Phase Contrast Microscopy using Coherent X-ray Diffraction

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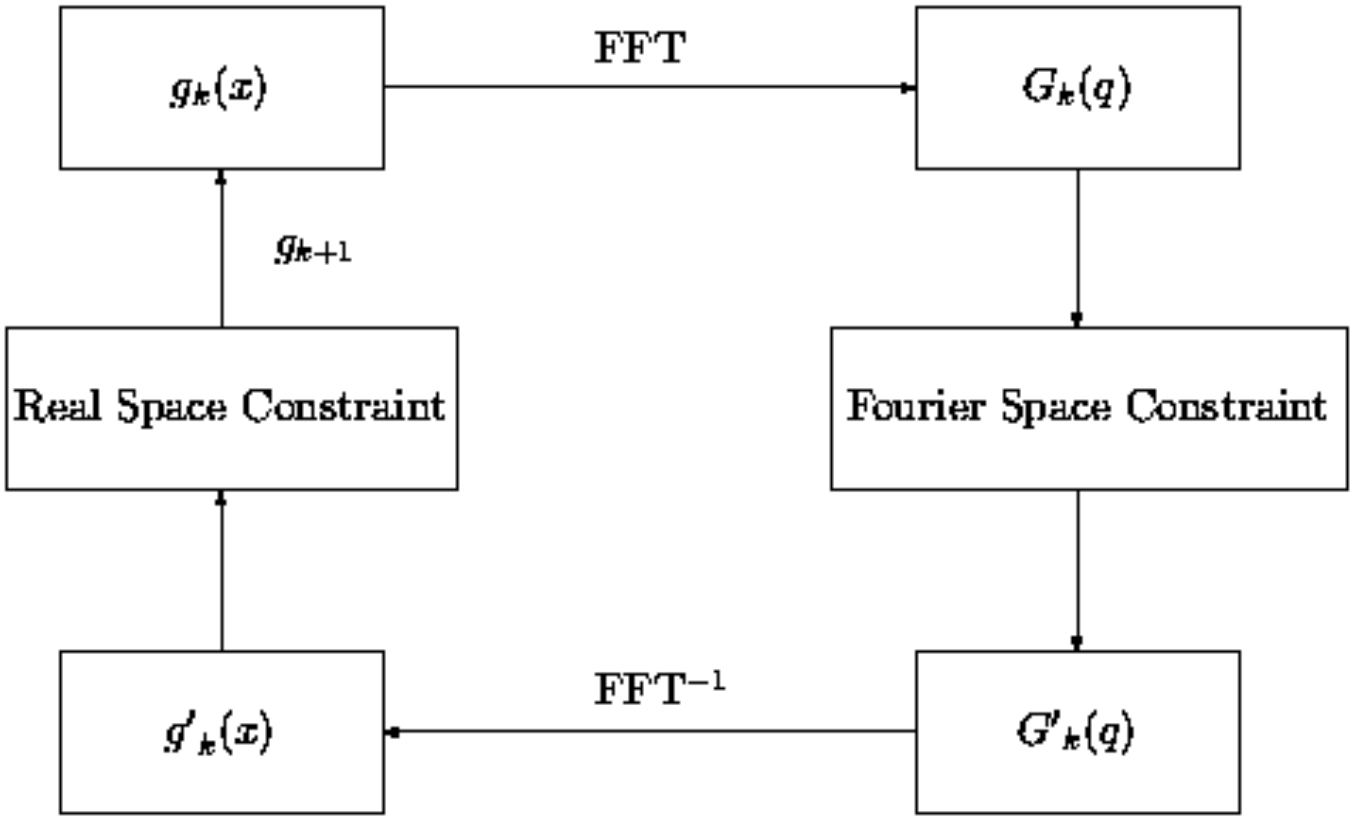
BESSY
Coherence Workshop
1 December 2004

Outline

- Coherence can be used for Structure
- The Phase Problem
- Nanocrystal Shapes
- Imaging of Phase Objects
- How small can we go?

Generic "Error Reduction" method

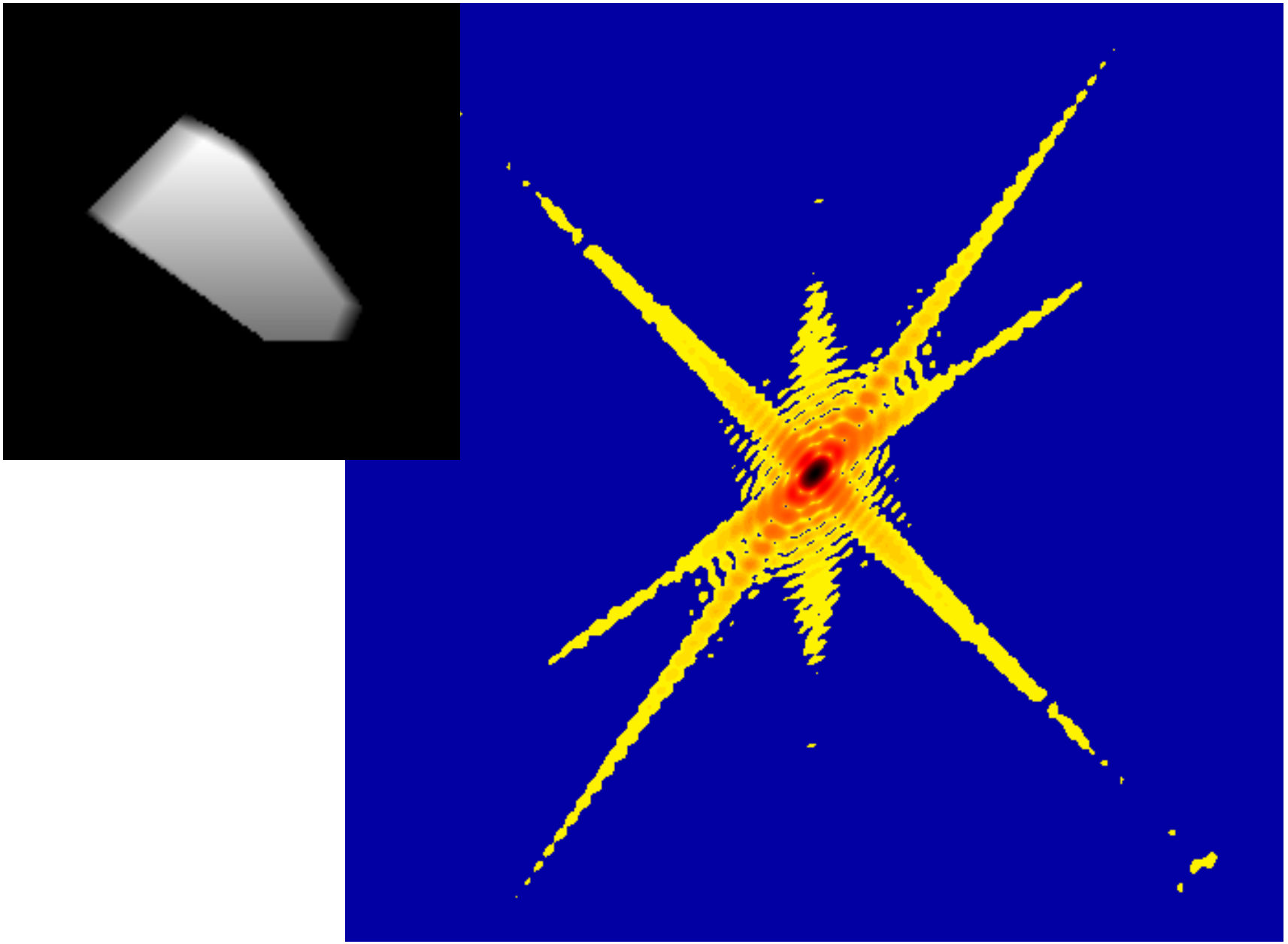


J. R. Fienup Appl. Opt. 21 2758 (1982)
R. W. Gerchberg and W. O. Saxton Optik 35 237 (1972)

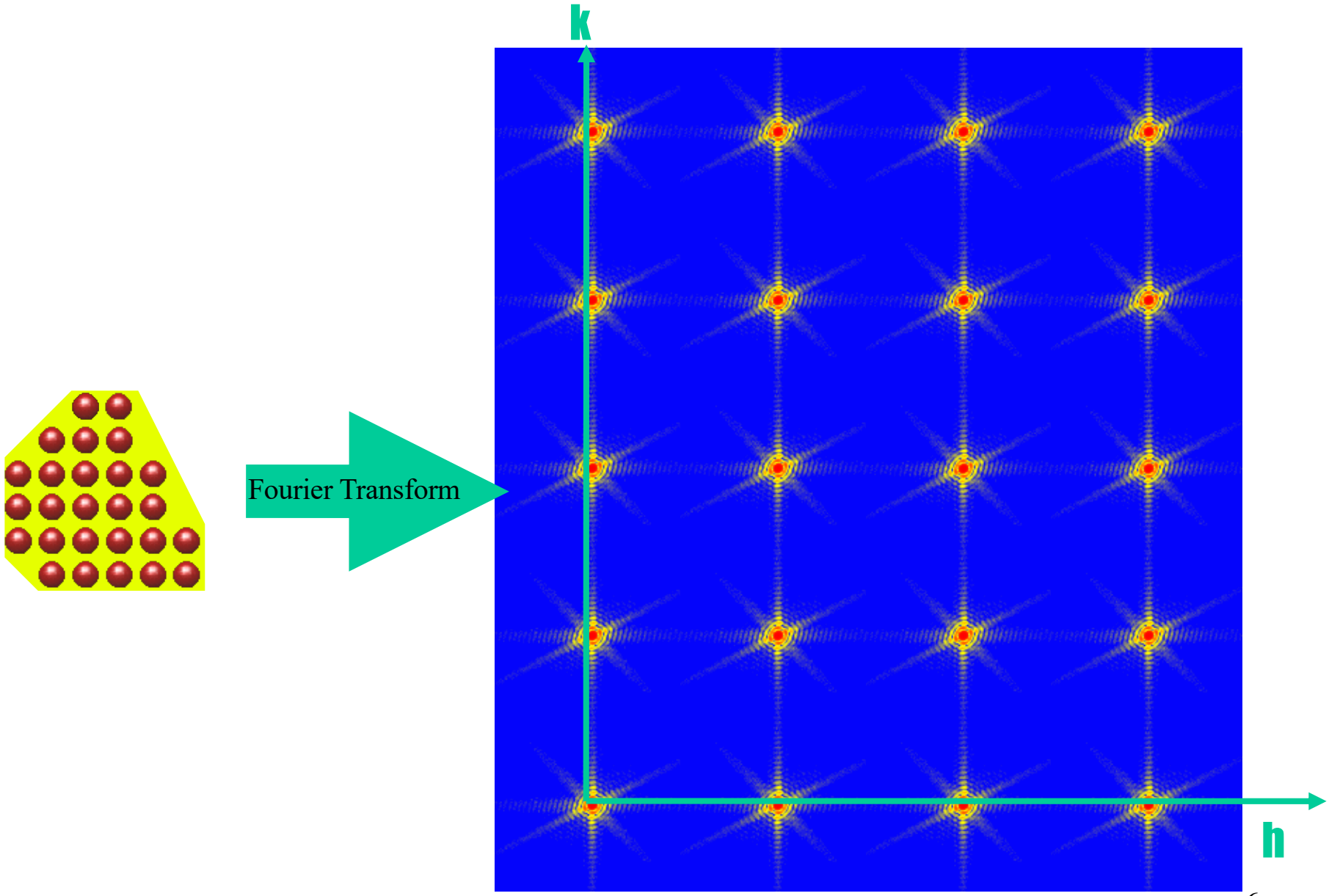
Real-space Constraints in Crystallograhy

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)

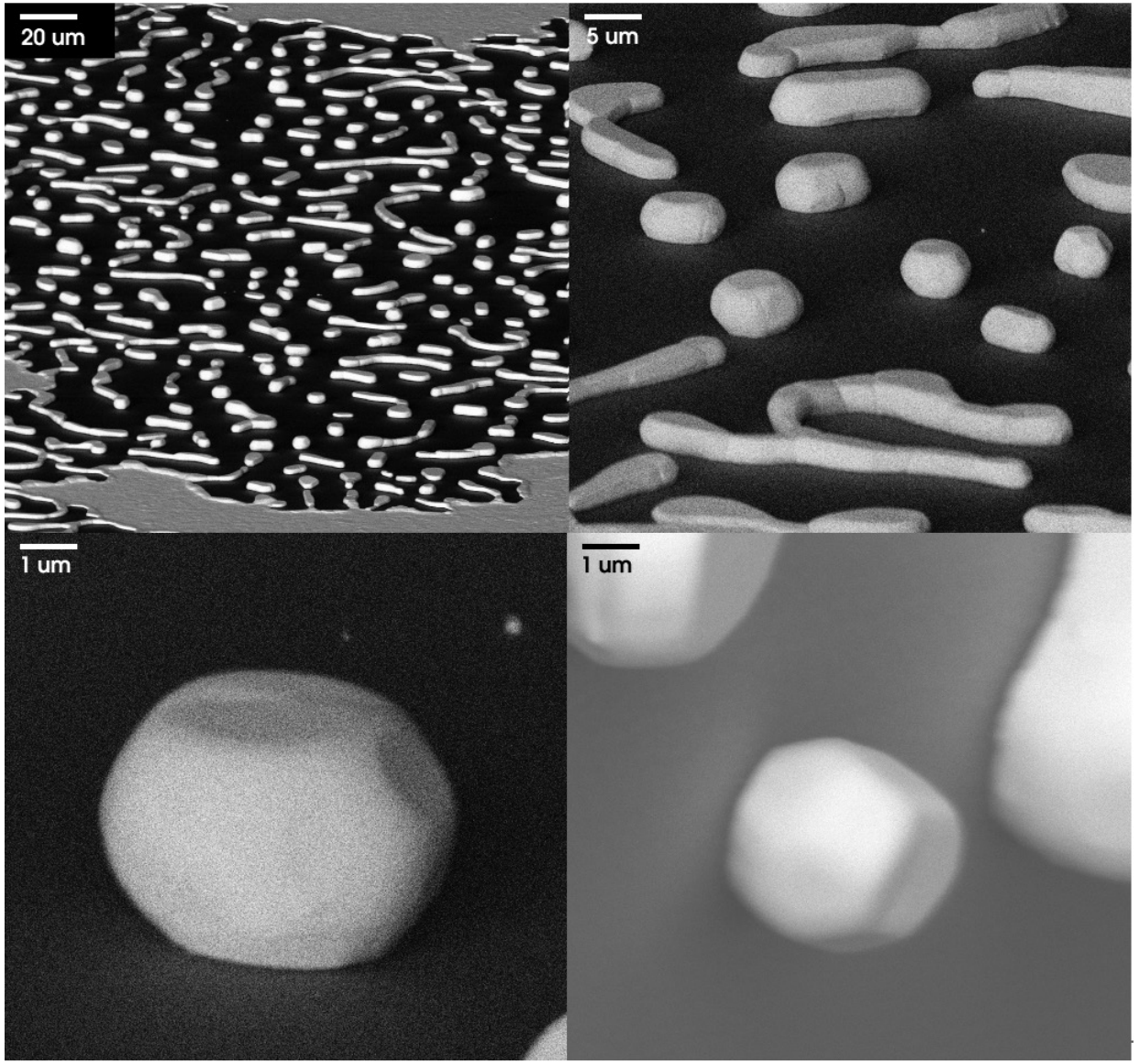


Coherent Diffraction from Crystals



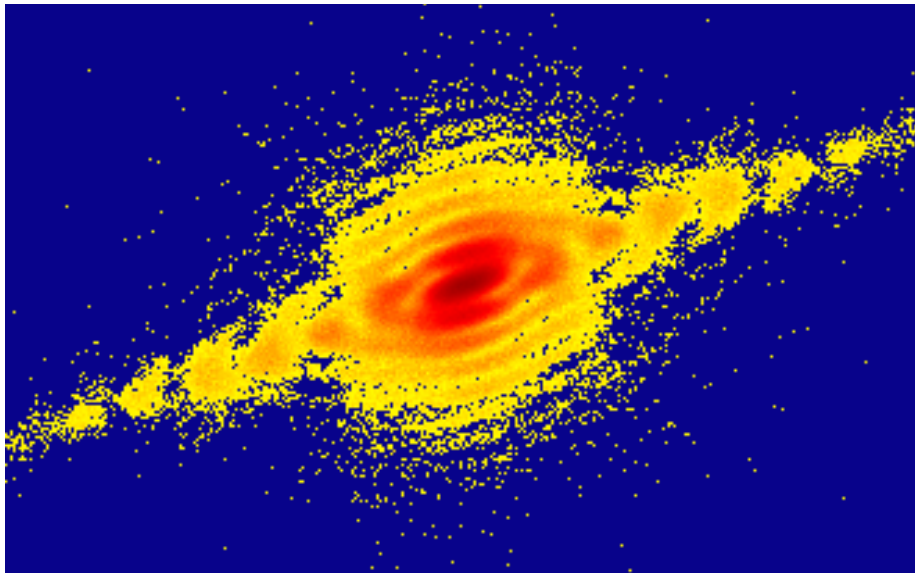
SEMS

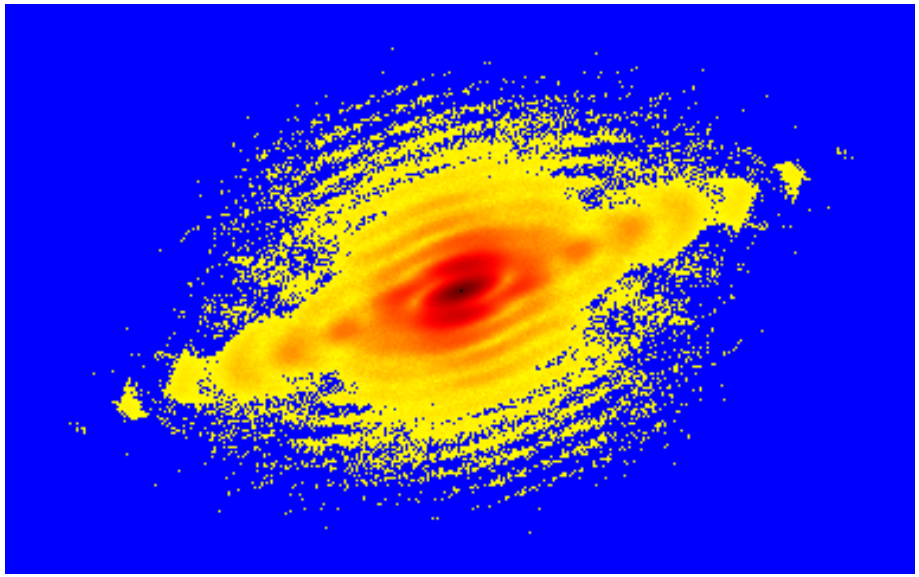
- Au blanket film
- Quartz substrate
- Annealed at 950°C for 70 hrs.

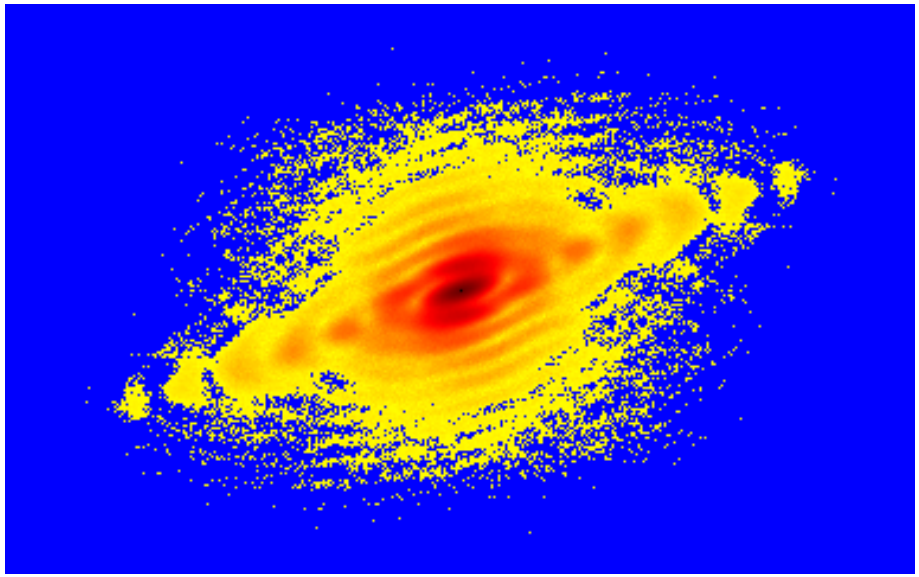


Symmetrized Data and two best fits

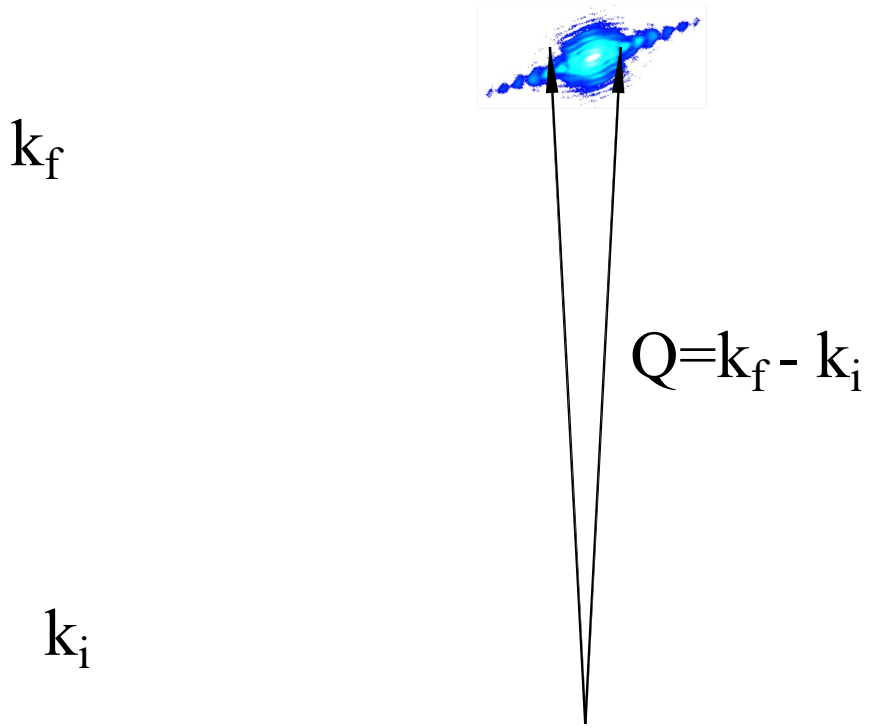
Chisq=0.0005

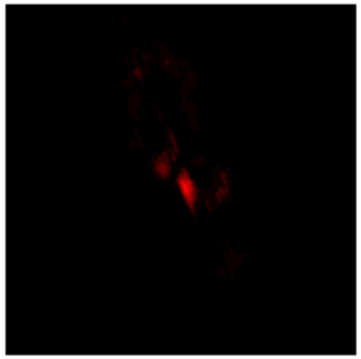
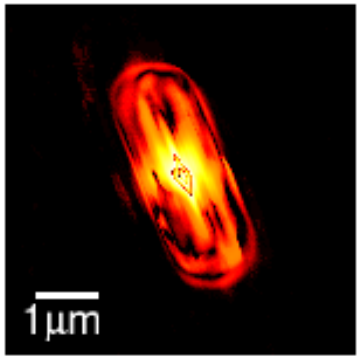


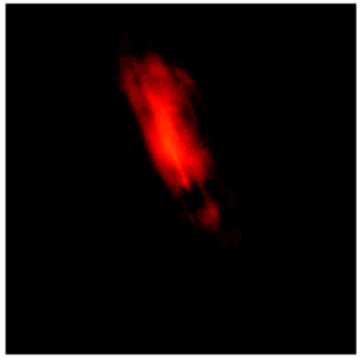
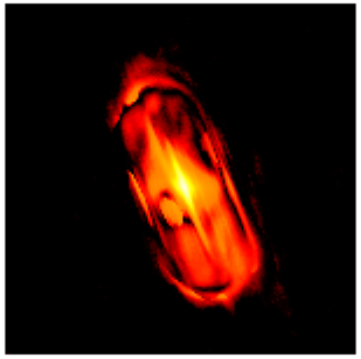
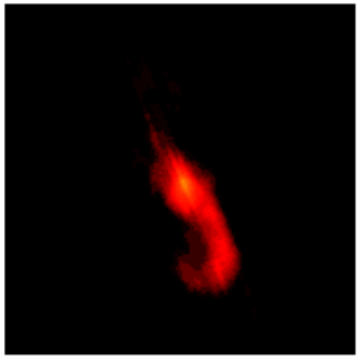
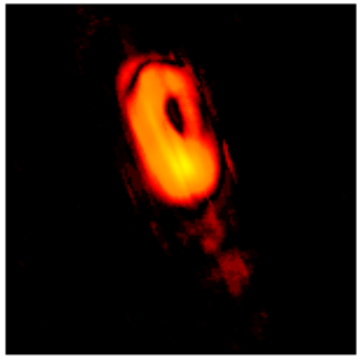
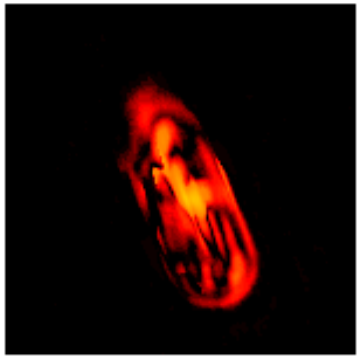
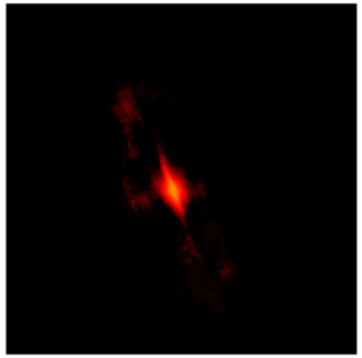
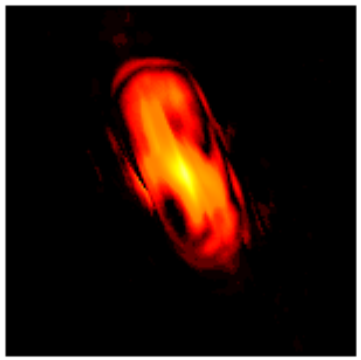
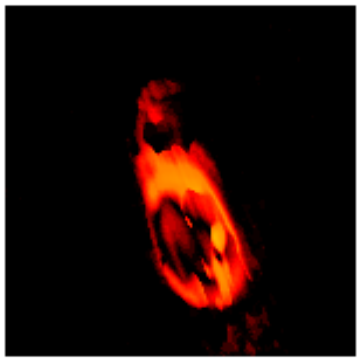
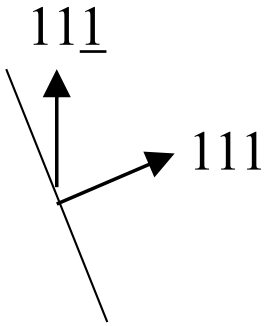




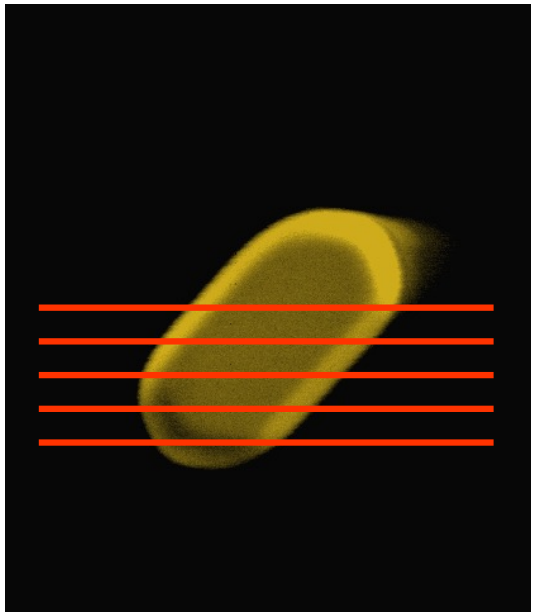
3D Diffraction Method



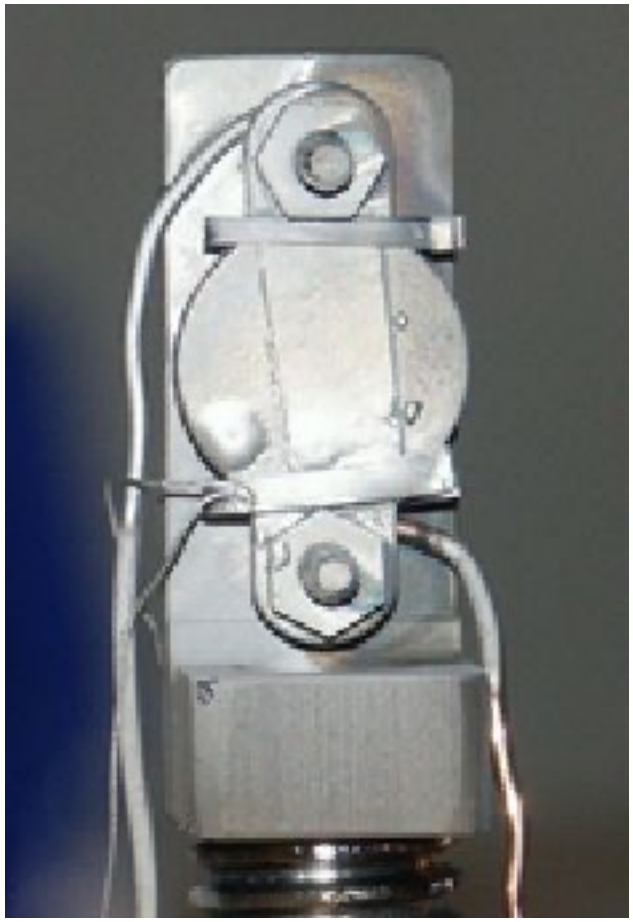



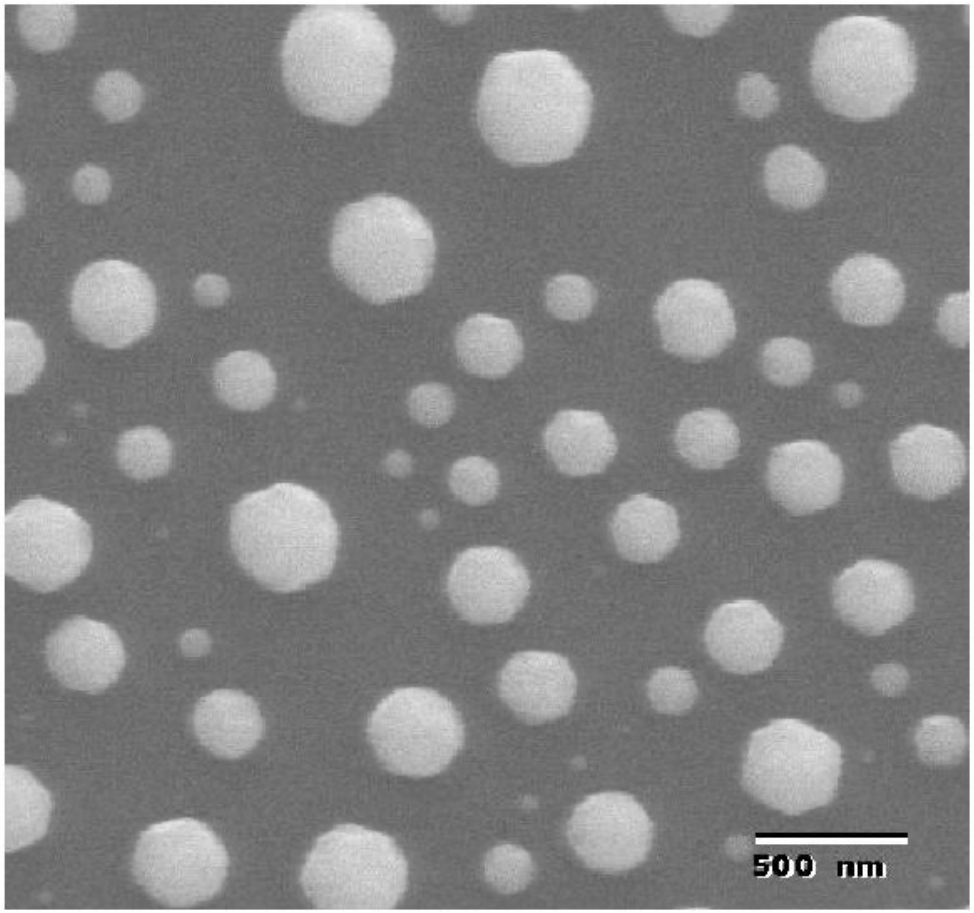










Slices through plan view SEM:



In situ growth of Pb crystals





Good statistics, 3D diffraction data

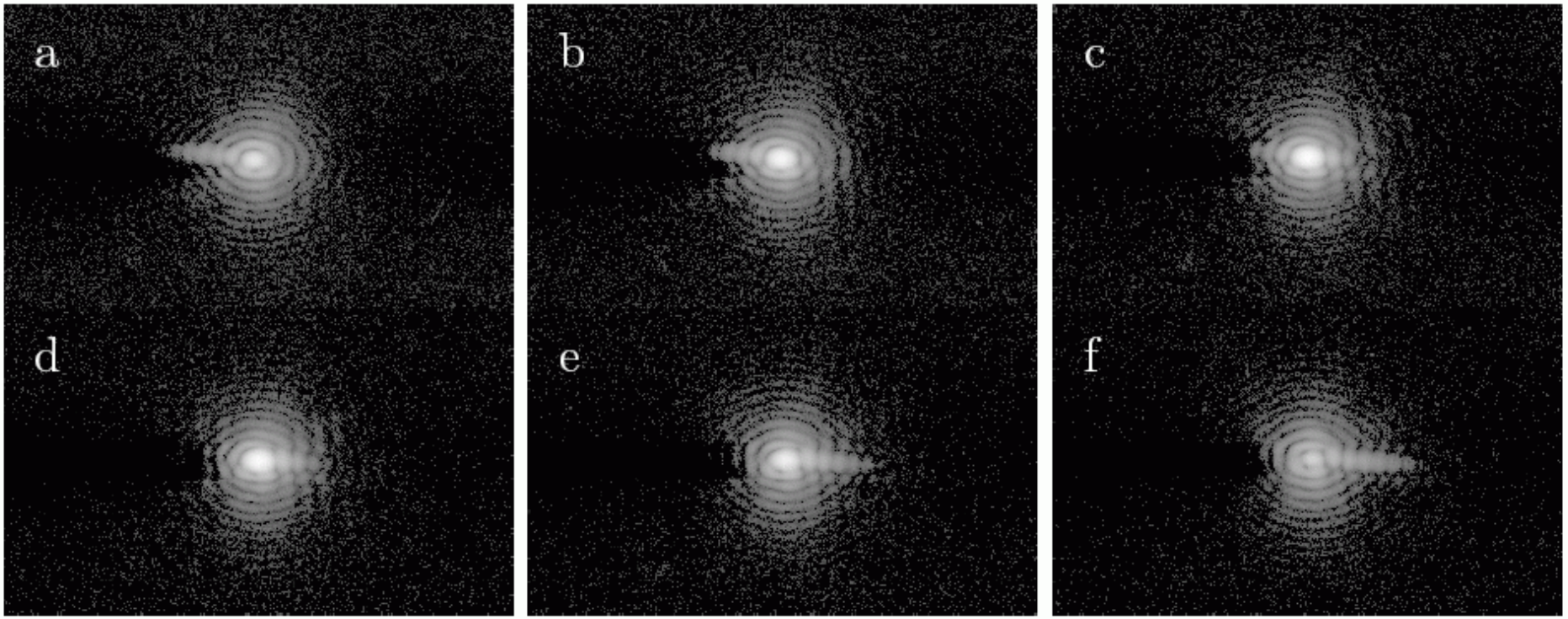
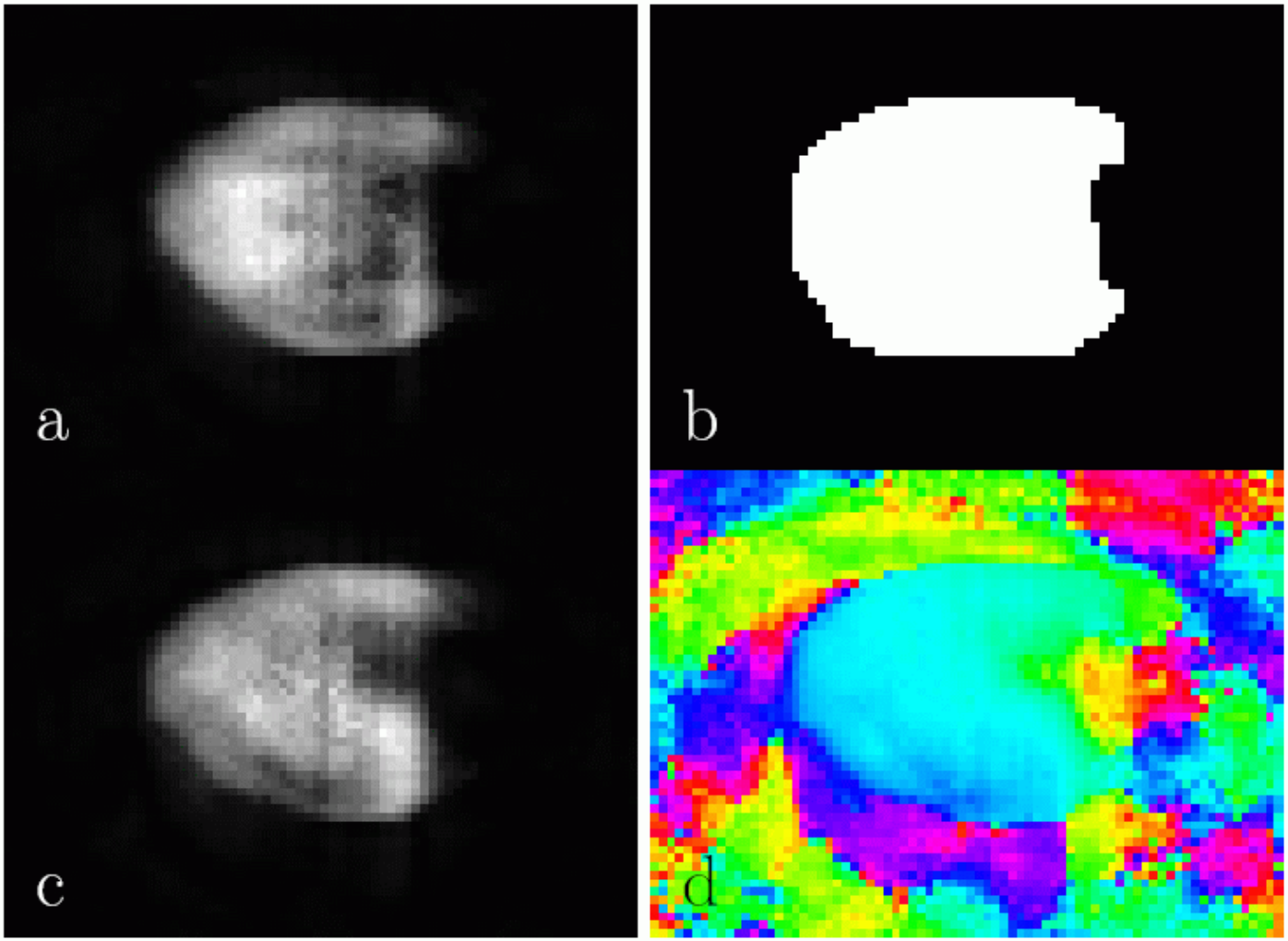
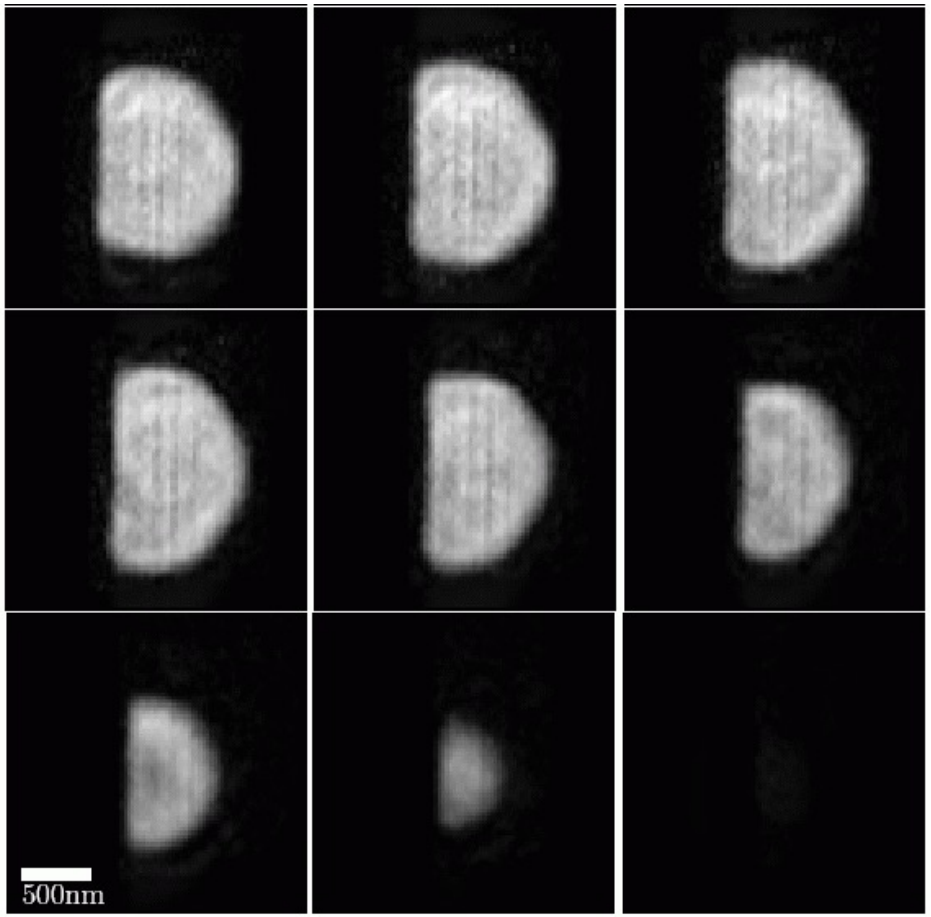


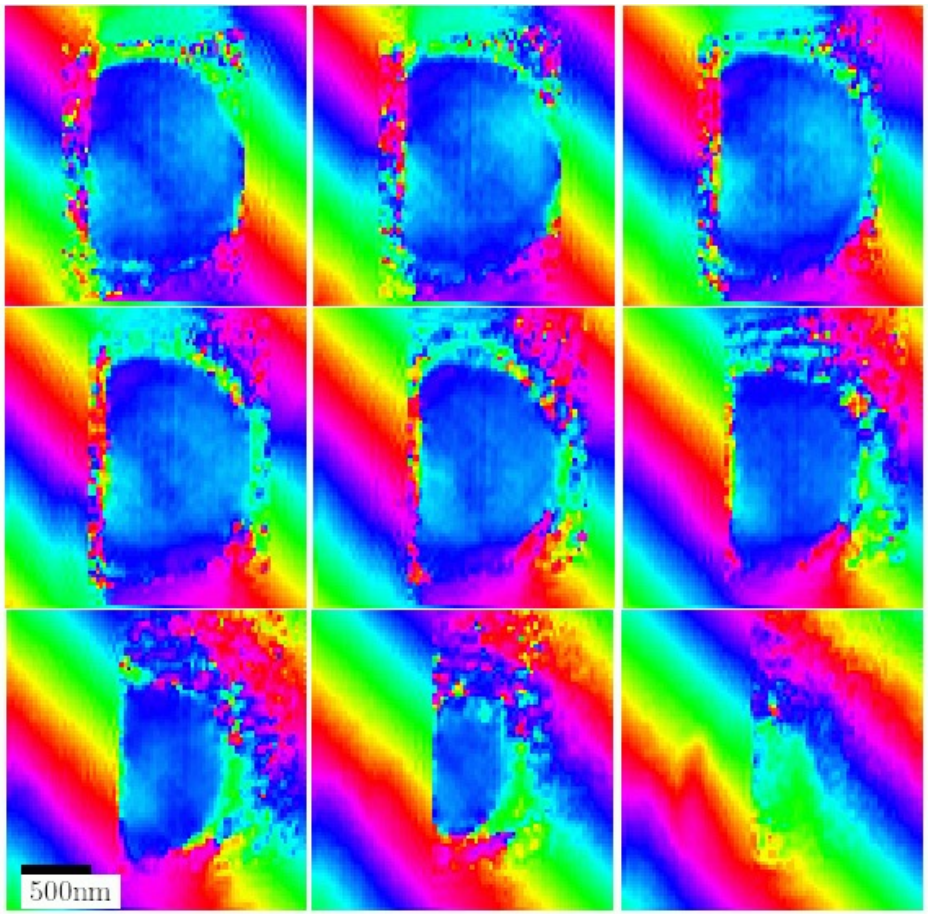
Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

Learn shape of “tight” support



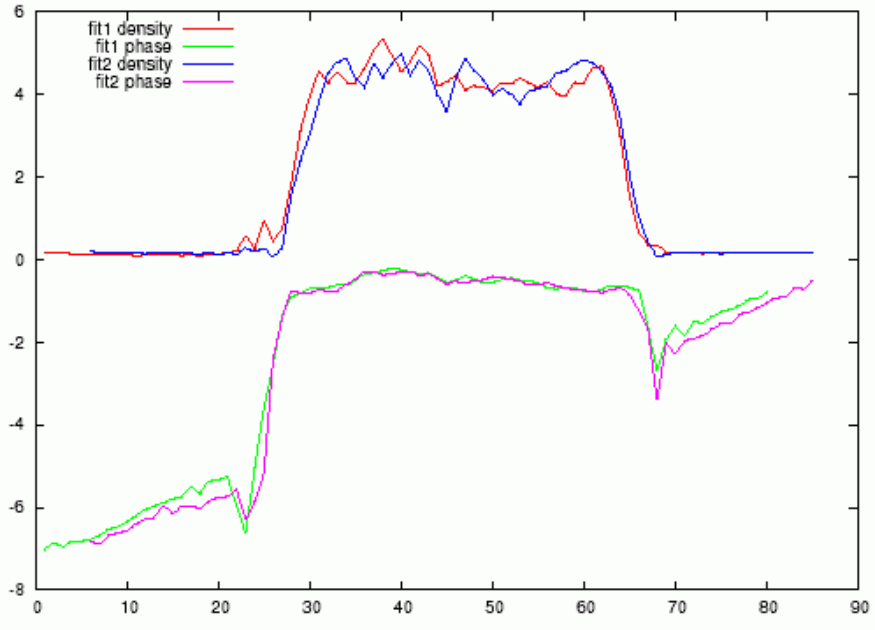
Then refine amplitude *and* phase



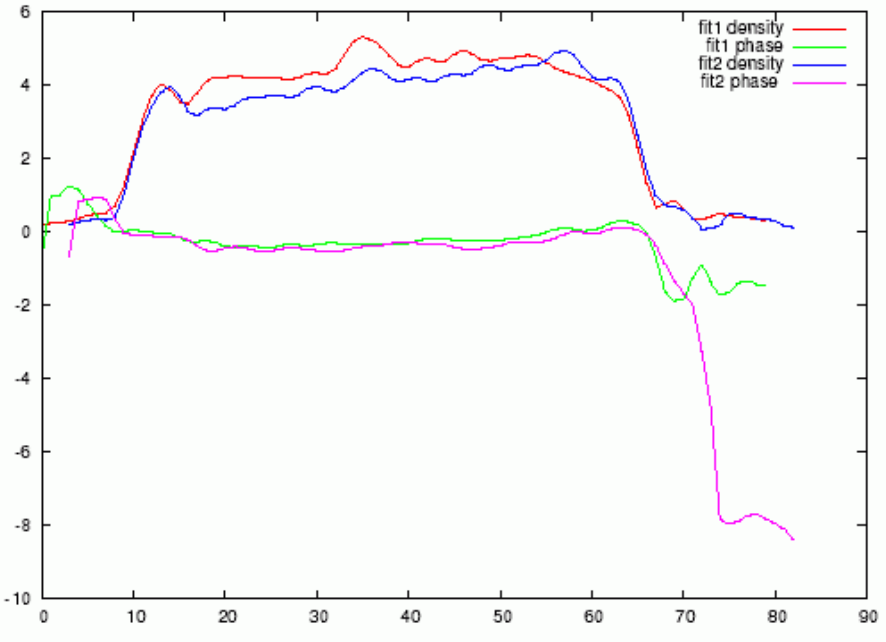


Amplitude/phase cross sections

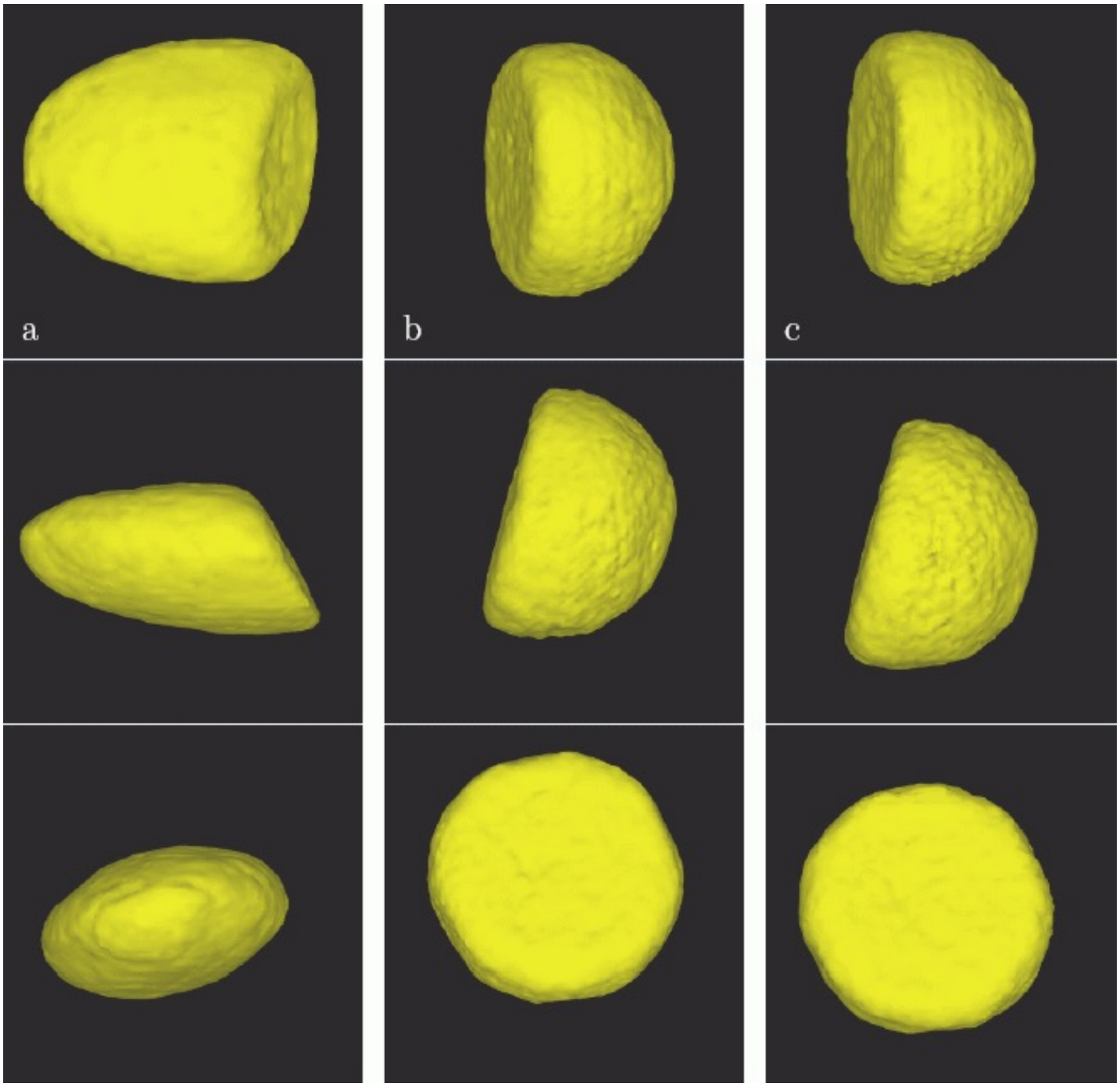
x-striations do not reproduce



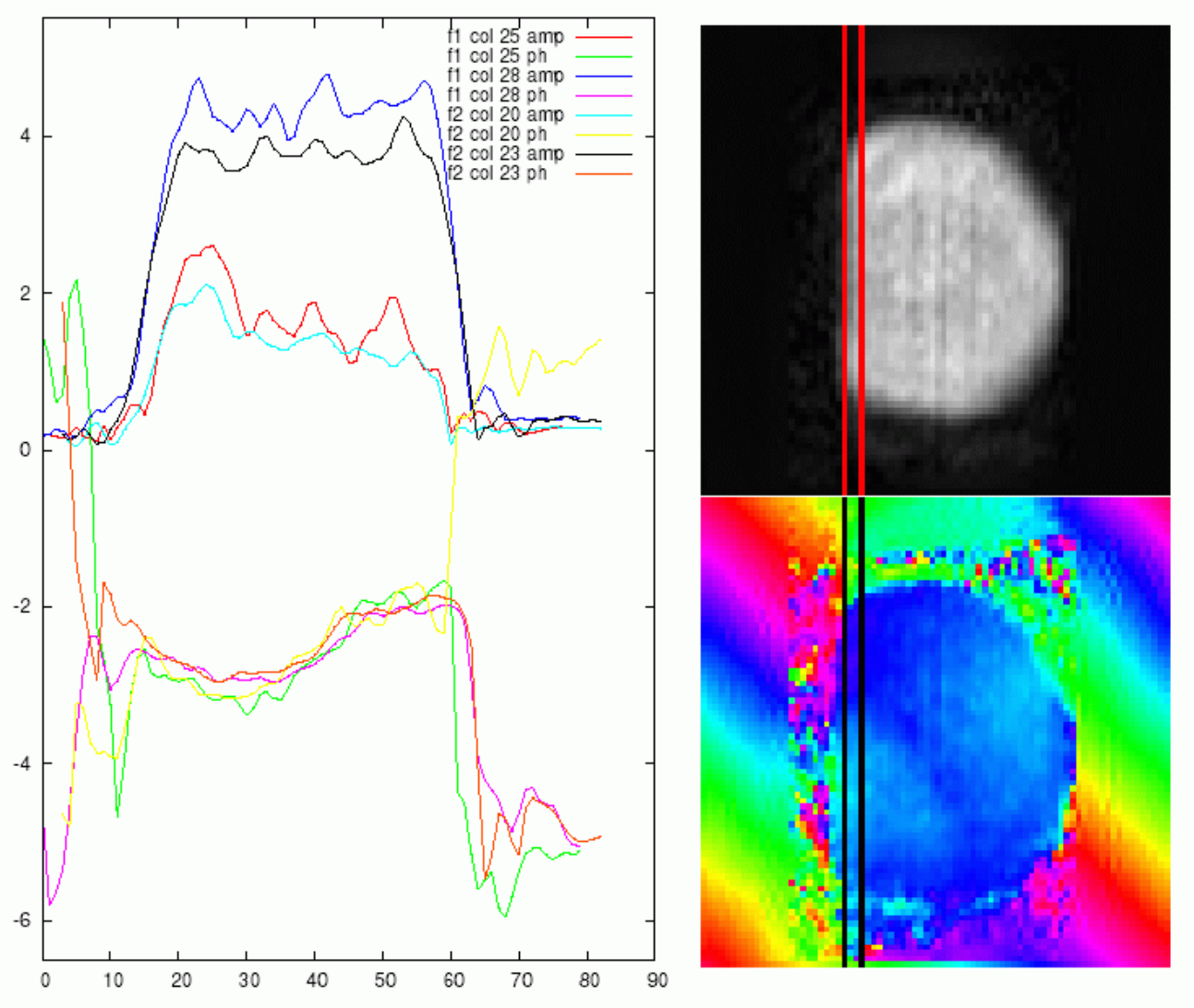
x-coordinate



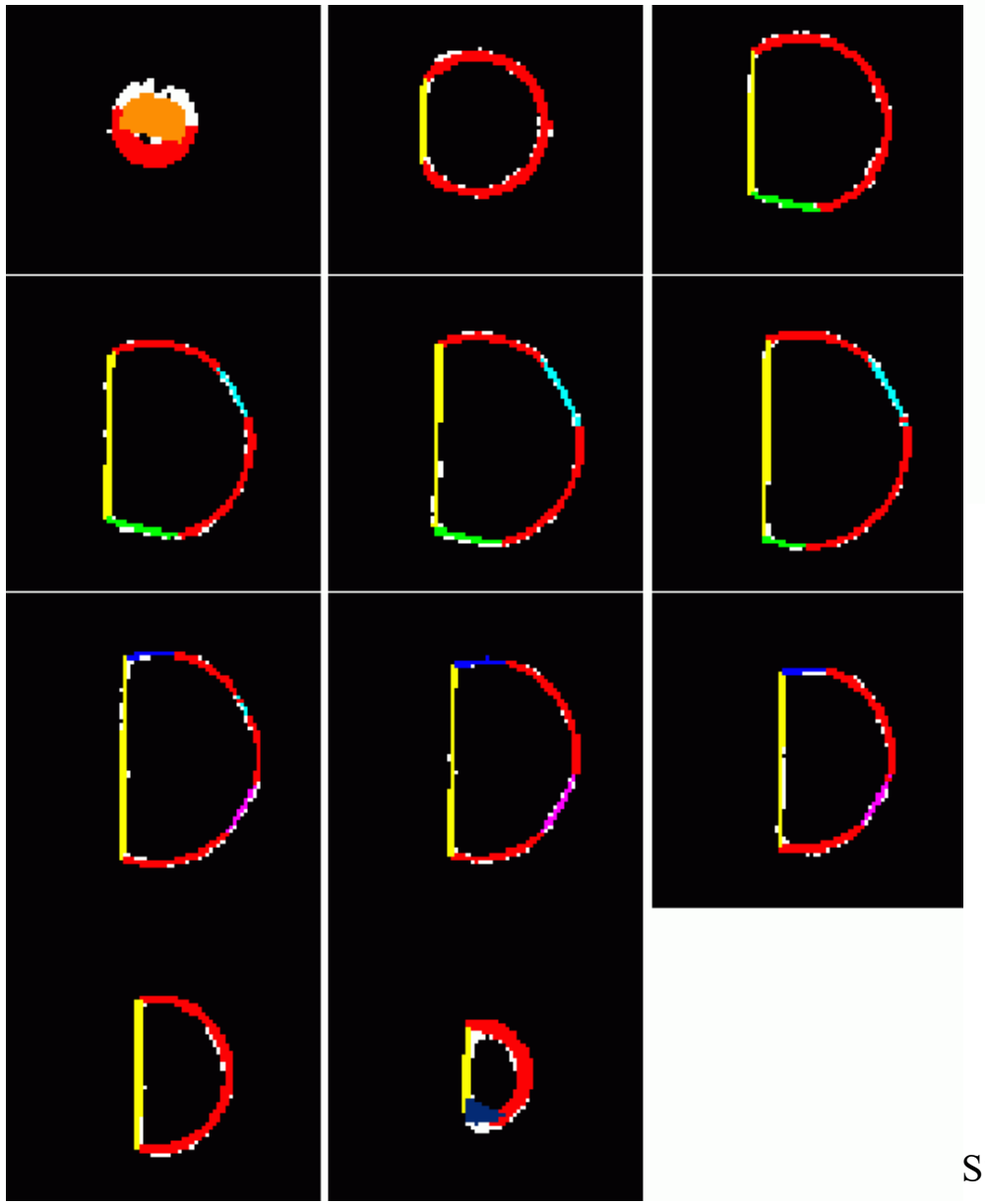
y-coordinate


a
b
c

Phase structure near substrate interface

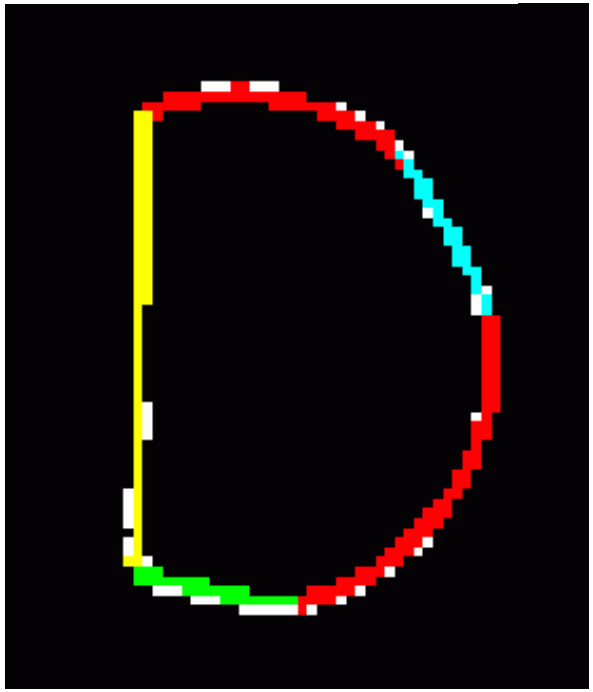


Fitting to facetted shape



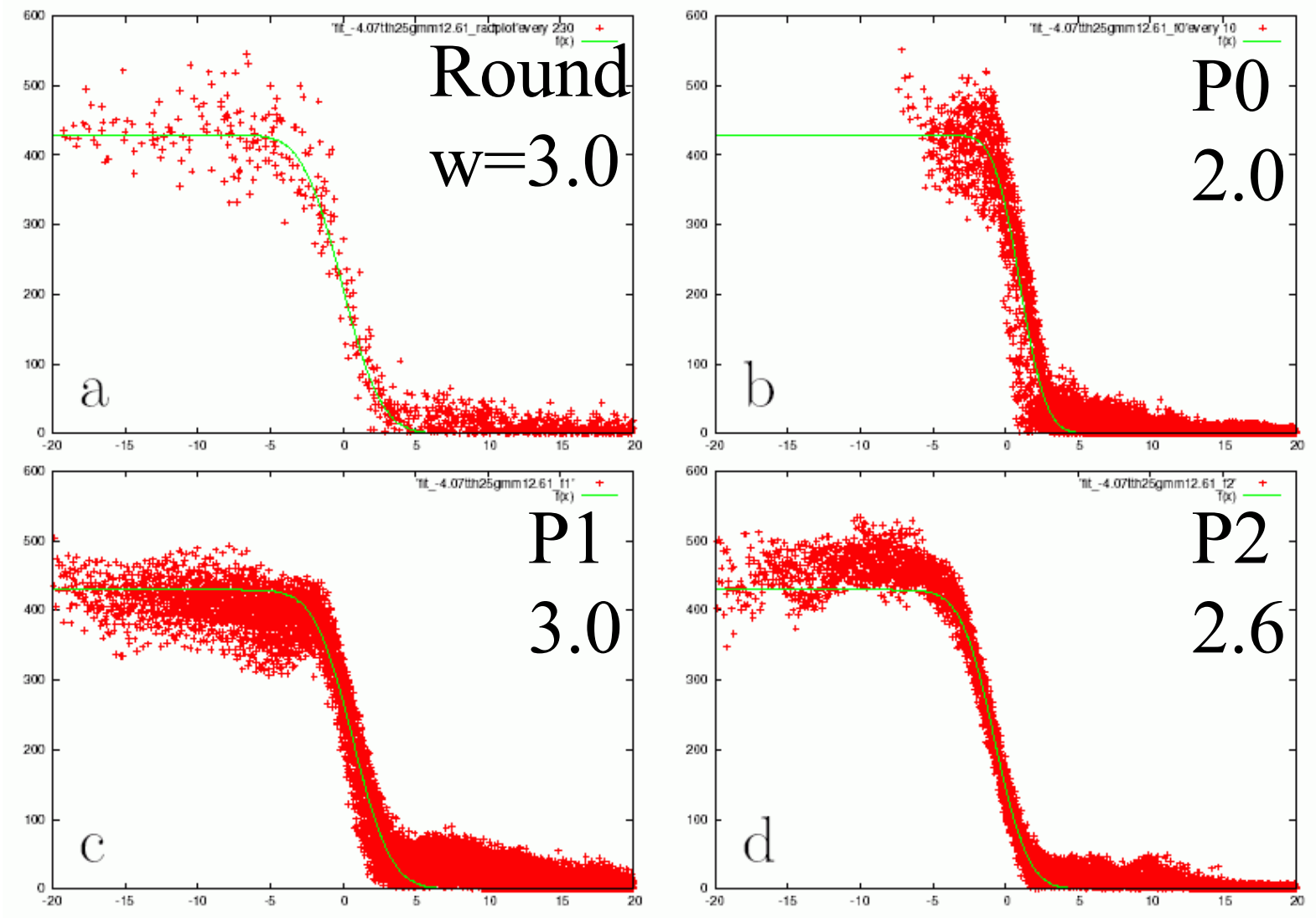
	$\|R\|$		P0	P1	P2	P3	P4	P5	P6
	9.4	P0	0	85	149	79	134	106	71
	25.7	P1		0	123	164	83	76	102
	25.1	P2			0	72	67	74	110
	25.9	P3				0	111	106	76
	25.4	P4					0	113	68
	25.4	P5						0	176
	26.0	P6							0 0

Angles between facets

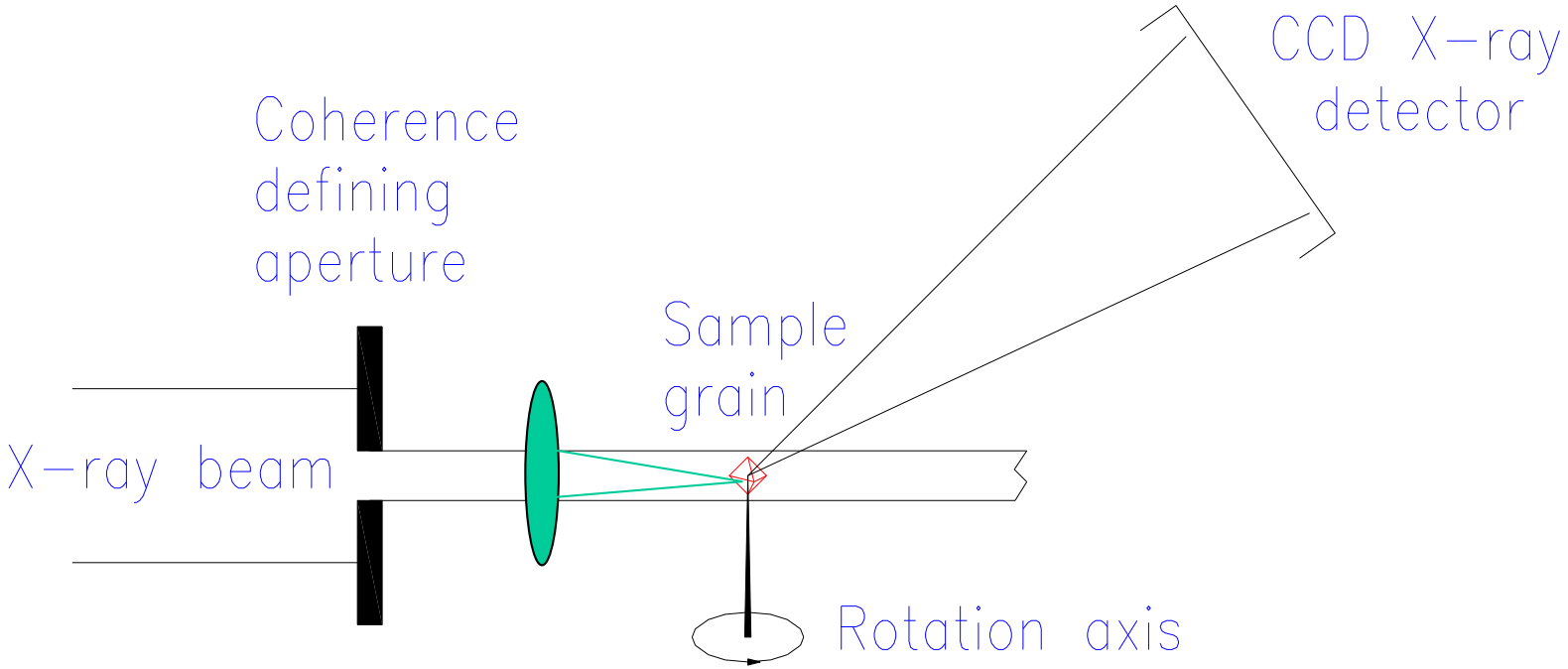


SSY, Dec 2004

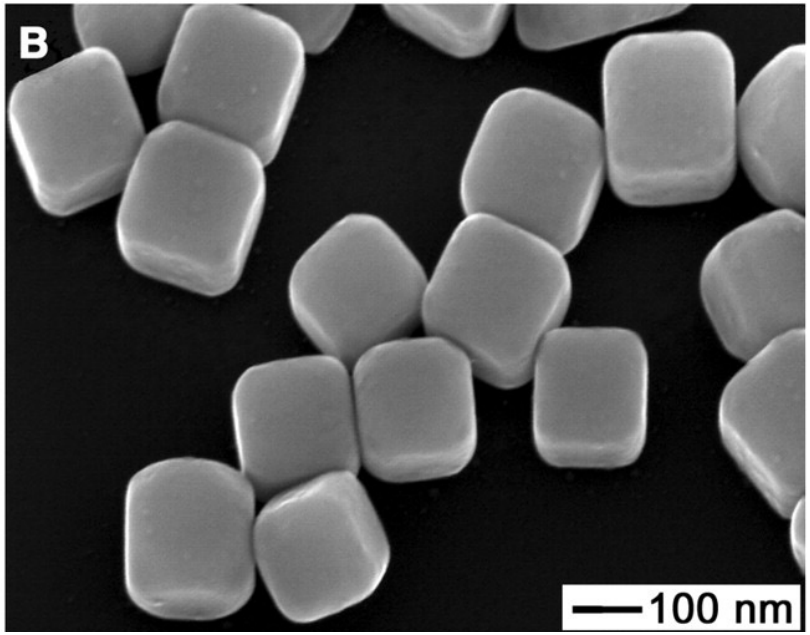
Density distribution across surface

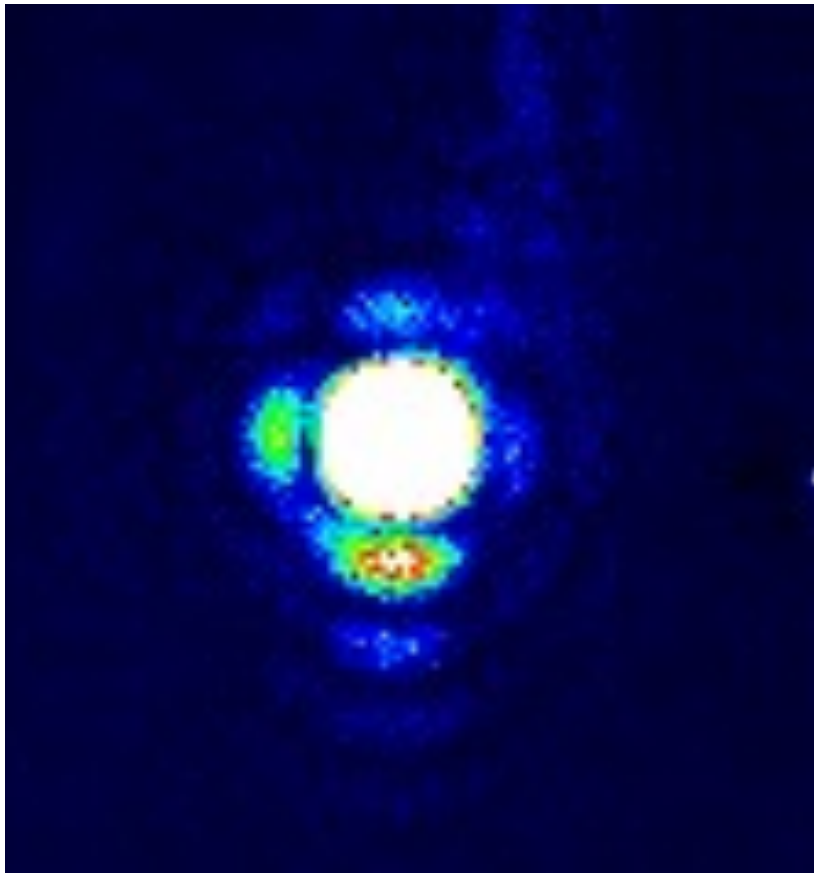


Lensless X-ray Microscope



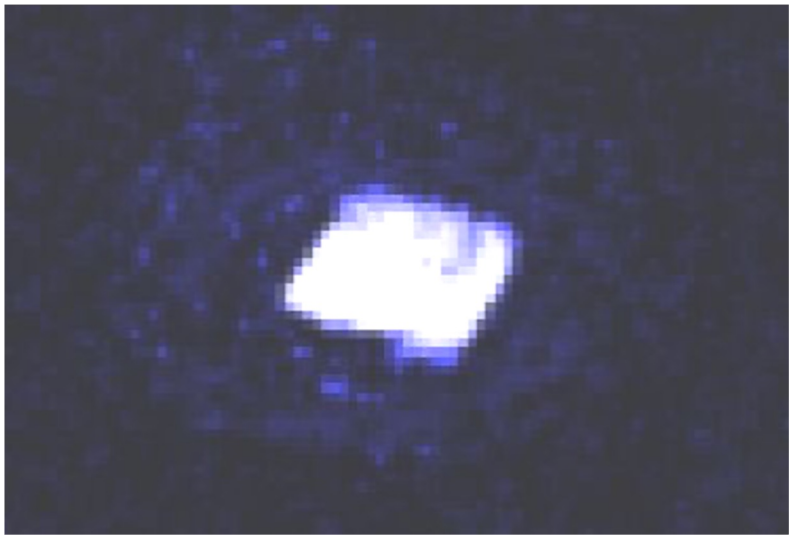
CXD from Silver Nanocubes



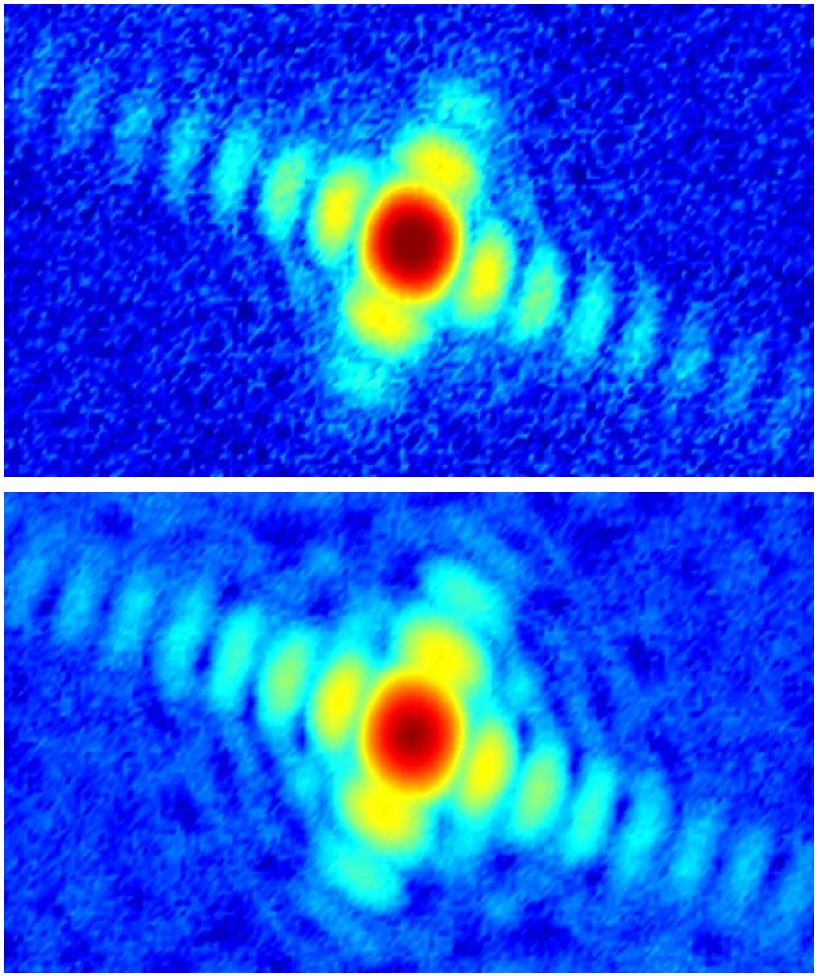


Yugang Sun and Younan Xia,
Science 298 2177 (2003)

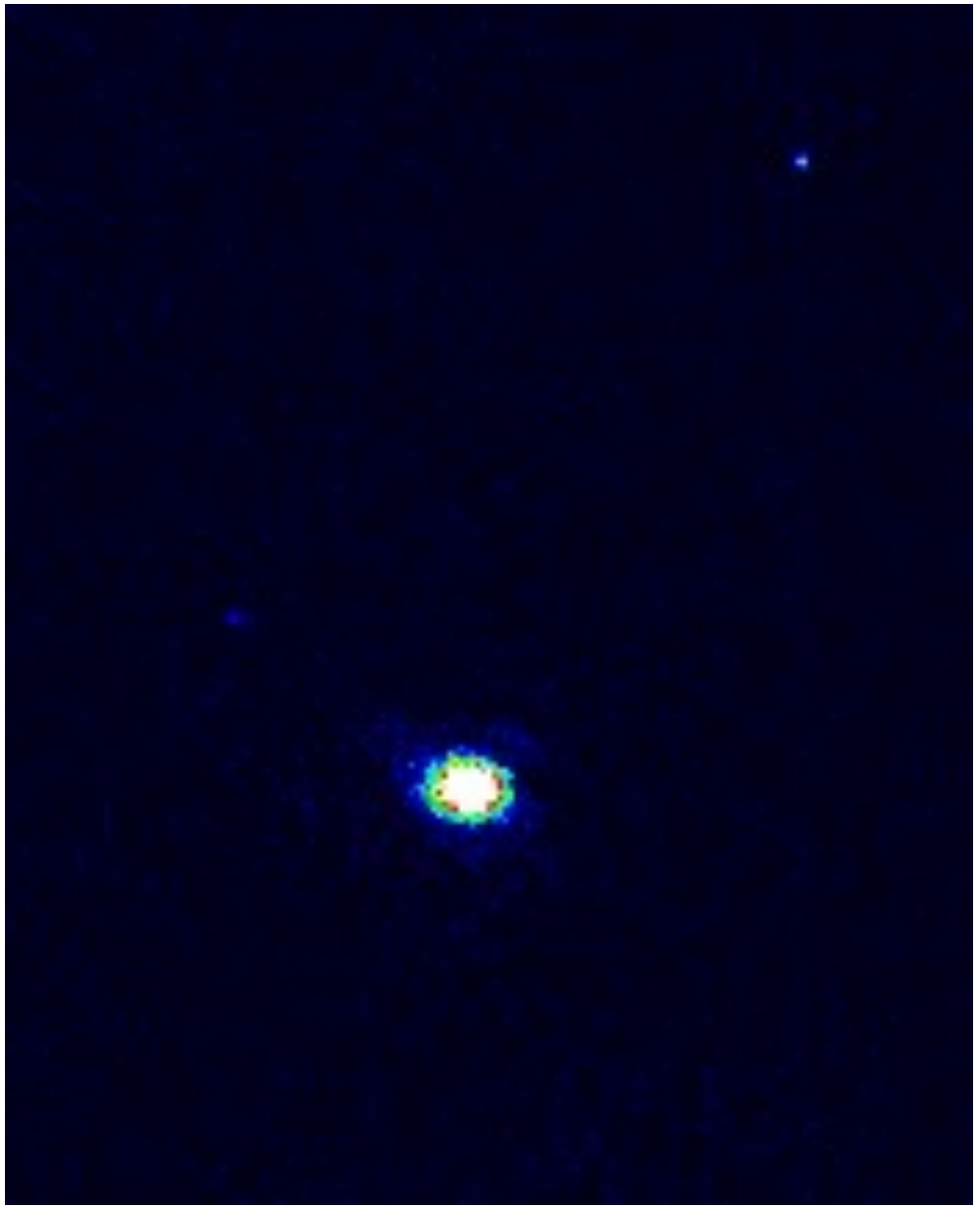
Reconstruction of Ag Nanocrystal



200nm

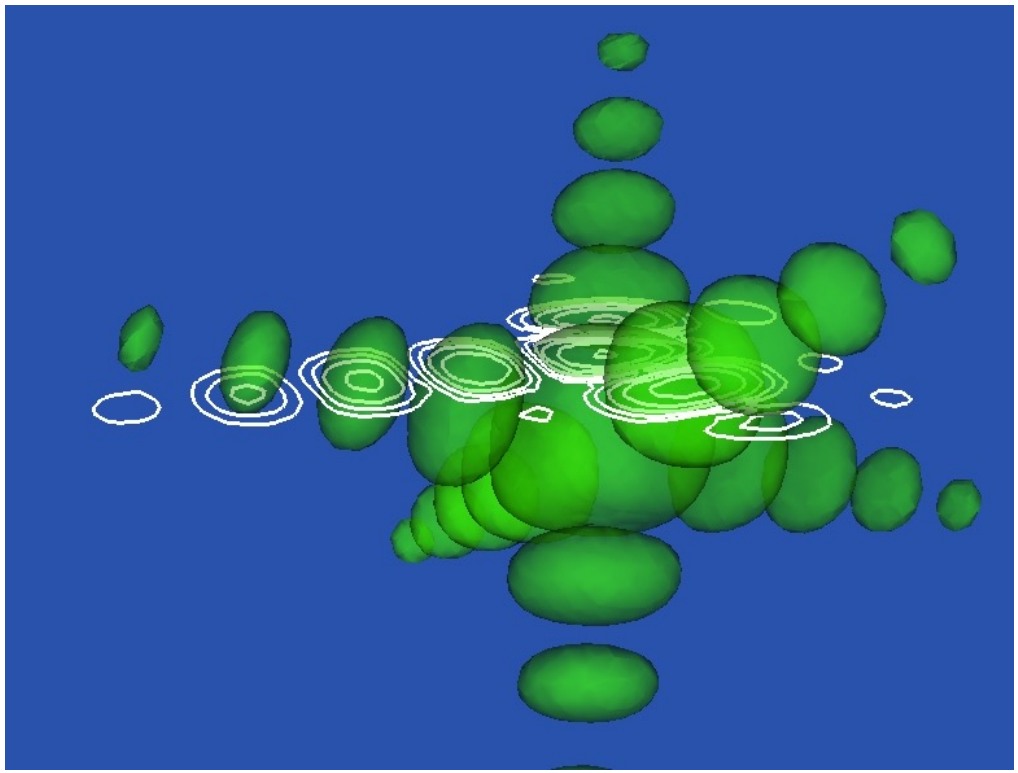


Rocking scan of Ag cubes with 0.01° steps



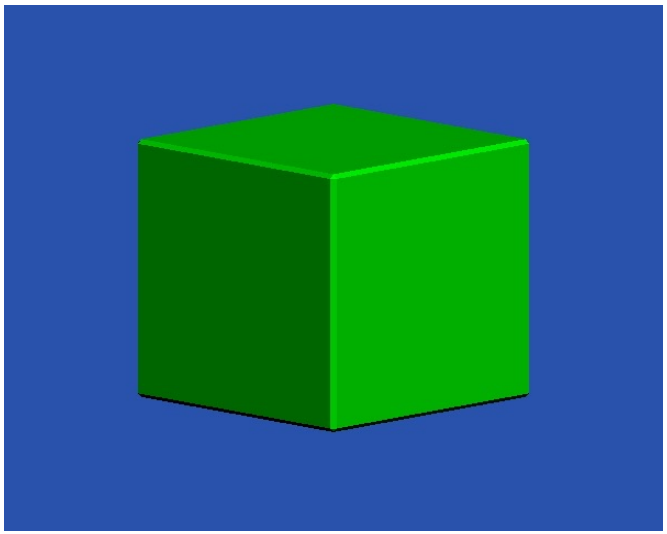
Miscentered Non-Centrosymmetric Reciprocal Space Slice

$$A_q \neq A^*_{\bar{q}}$$

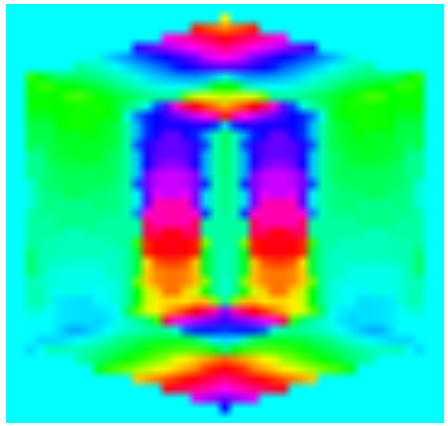


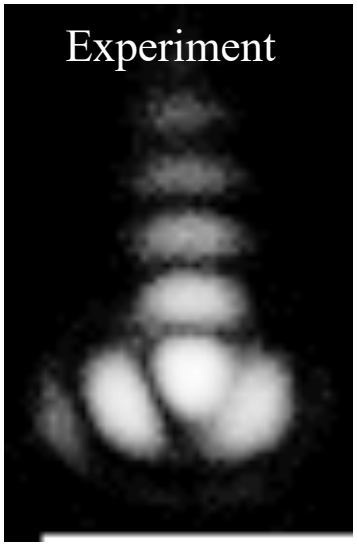
Real-space phase.

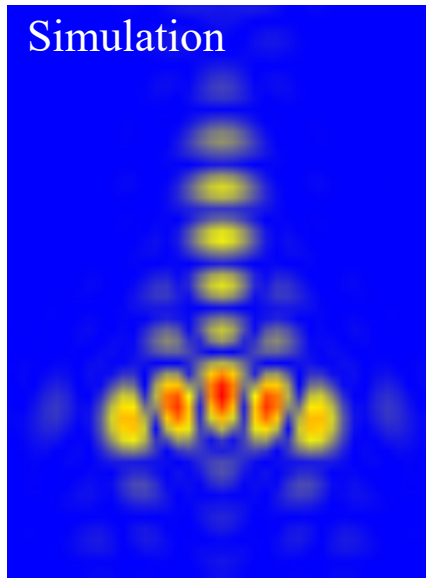
What can we expect to see?



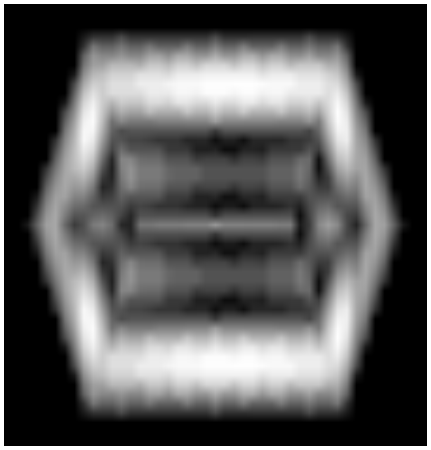
$$A(\bar{q}_o+\bar{q}_z)=\sum_i \sum_z \underbrace{\rho(x,y,z)}_{u_i(x,y)} e^{2\pi i \bar{q}_z\cdot\bar{z}_i} e^{2\pi i(\bar{q}_o)\cdot\bar{r}_i}$$

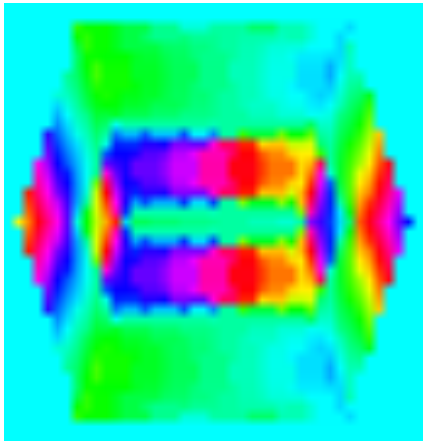


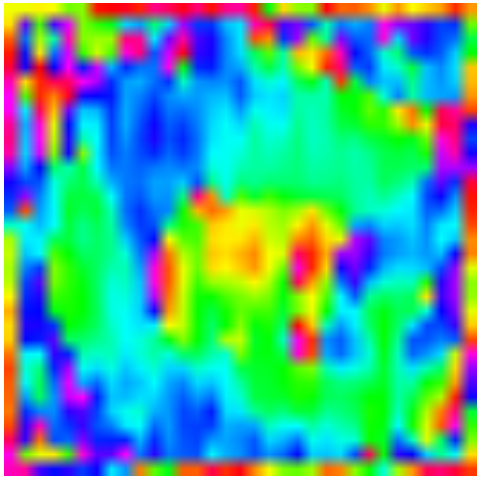


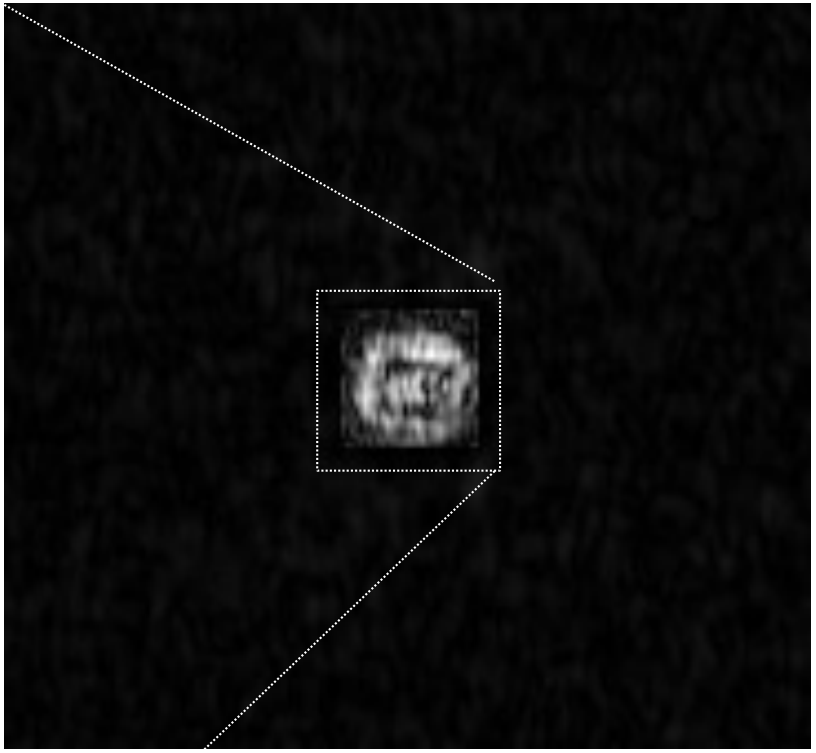


Direct Space Result (1000 Iterations)

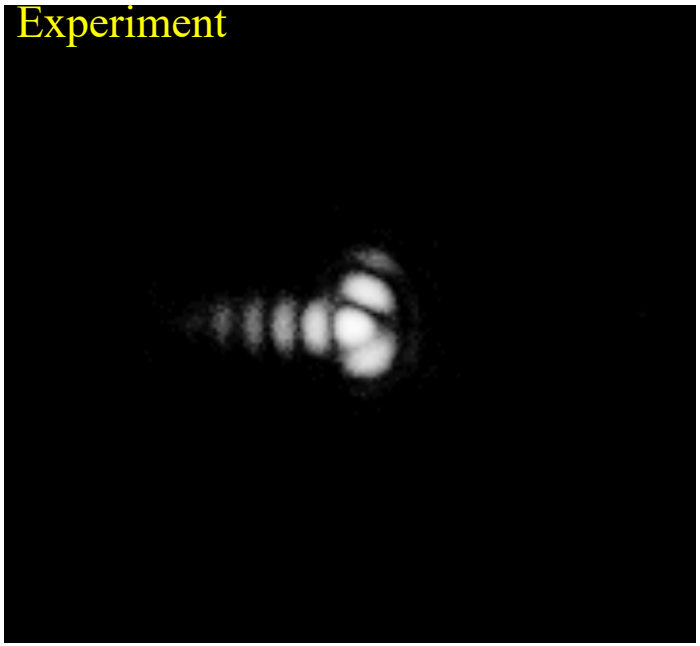


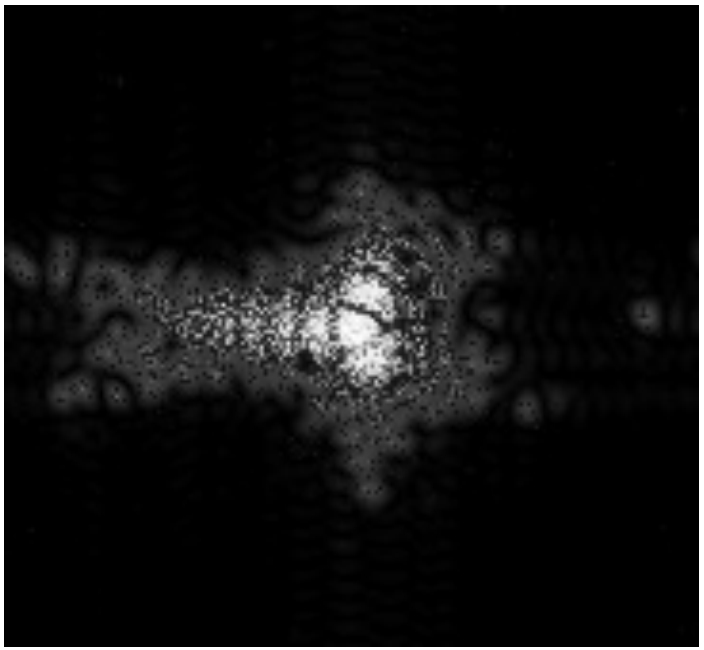


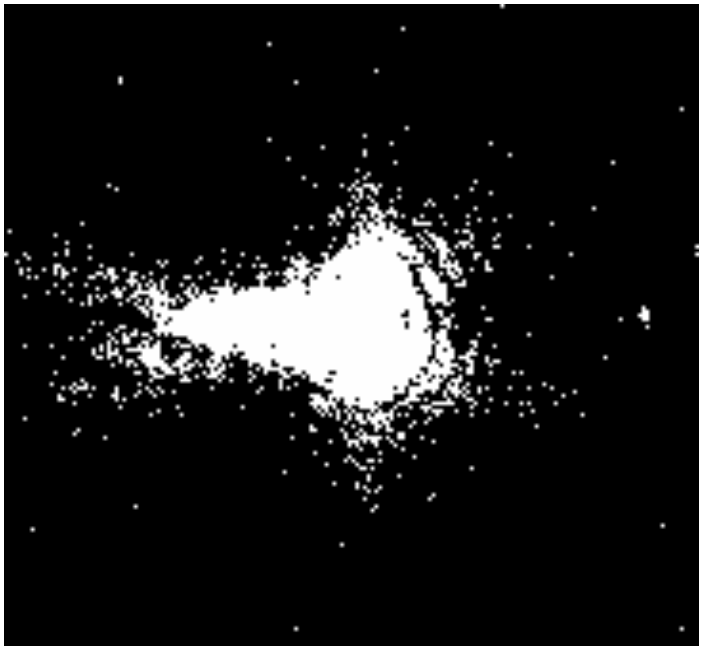


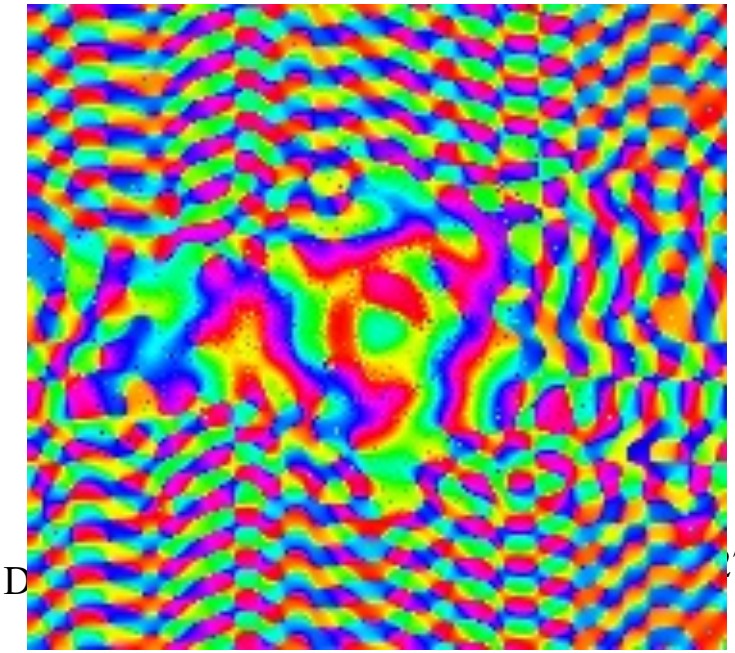


Reciprocal Space Result (1000 iterations)

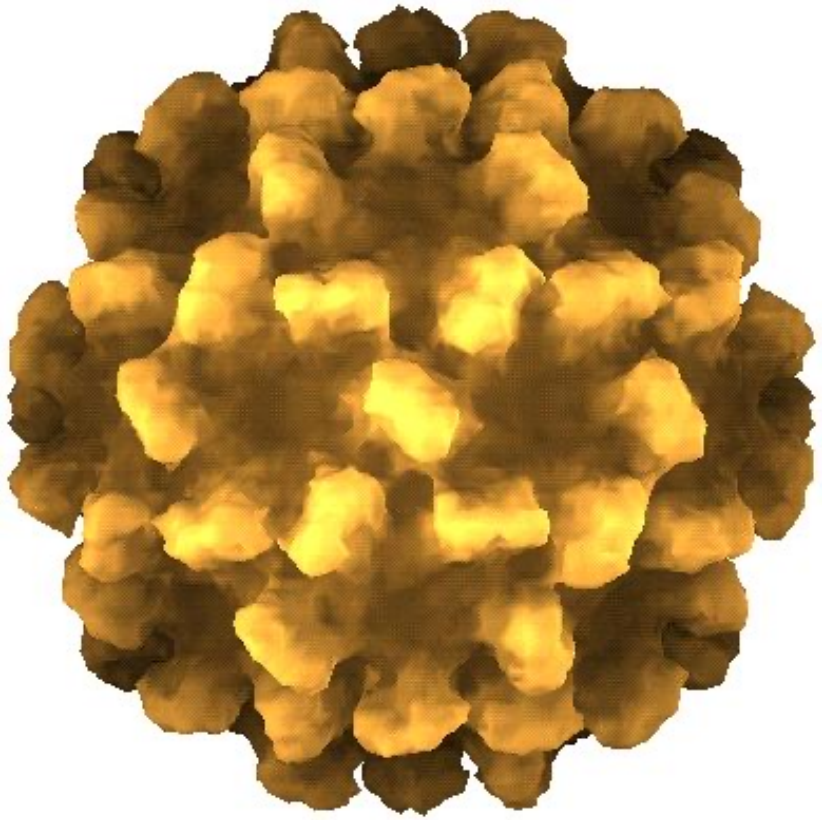








Tomato Bushy Stunt Virus
1980



Conclusions and Outlook

- Inversion of CXD demonstrated
- Internal structure of Au Nanocrystals
- Phase structure visible in Pb Nanocystals
- Off-center diffraction gives complex image
- Single molecules one day