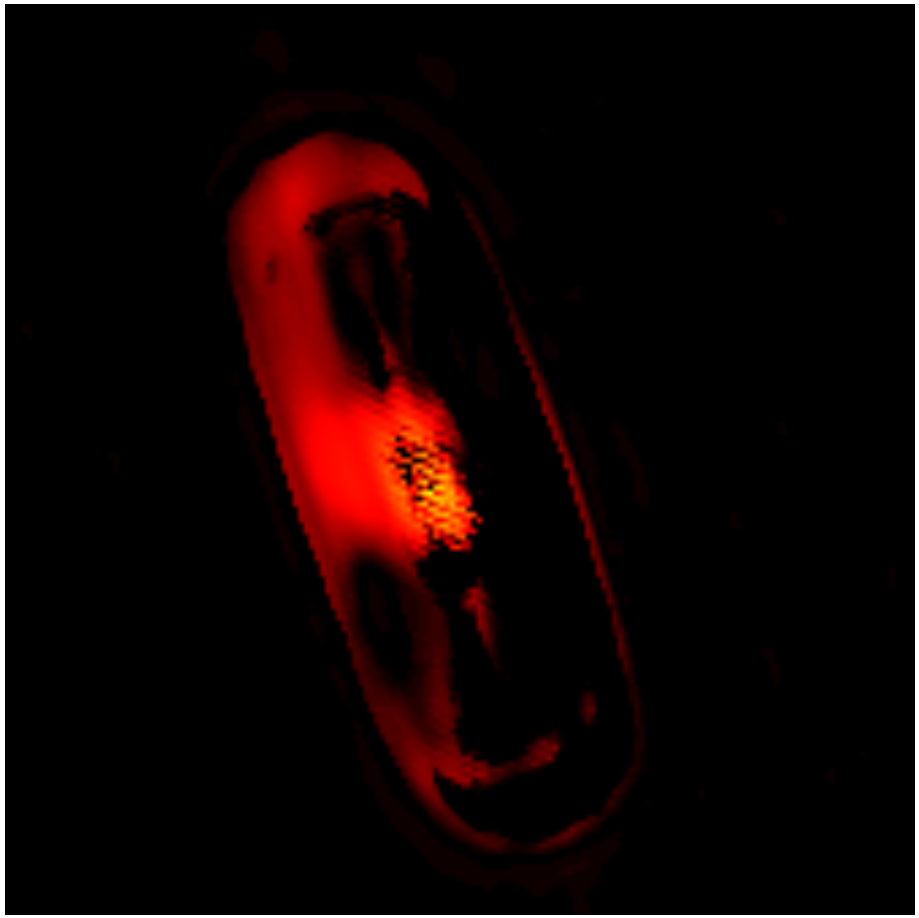


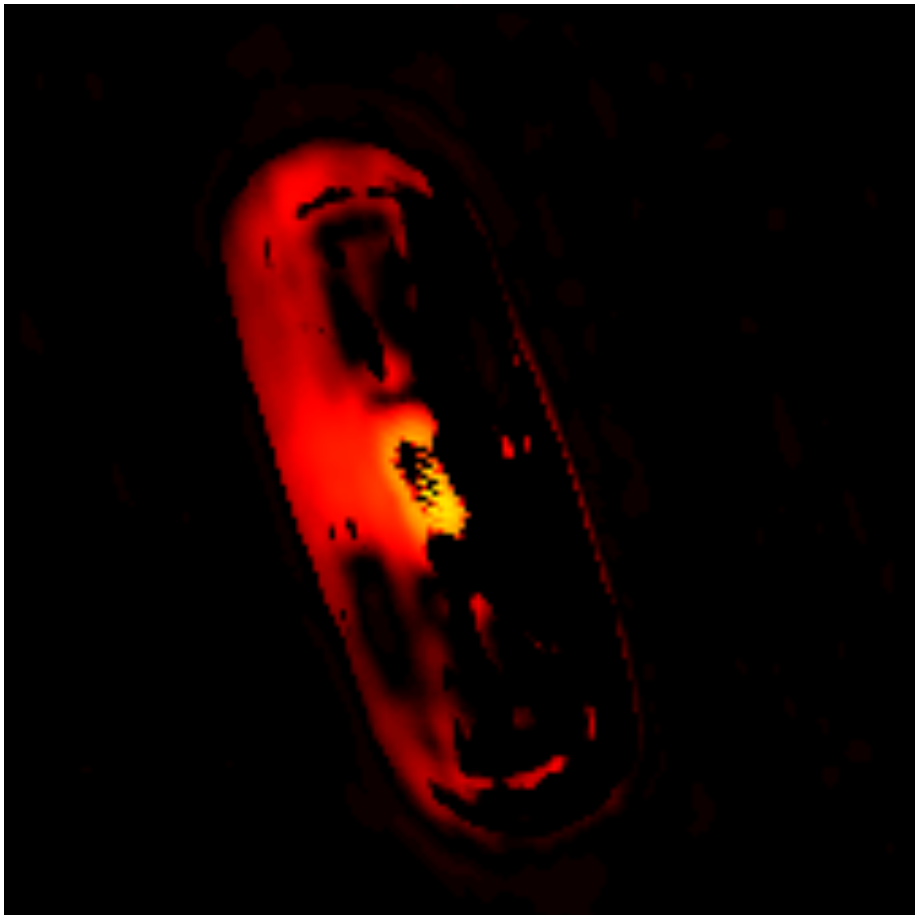




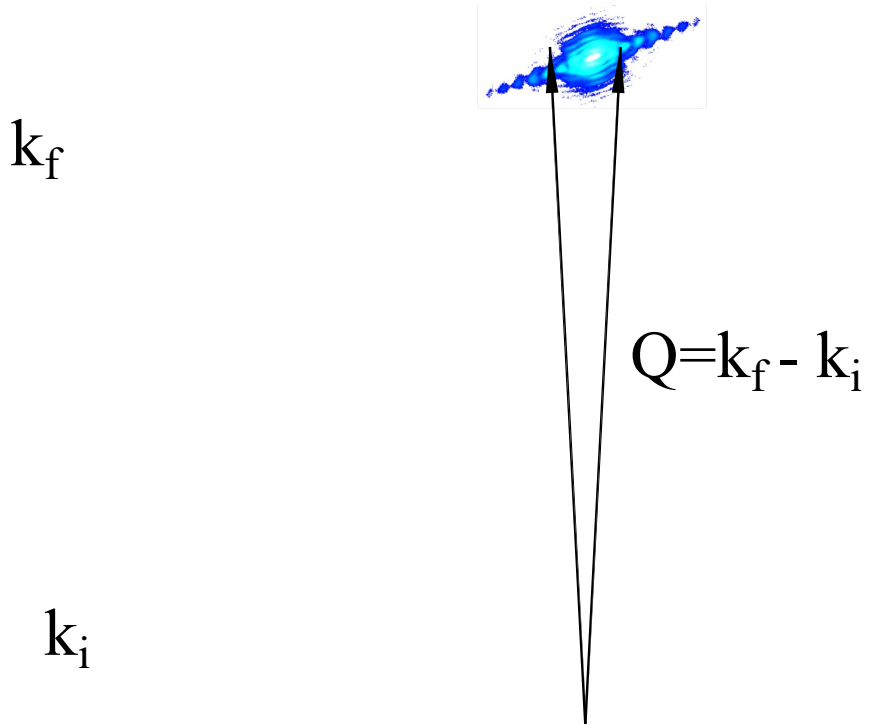
2D Reconstructions

chisquare = 0.0005

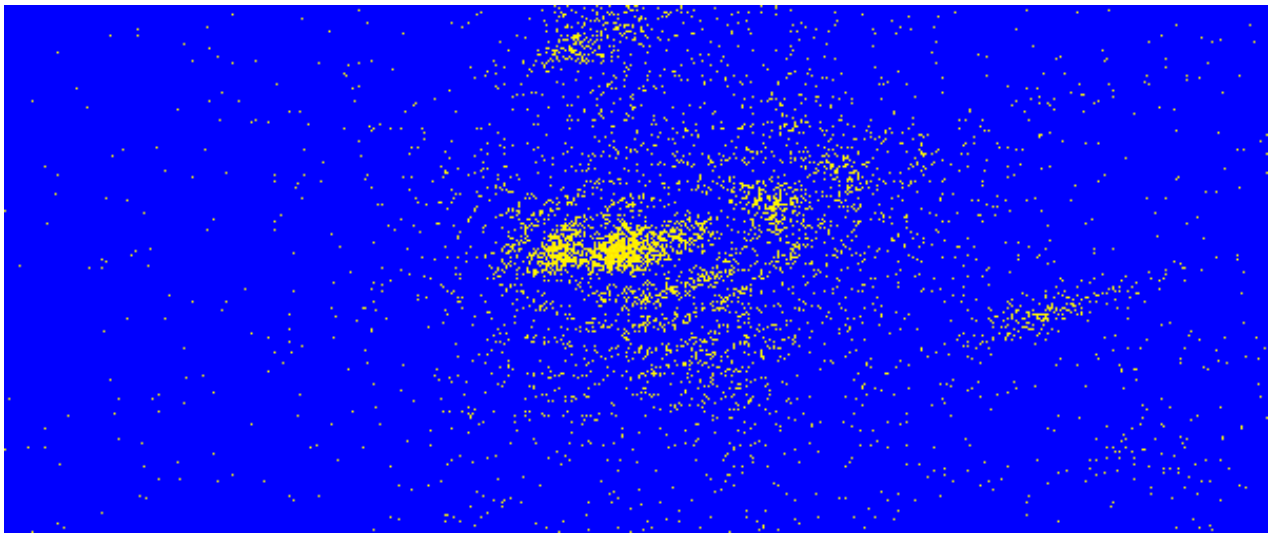




3D Diffraction Method

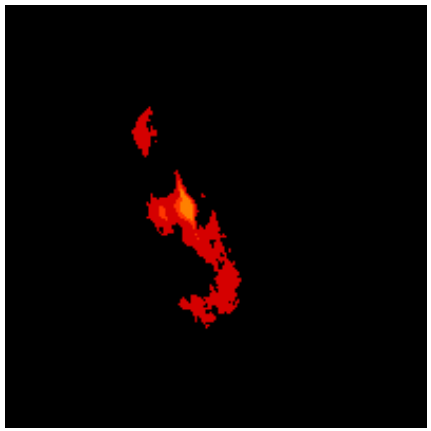


3D Diffraction Data
1 micron Au crystal

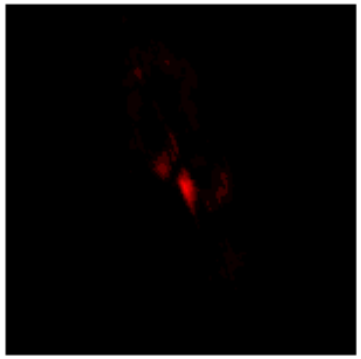
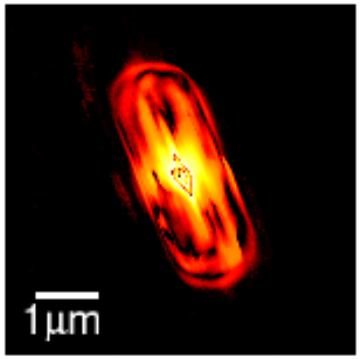


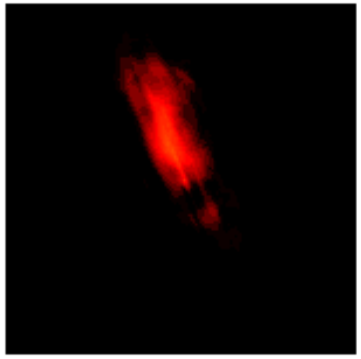
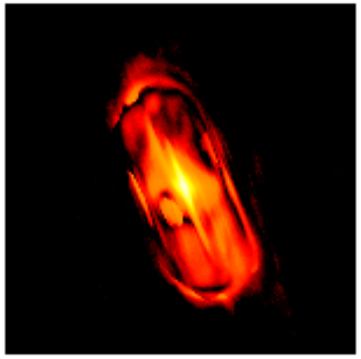
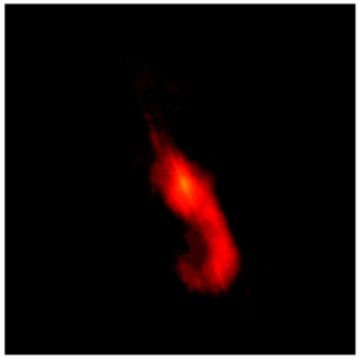
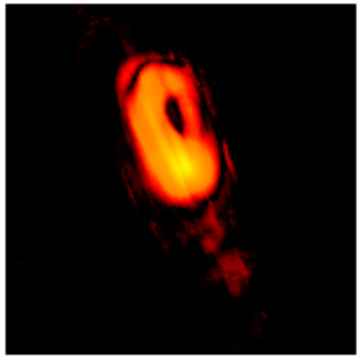
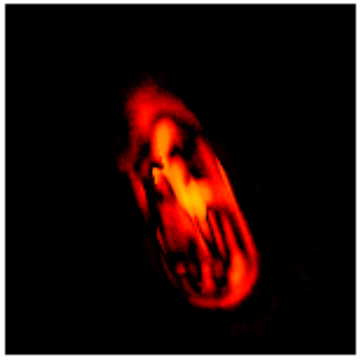
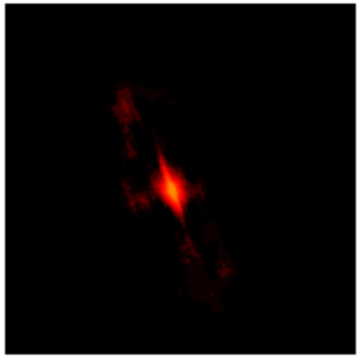
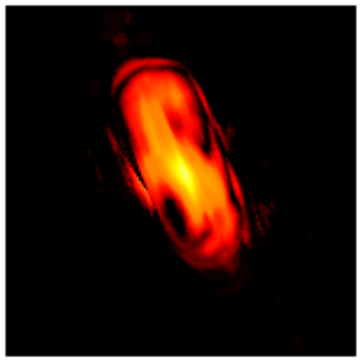
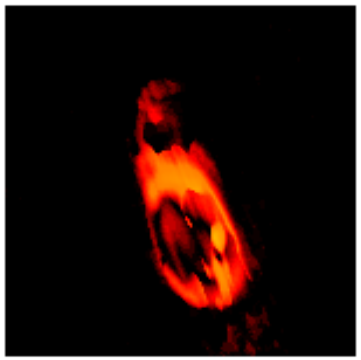
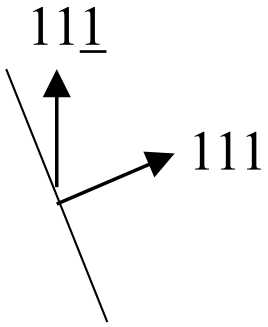
* Center is Symmetric *

30 frames of 3D reconstruction
1 micron gold crystal

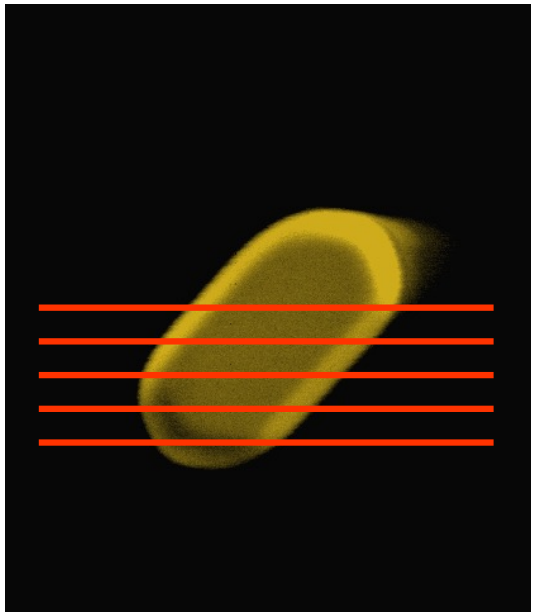


* CENTER *

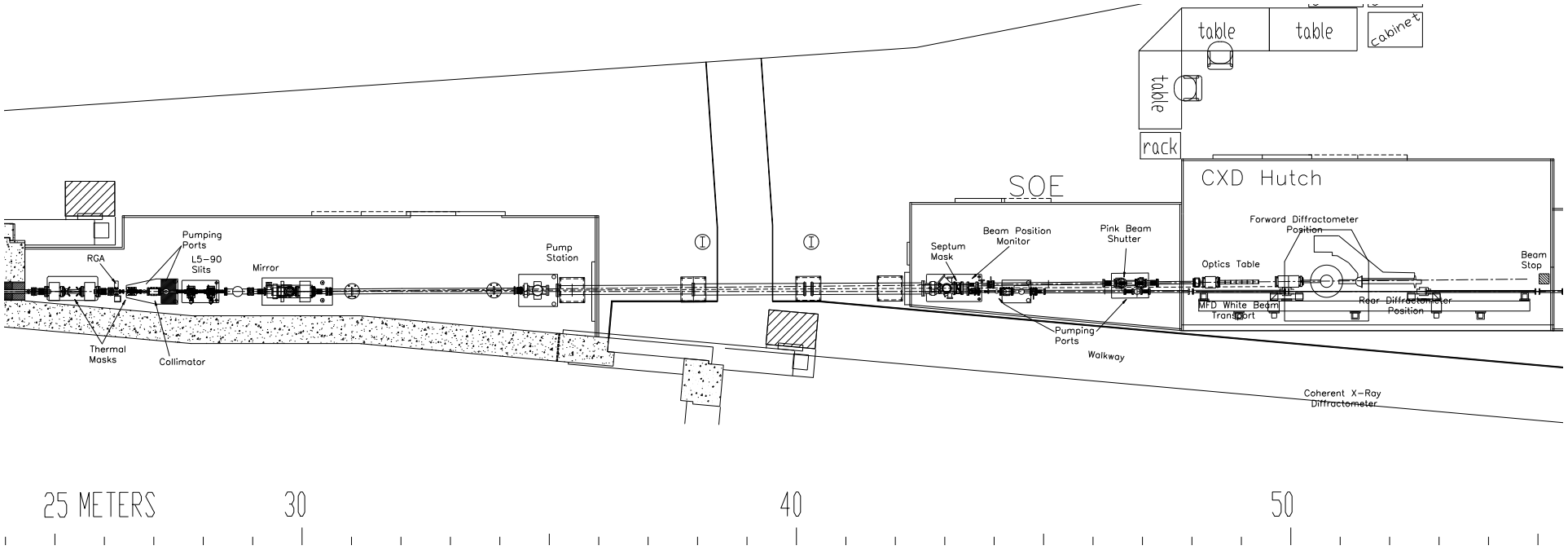



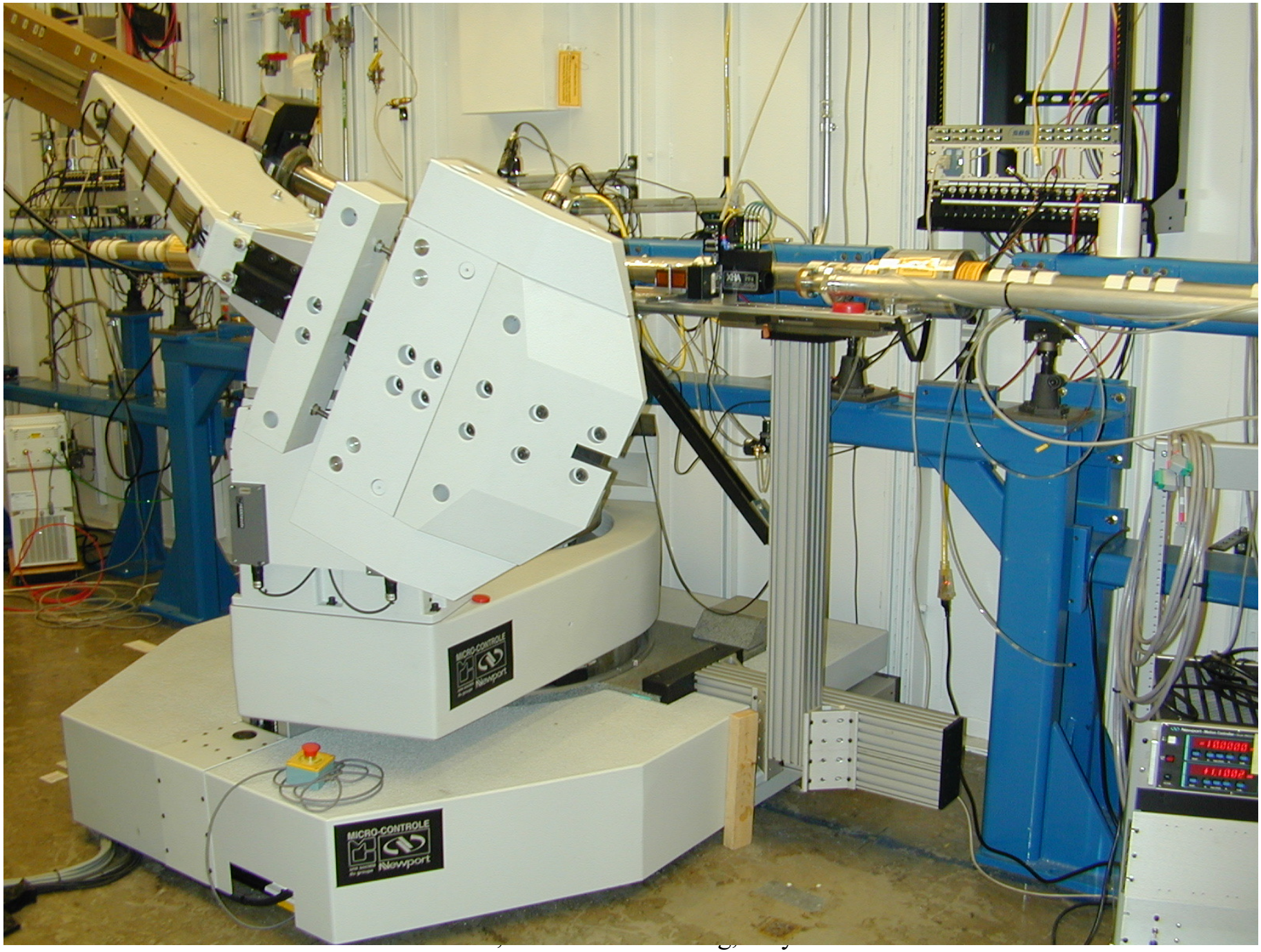










Slices through plan view SEM:

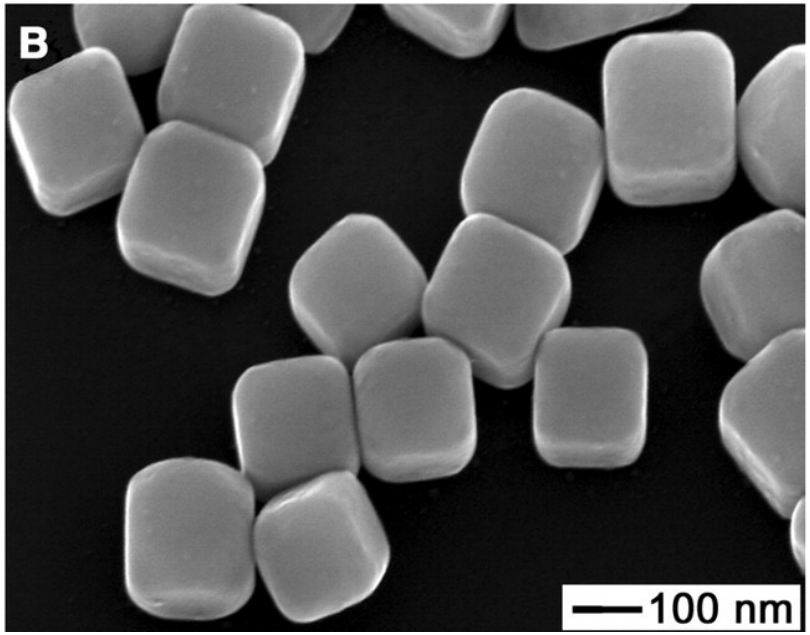


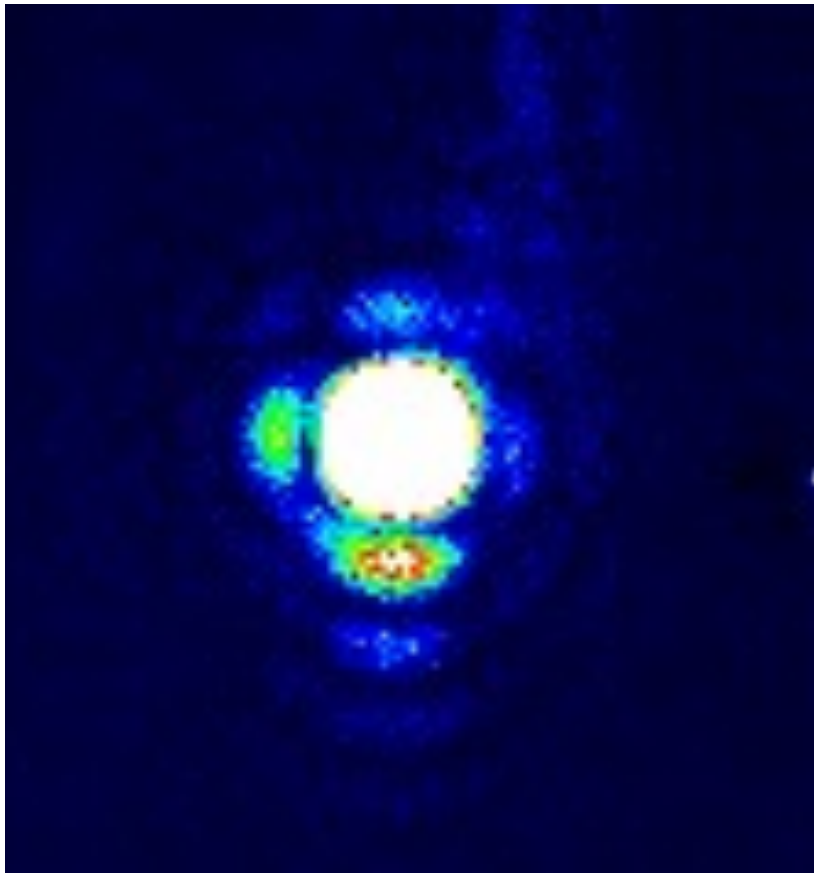
CXD Beamline at APS Sector 34




MICRO-CONTROLE
Newport
MICRO-CONTROLE
Newport

CXD from Silver Nanocubes

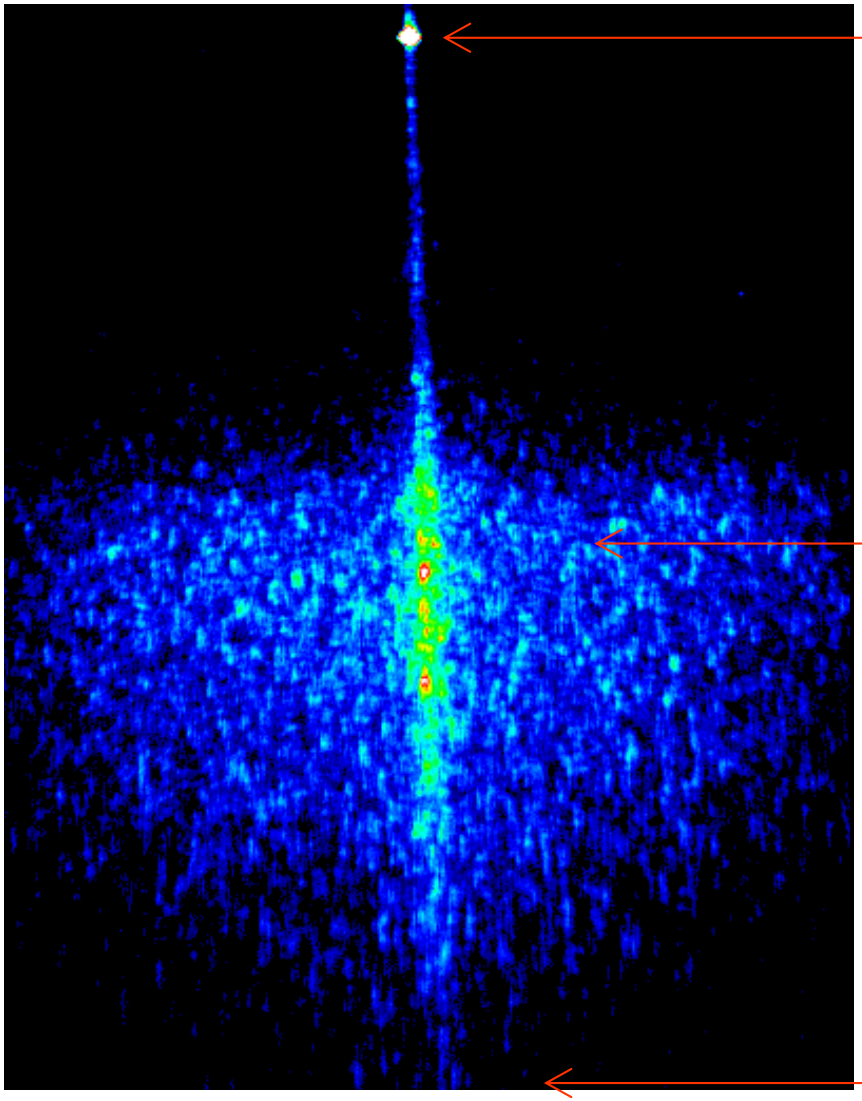




Yugang Sun and Younan Xia,
Science 298 2177 (2003)

Structure in "Yoneda" Peak

Grazing-exit diffraction from a 1000A Au polycrystalline film



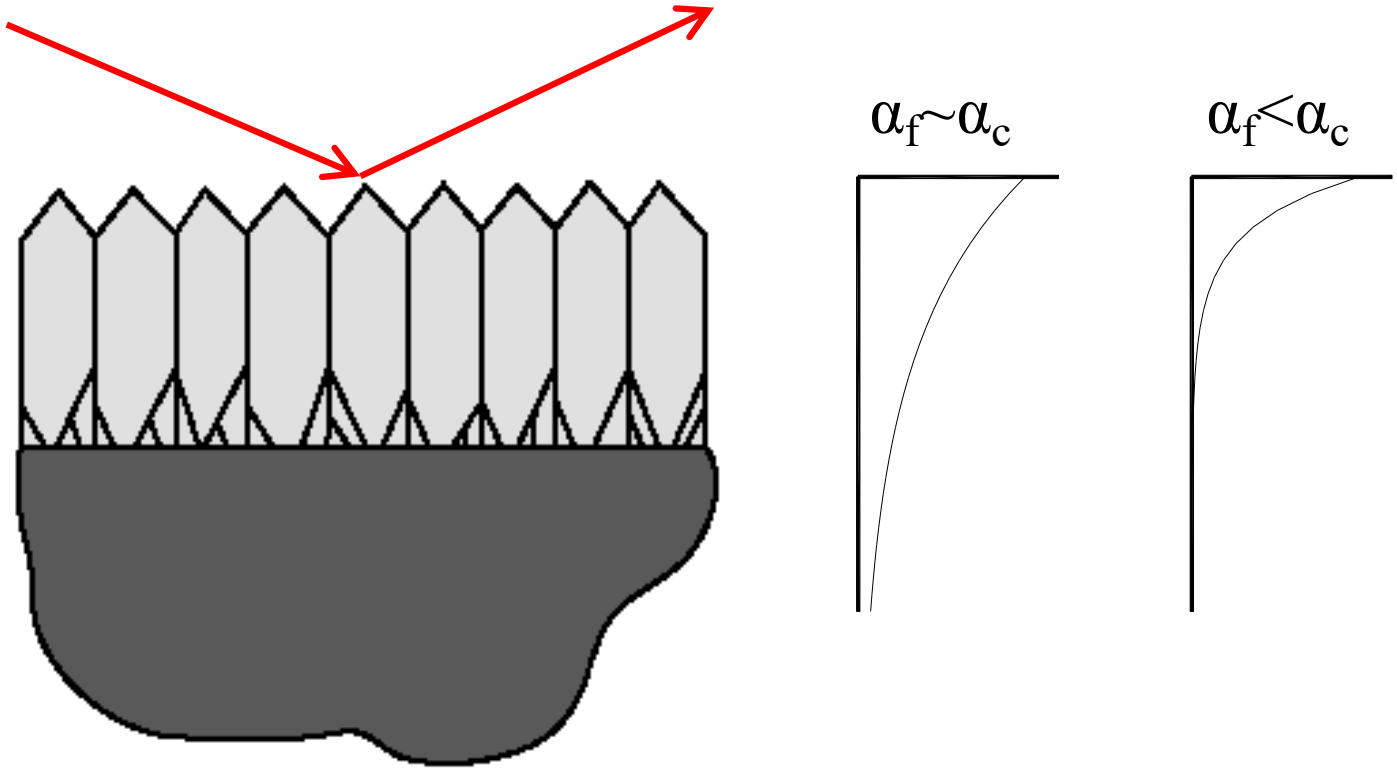
Specular ($\alpha_f \sim \alpha_i$)

$\alpha_f \sim \alpha_c$

$\alpha_f \sim 0$

Competitive Grain Growth

C. V. Thompson, Ann. Rev. Mat. Sci. **30** 159 (2000)

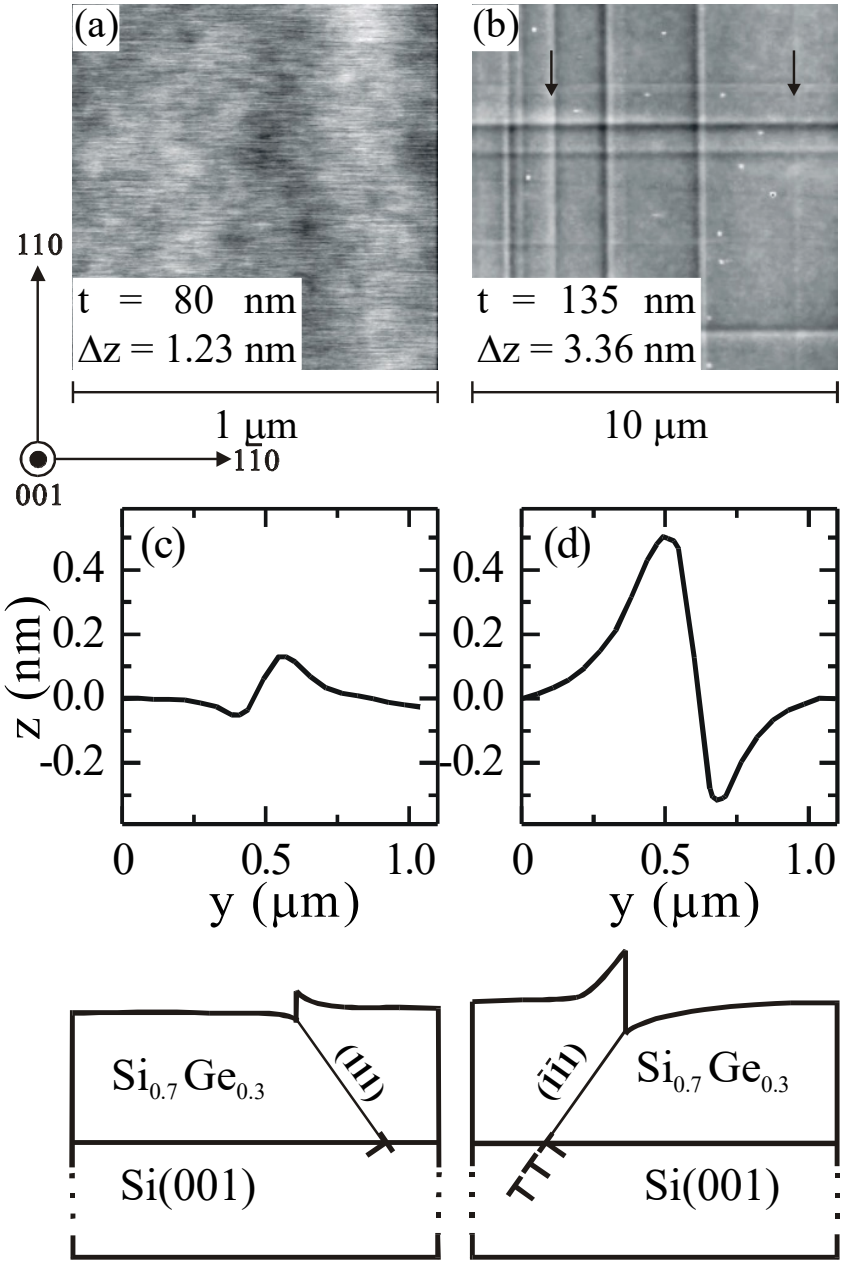


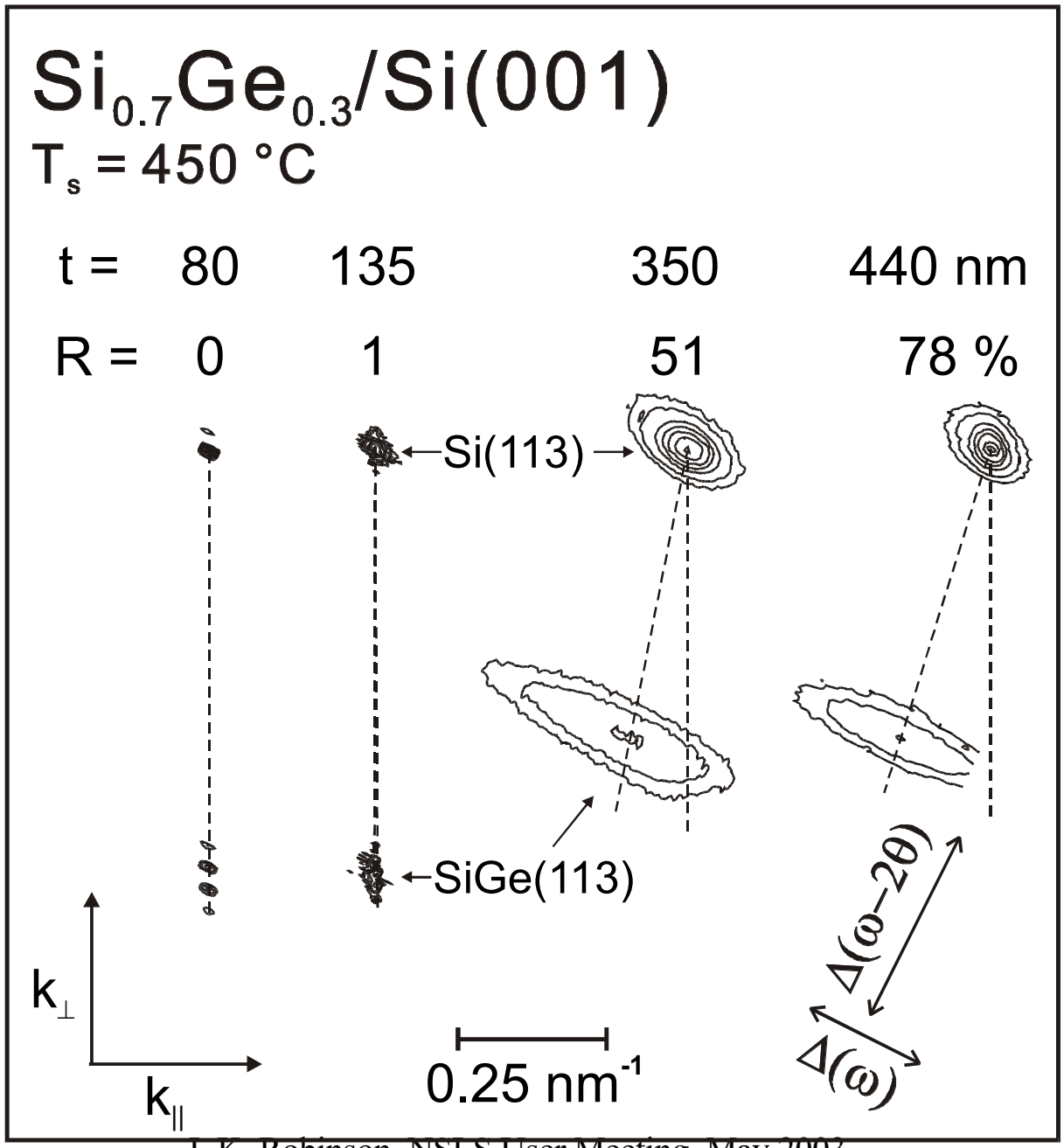
Low dislocation density GeSi films

Thickness close to critical thickness

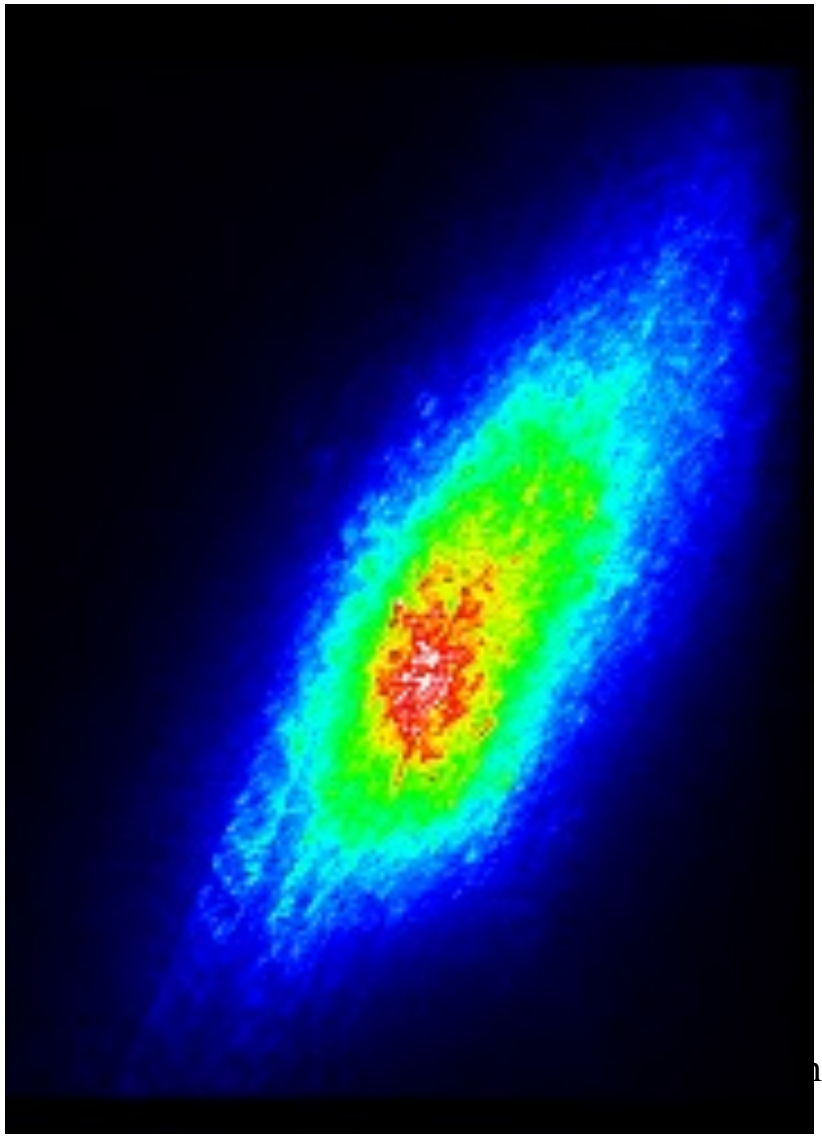
Dislocations aggregate at interface and glide to surface along {111}

T. Spila, UIUC Thesis



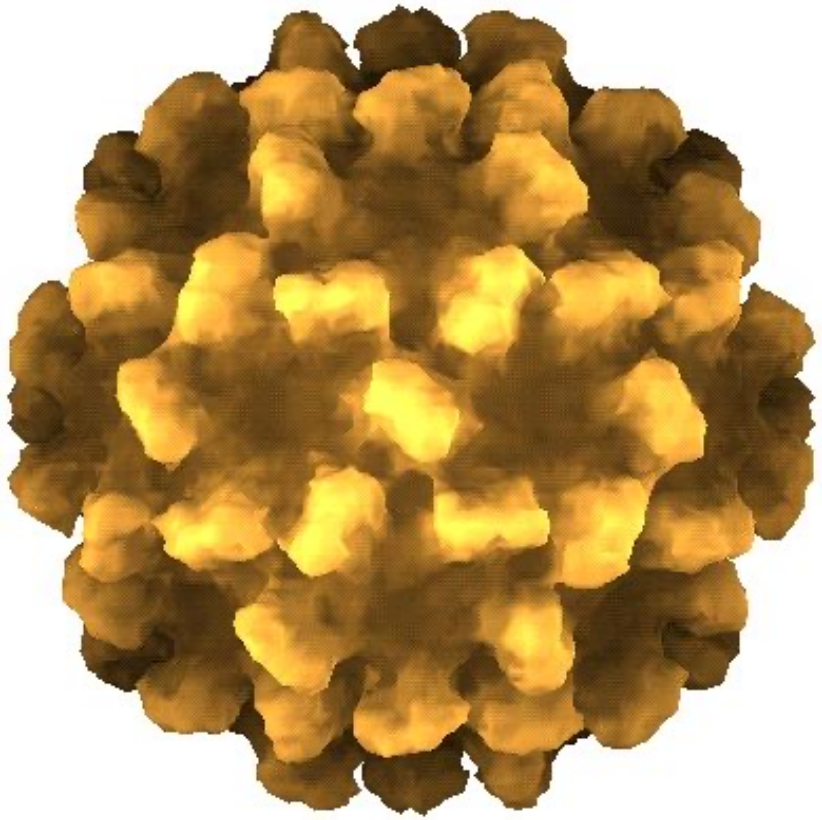

Si0.7Ge0.3/Si(001)
Ts = 450 °C
t = 80 135 350 440 nm
R = 0 1 51 78 %
Si(113)
SiGe(113)
k⊥
k||
0.25 nm-1
Δ(ω–2θ)
Δ(ω)

Ge_xSi_{1-x} Film Diffraction



- 202 Bragg Peak
- 2800A film
- 2° incidence angle
- 8.5 keV
- 20μm ×40μm beam onto KB mirror
- 1μm ×1μm focus
- 0.5μm sample steps
- APS 34-ID-C

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