Strain Mapping by Coherent X-ray Diffraction

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ERL workshop,
Cornell University
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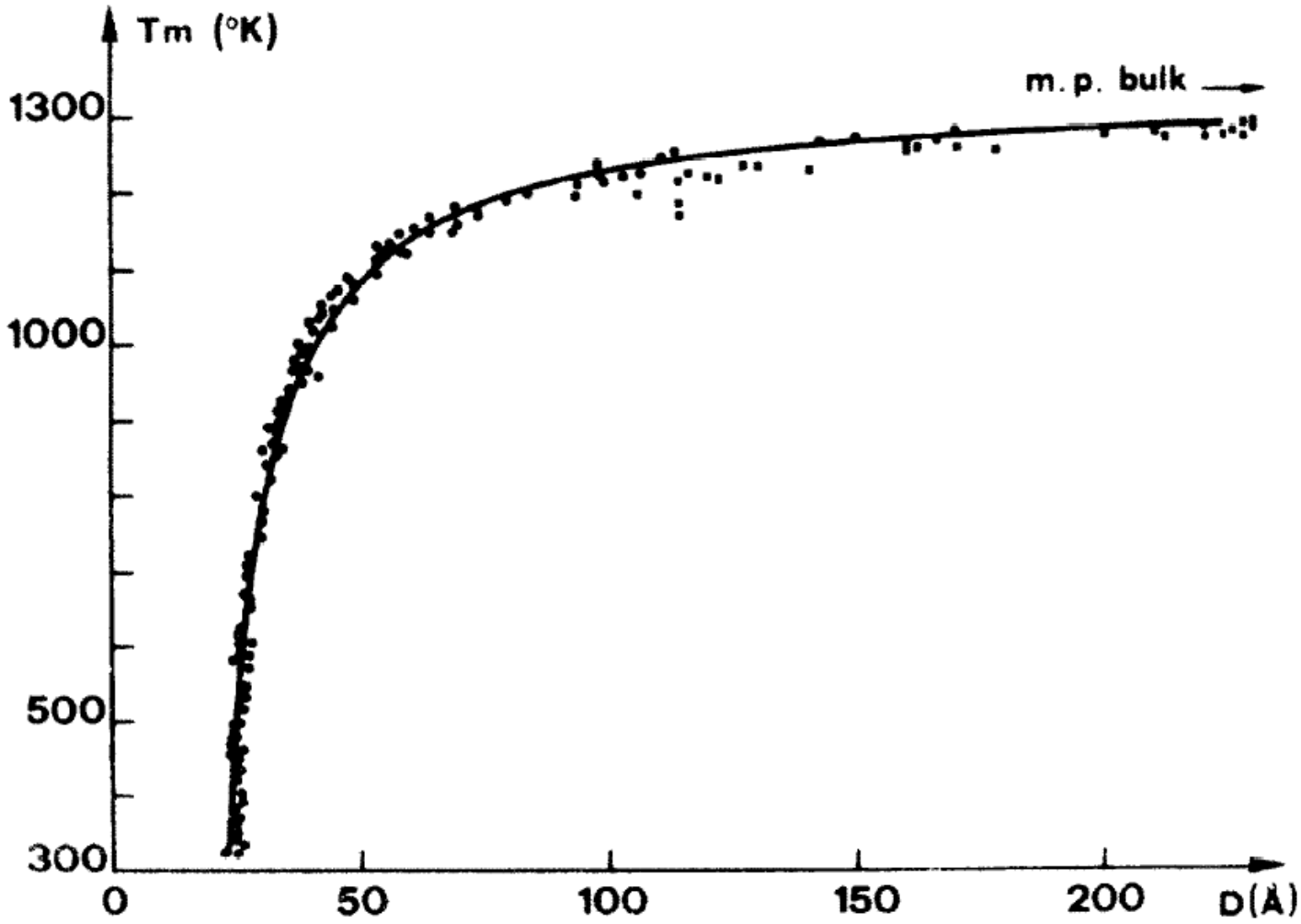
Outline

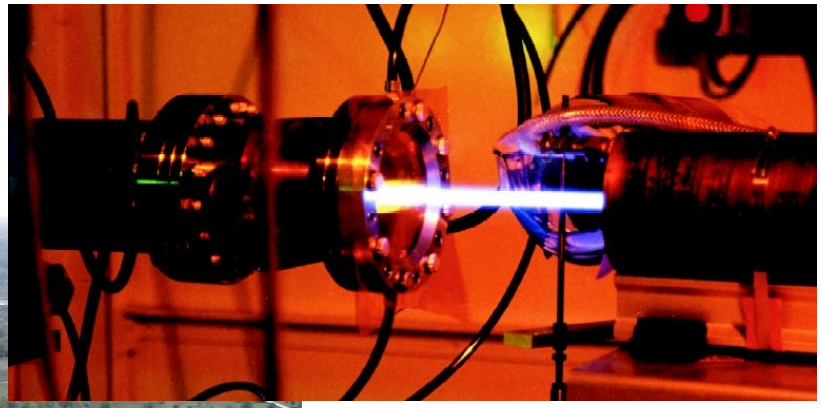
- Coherent X-ray Diffraction
- How to Solve the Phase Problem
- Nanocrystal Shapes
- Extension to Phase Objects
- New Beamline Concepts
- New Opportunities with ERLs

Size-dependent Melting of Au Particles

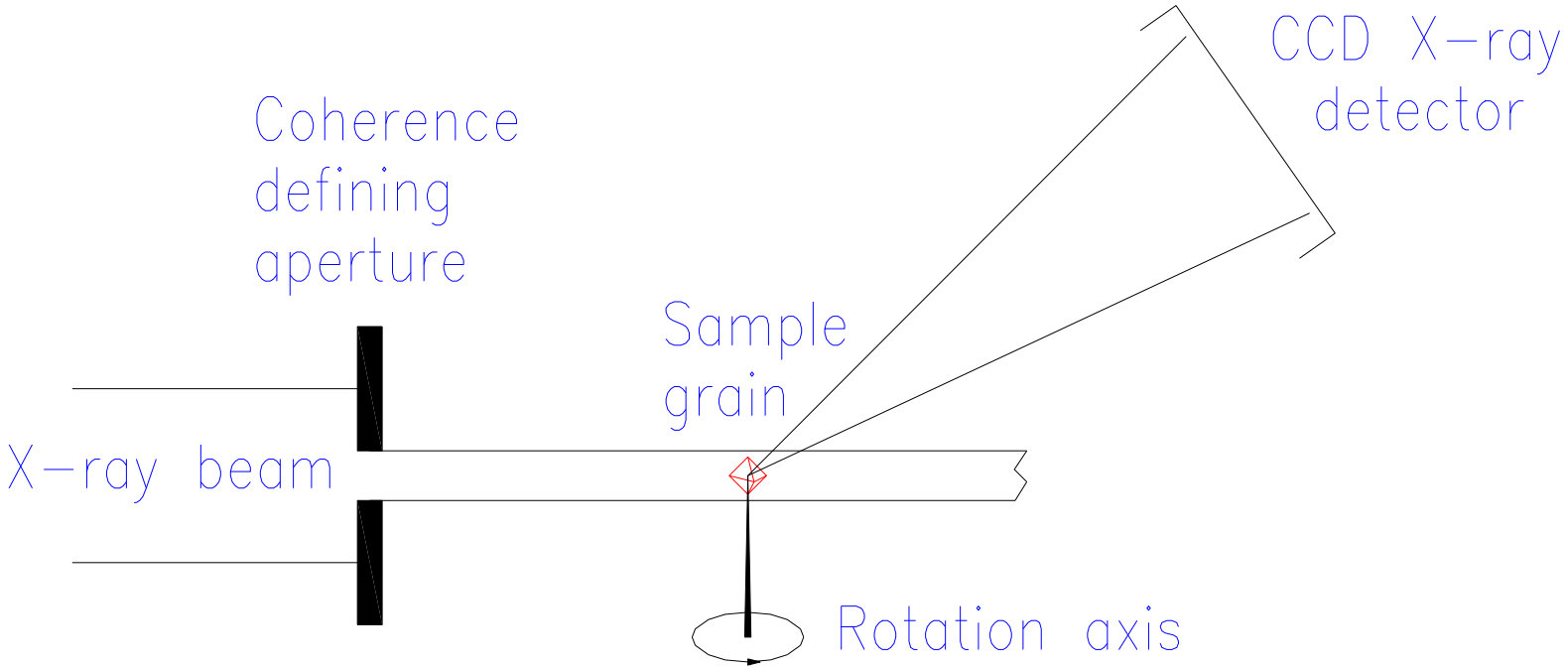
P. Buffat and J-P. Borel, Phys. Rev. A 2287-97 (1975)

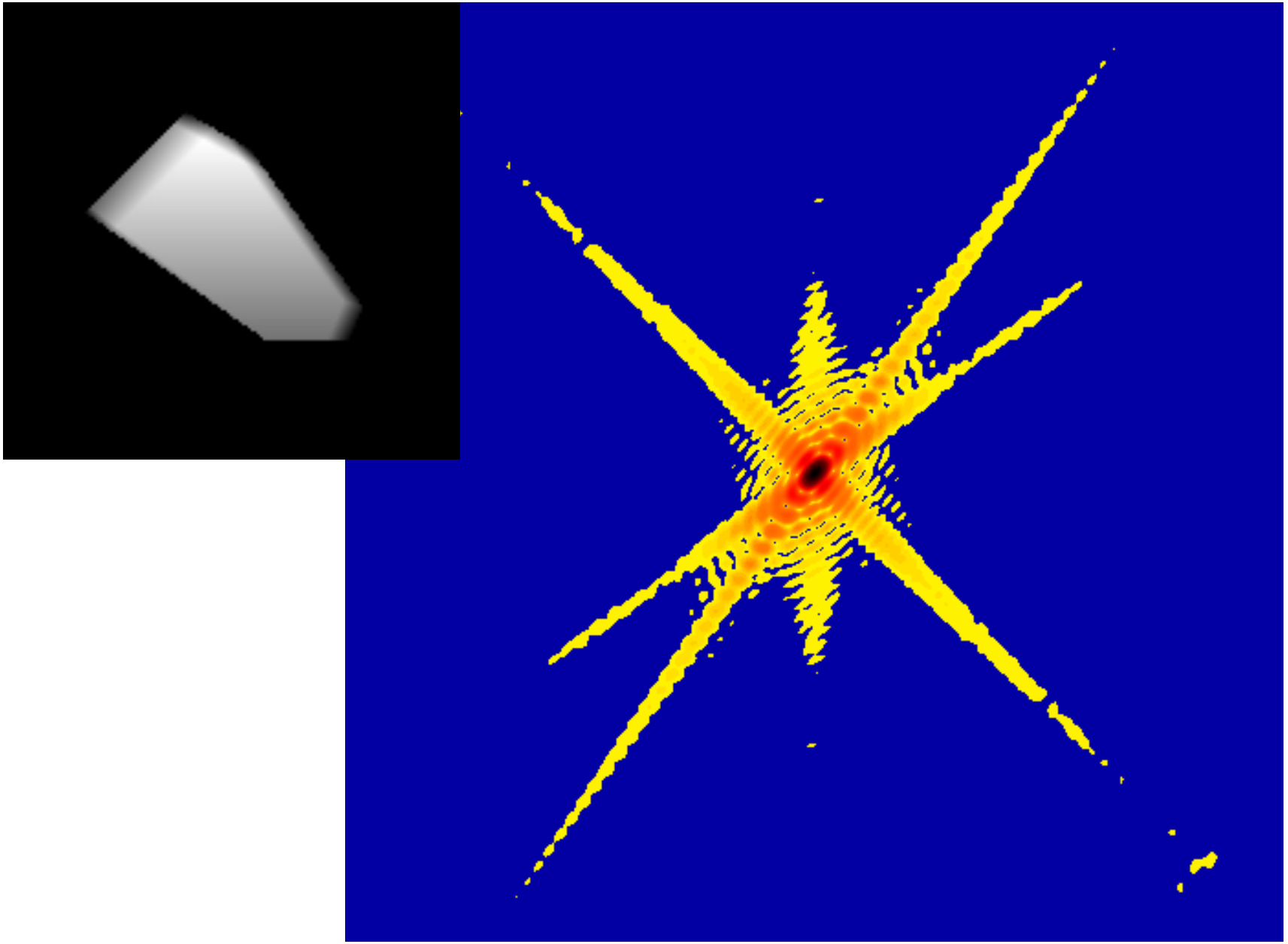


Synchrotron Radiation



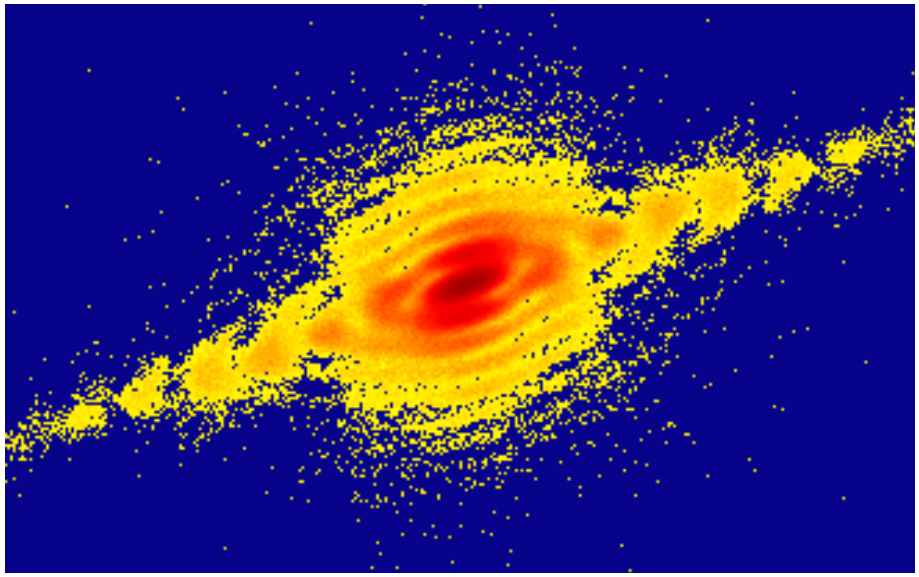
Lensless X-ray Microscope

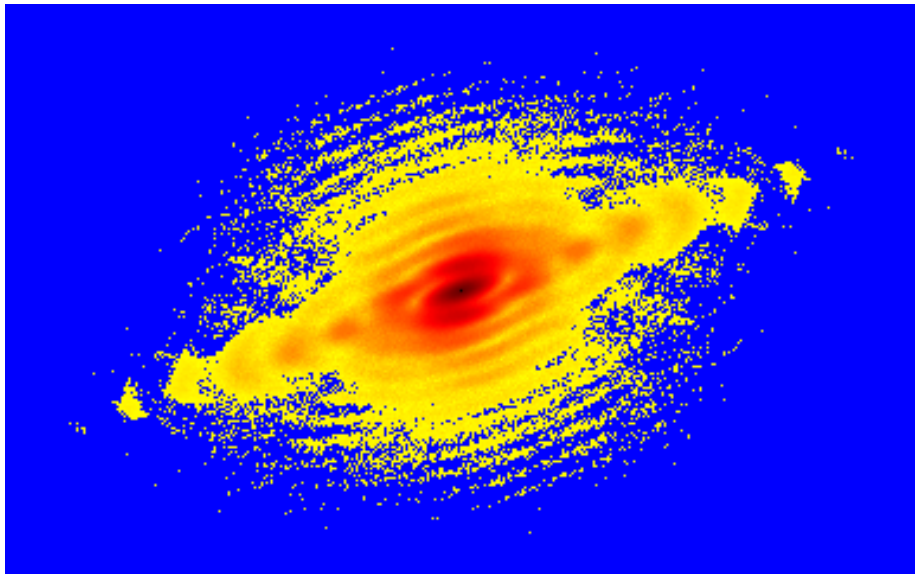


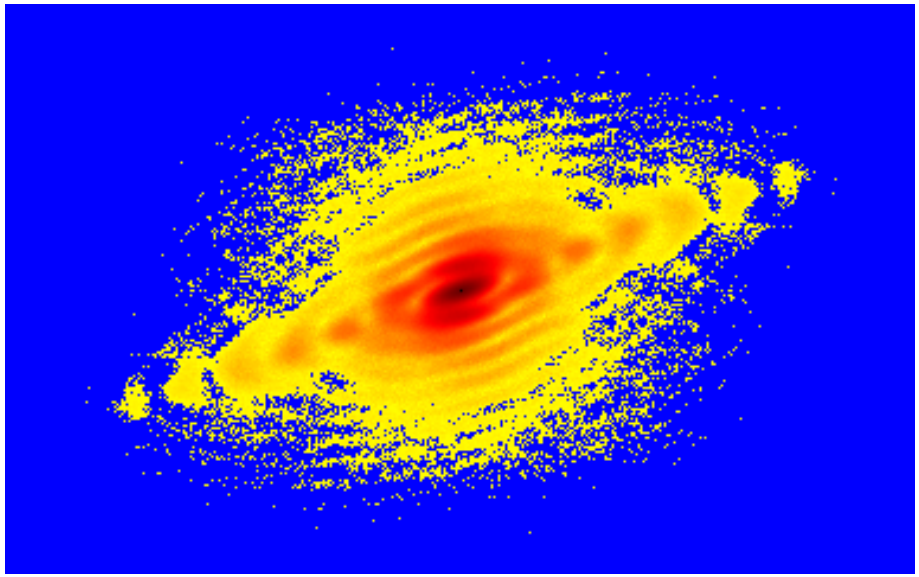


Symmetrized Data and two best fits

Chisq=0.0005

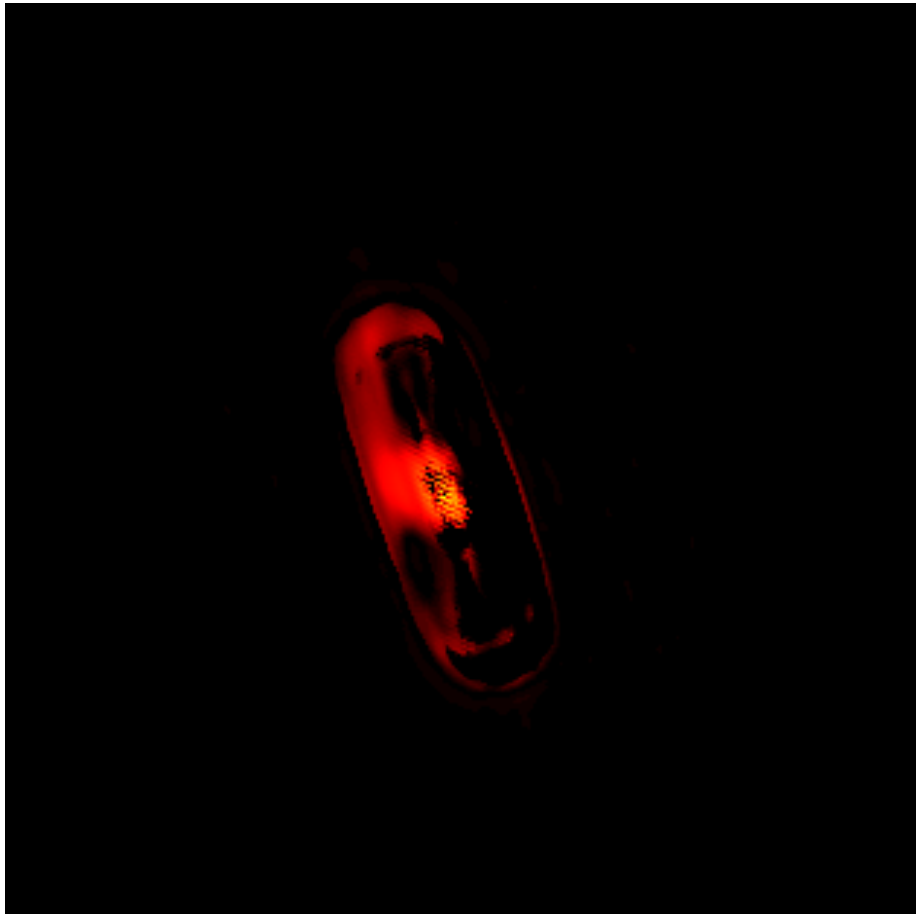


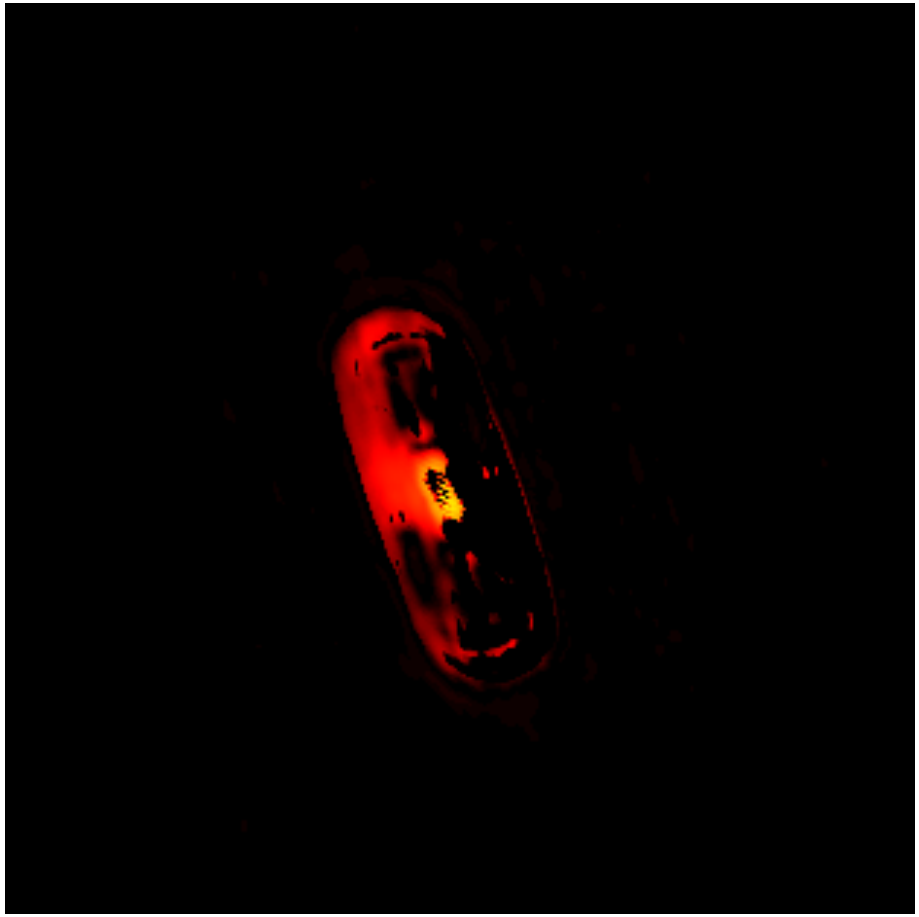


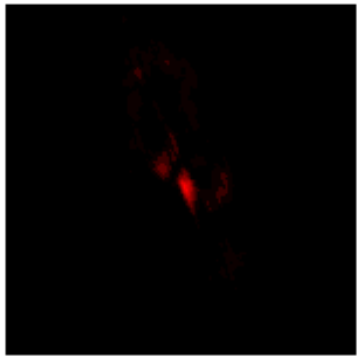
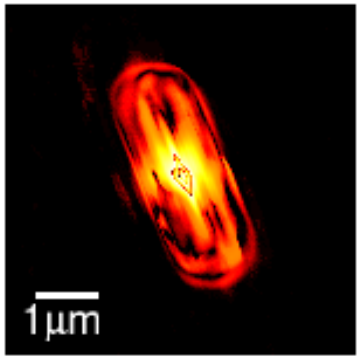


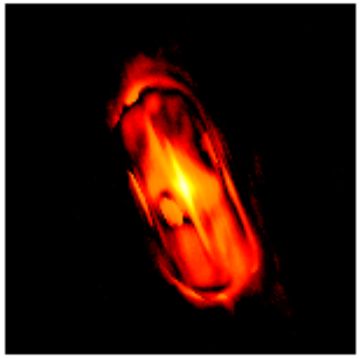
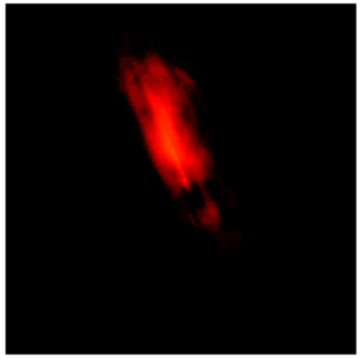
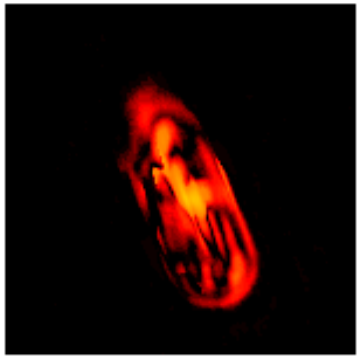
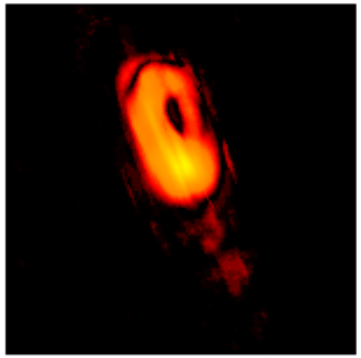
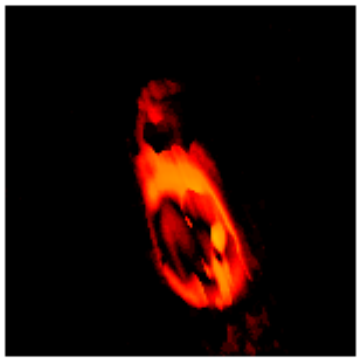
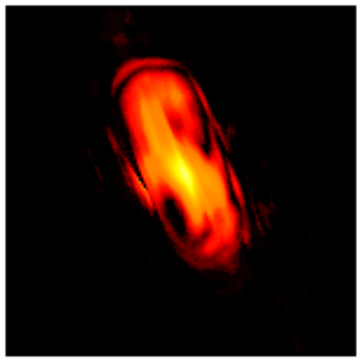
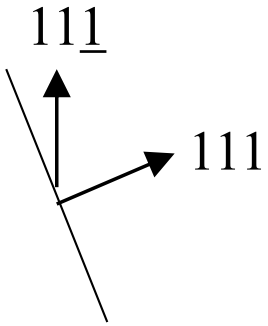
2D Reconstructions

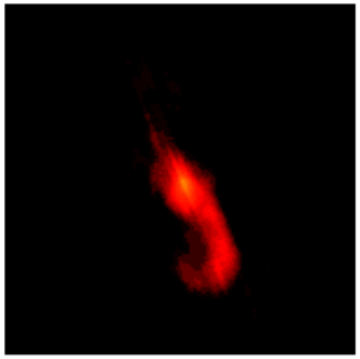
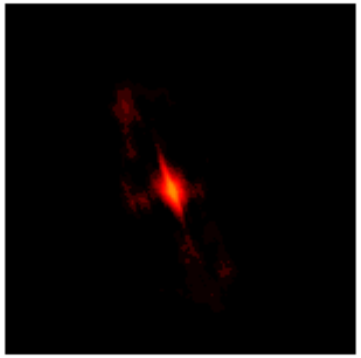
chisquare = 0.0005



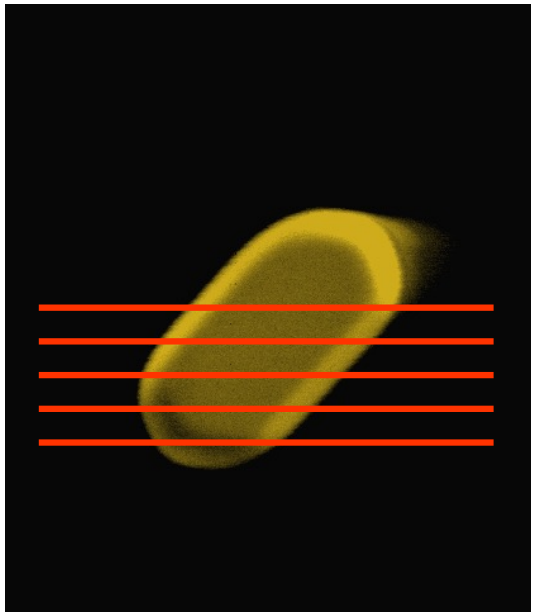


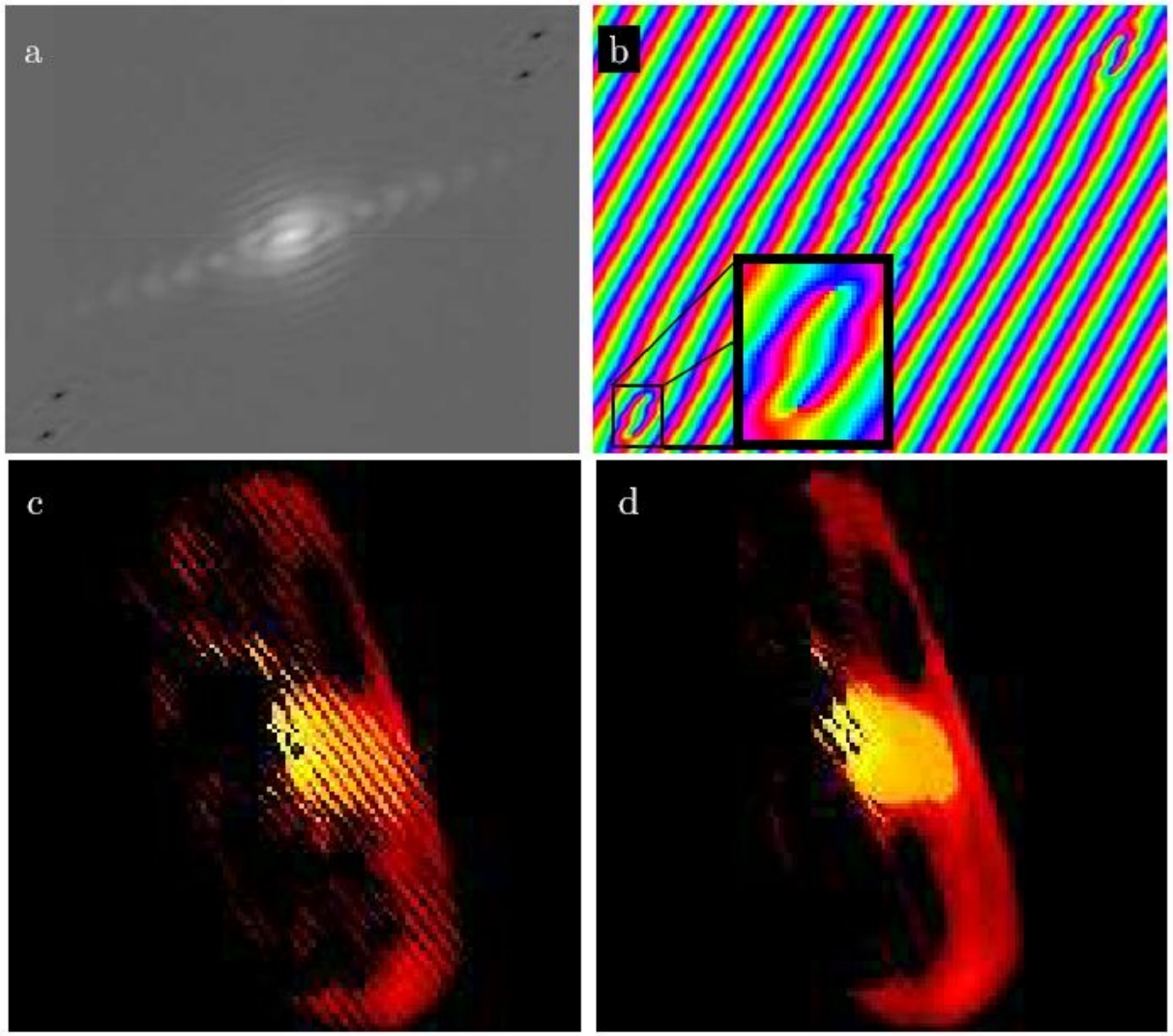








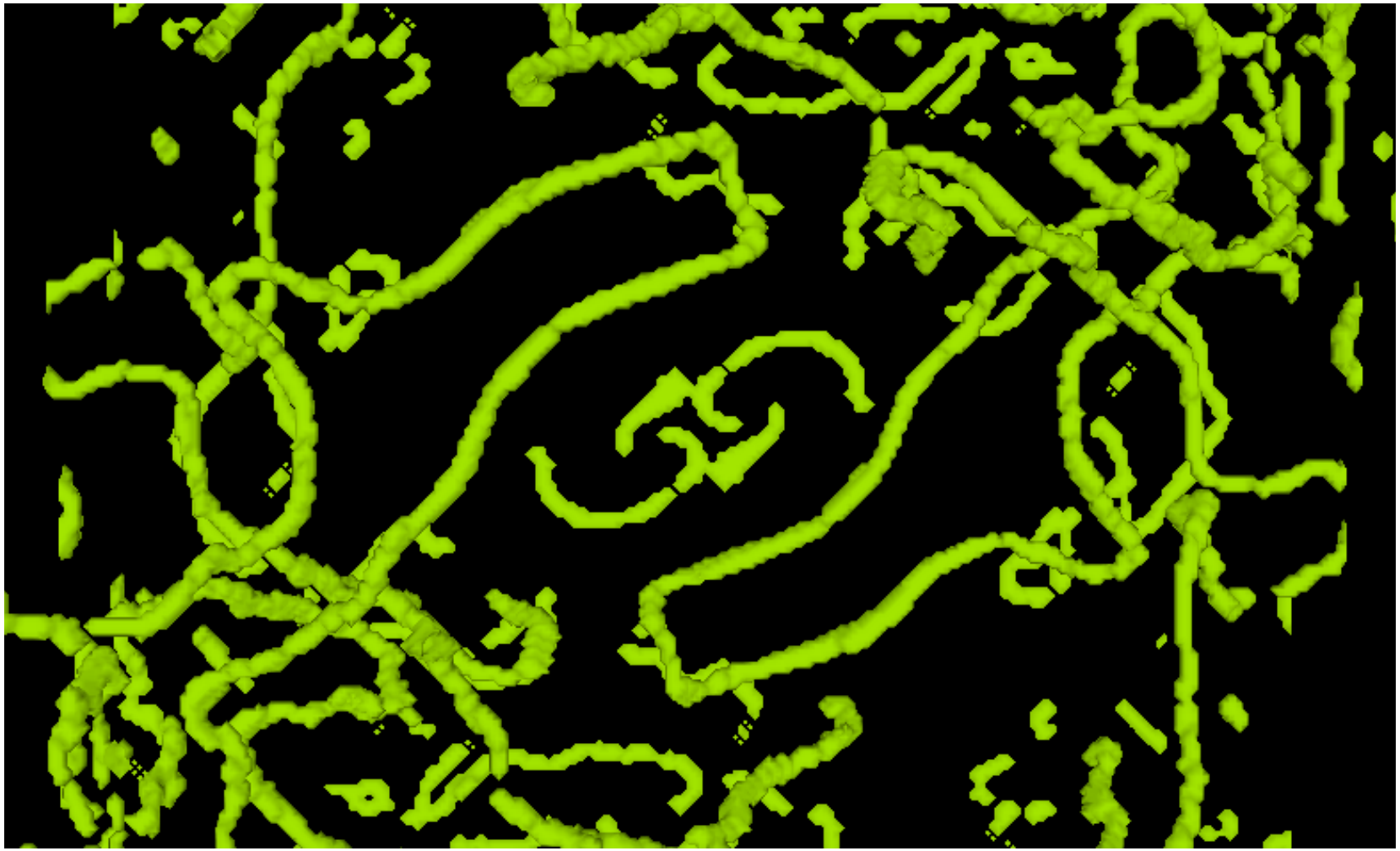
Slices through plan view SEM:



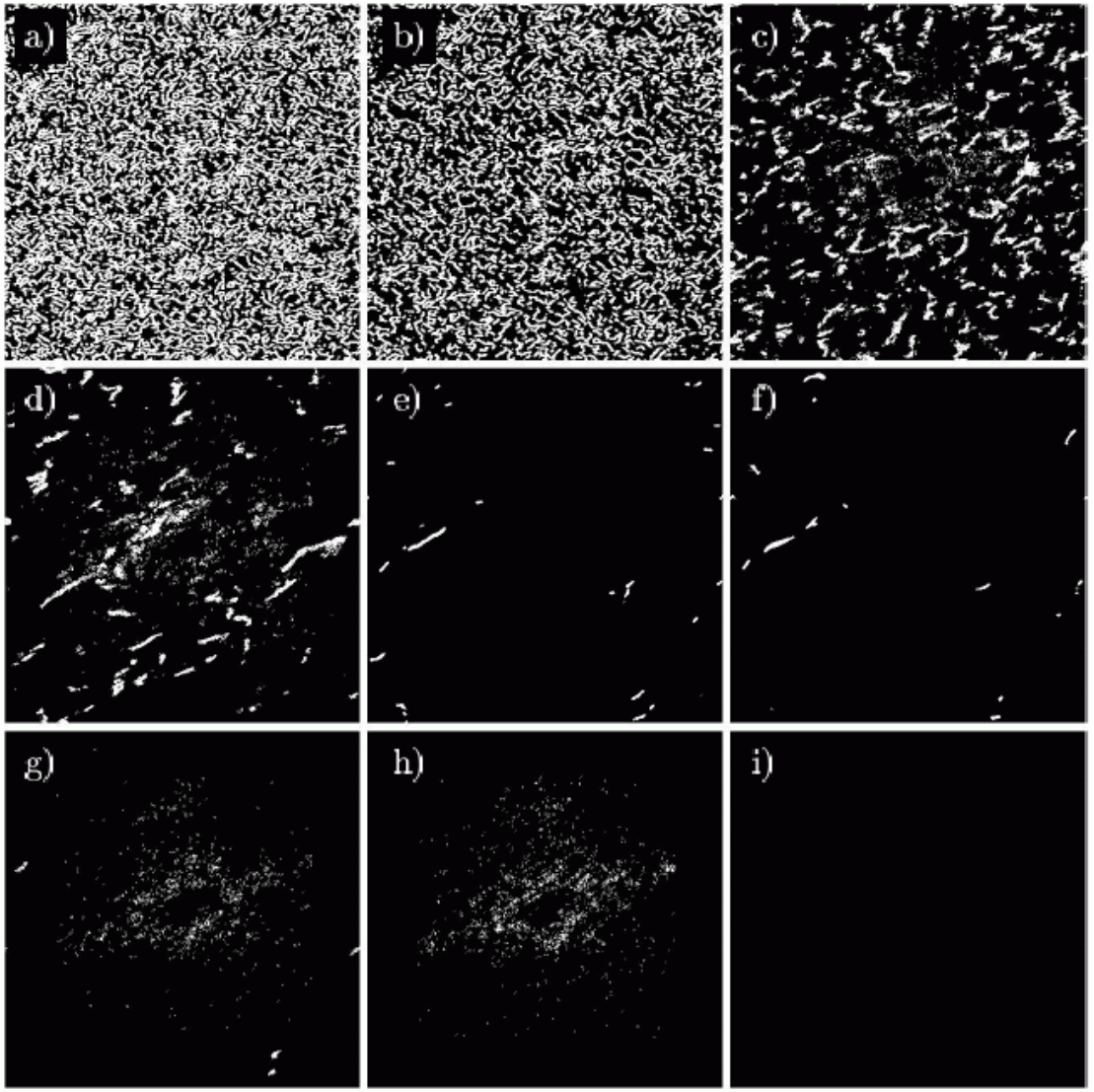
Phase Vortices and patching



‘Vortices’ Form Loops in 3D

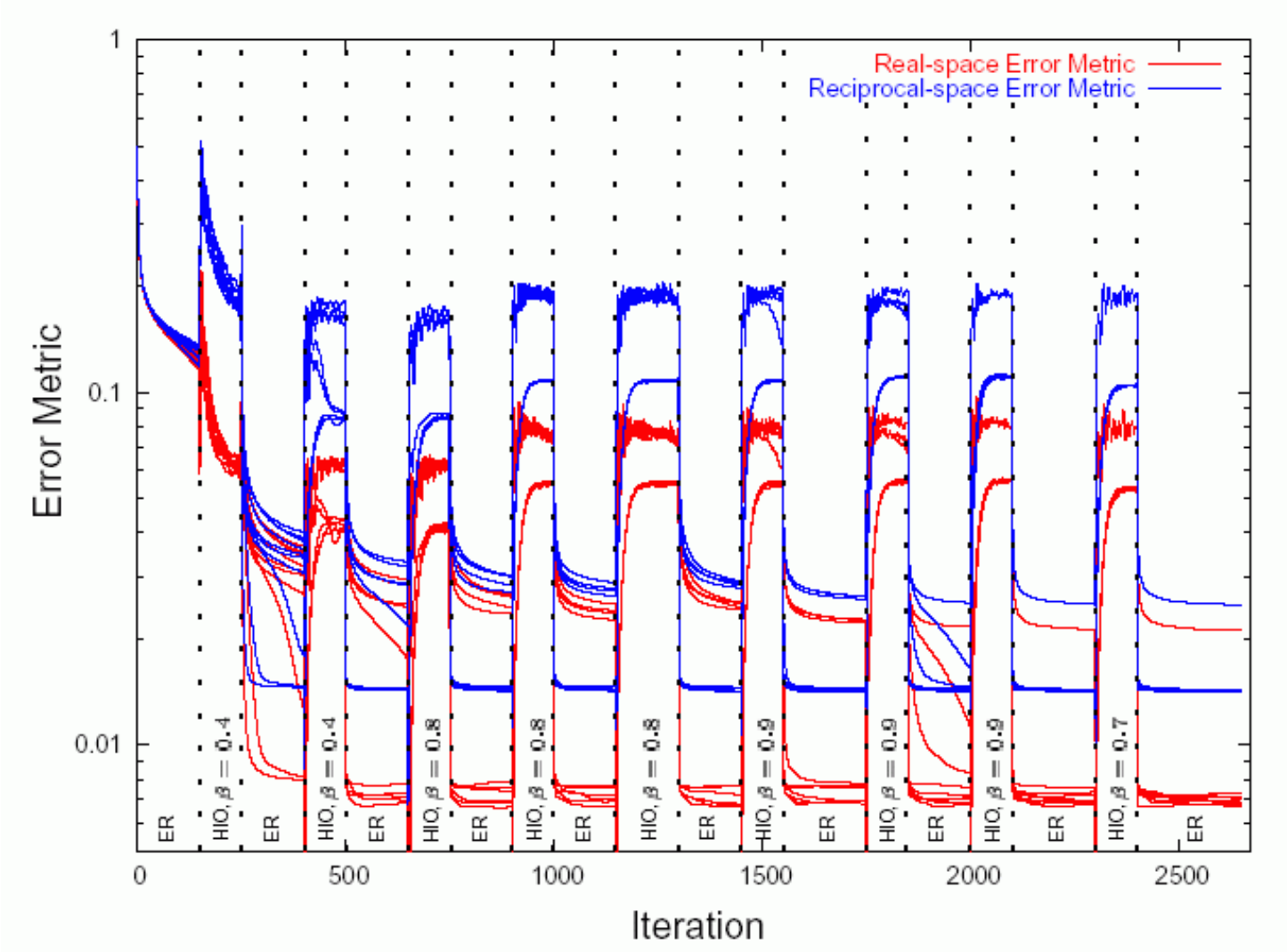


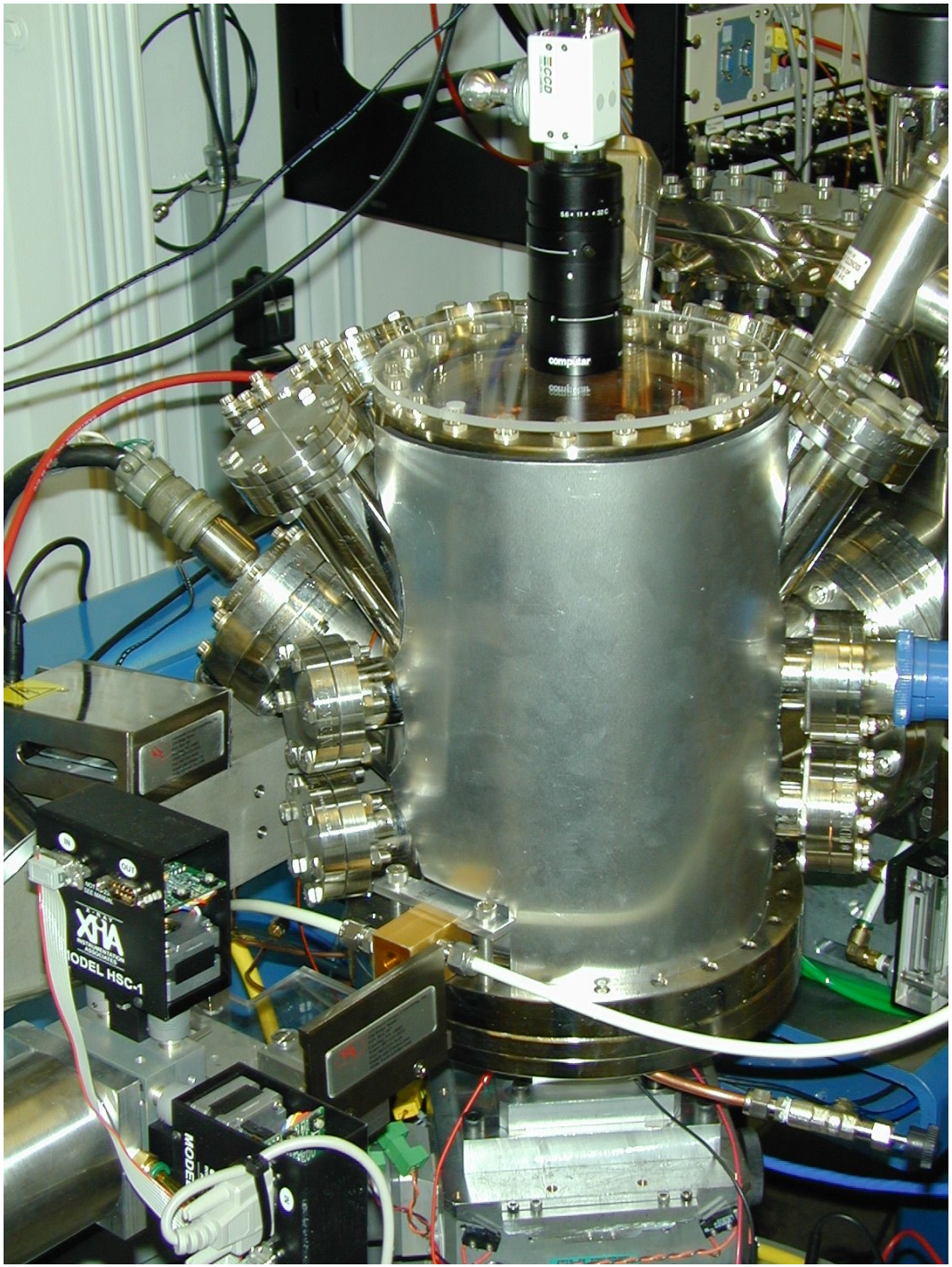
Clearing of Vortices during HIO



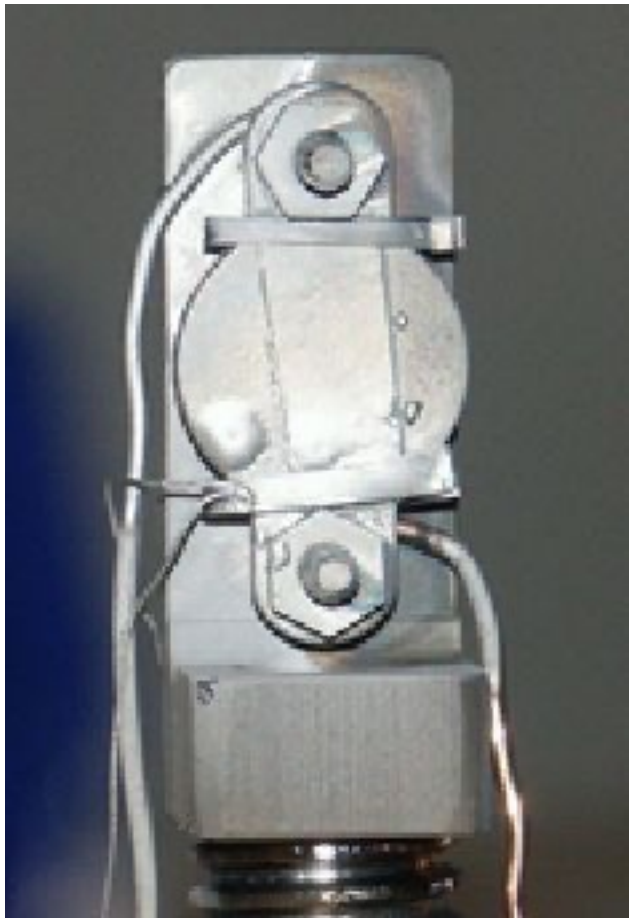
ER ER HIO
HIO ER ER
HIO HIO ER

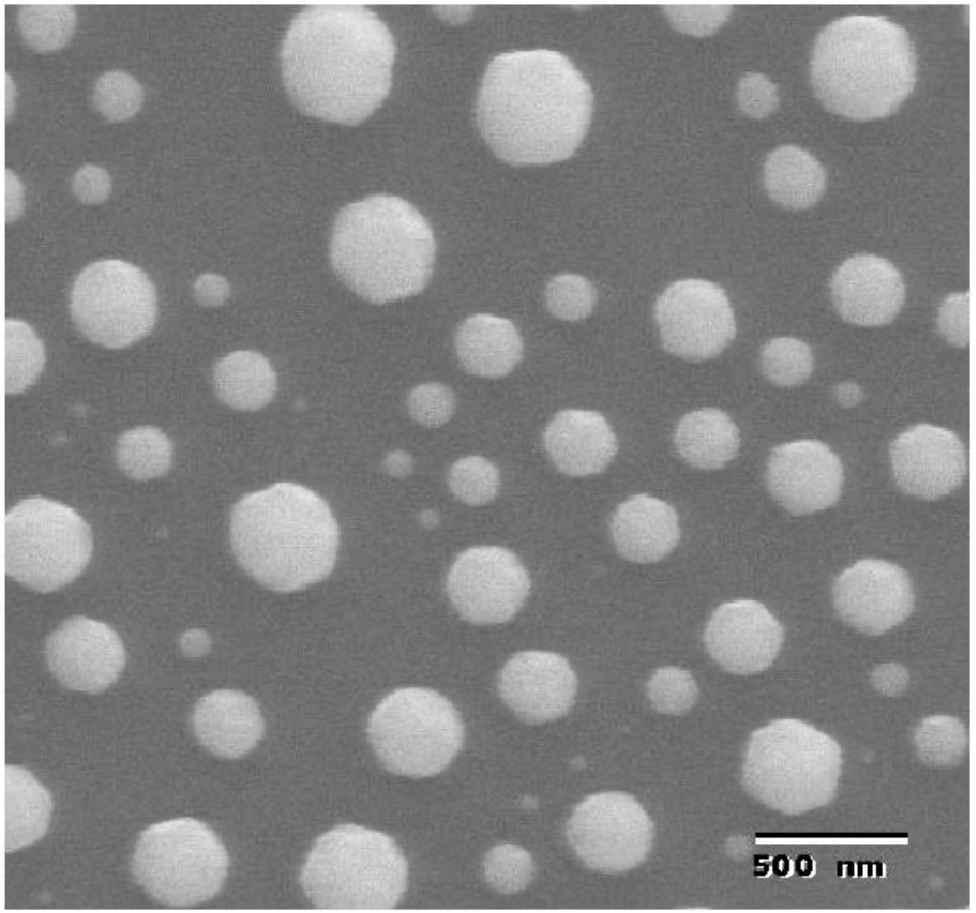
Progress of Phase Retrieval



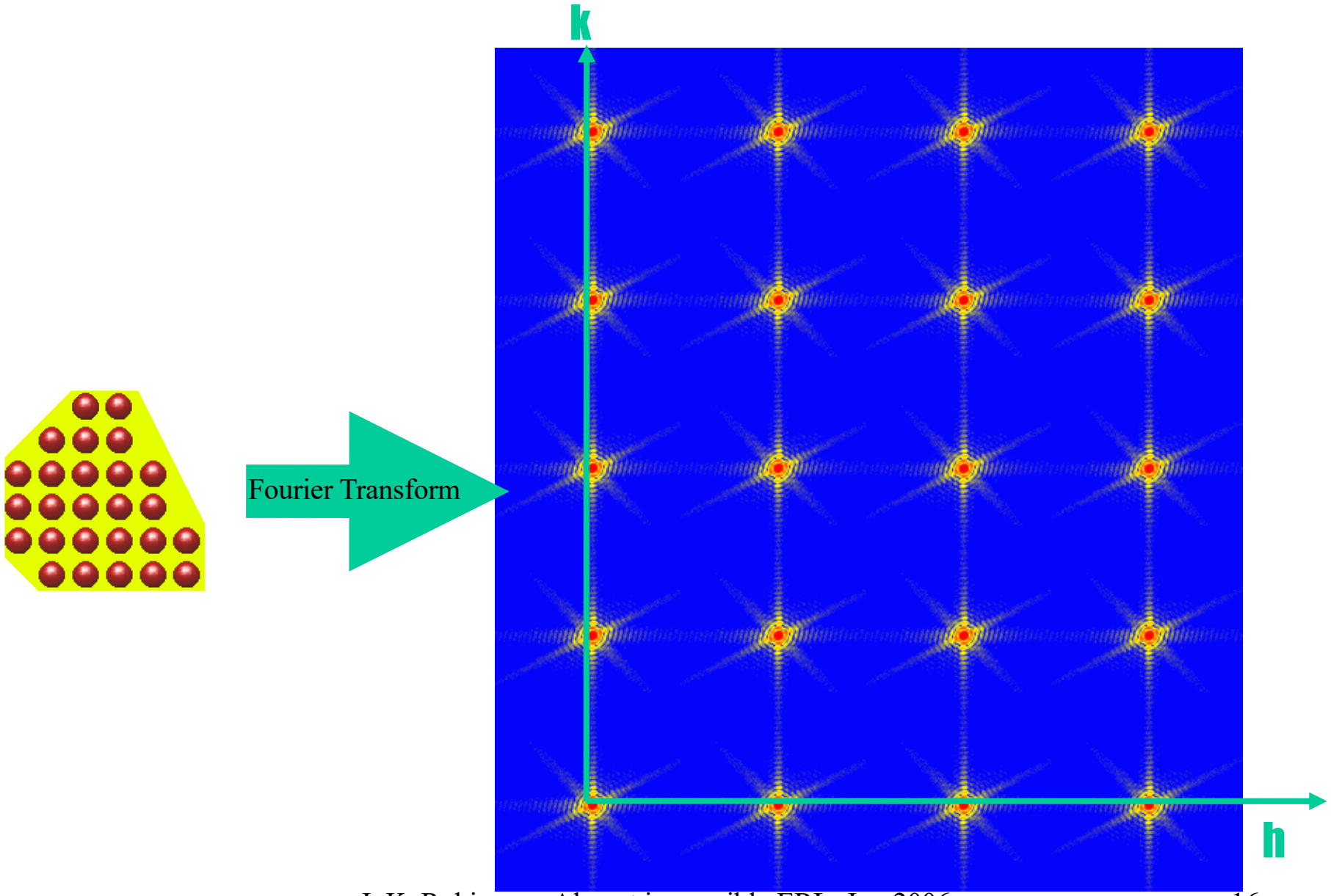

MODEL HSC-1

In situ growth of Pb crystals





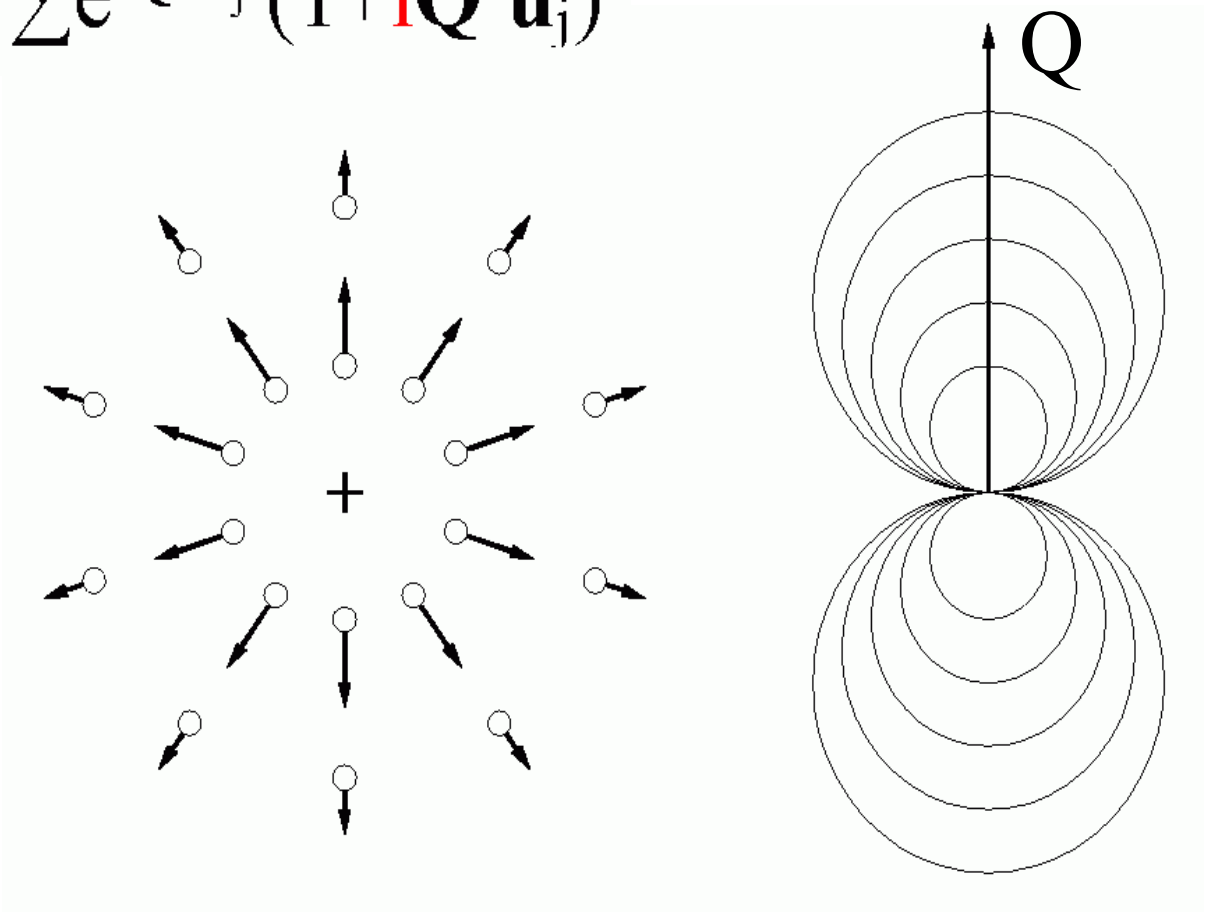
Coherent Diffraction from Crystals



Diffraction by Strain of Point Defect

$$A \sim \sum e^{i\mathbf{Q}\cdot(\mathbf{R}_j+\mathbf{u}_j)}$$
$$\approx \sum e^{i\mathbf{Q}\cdot\mathbf{R}_j}(1+i\mathbf{Q}\cdot\mathbf{u}_j)$$

Imaginary density



Good statistics, 3D diffraction data

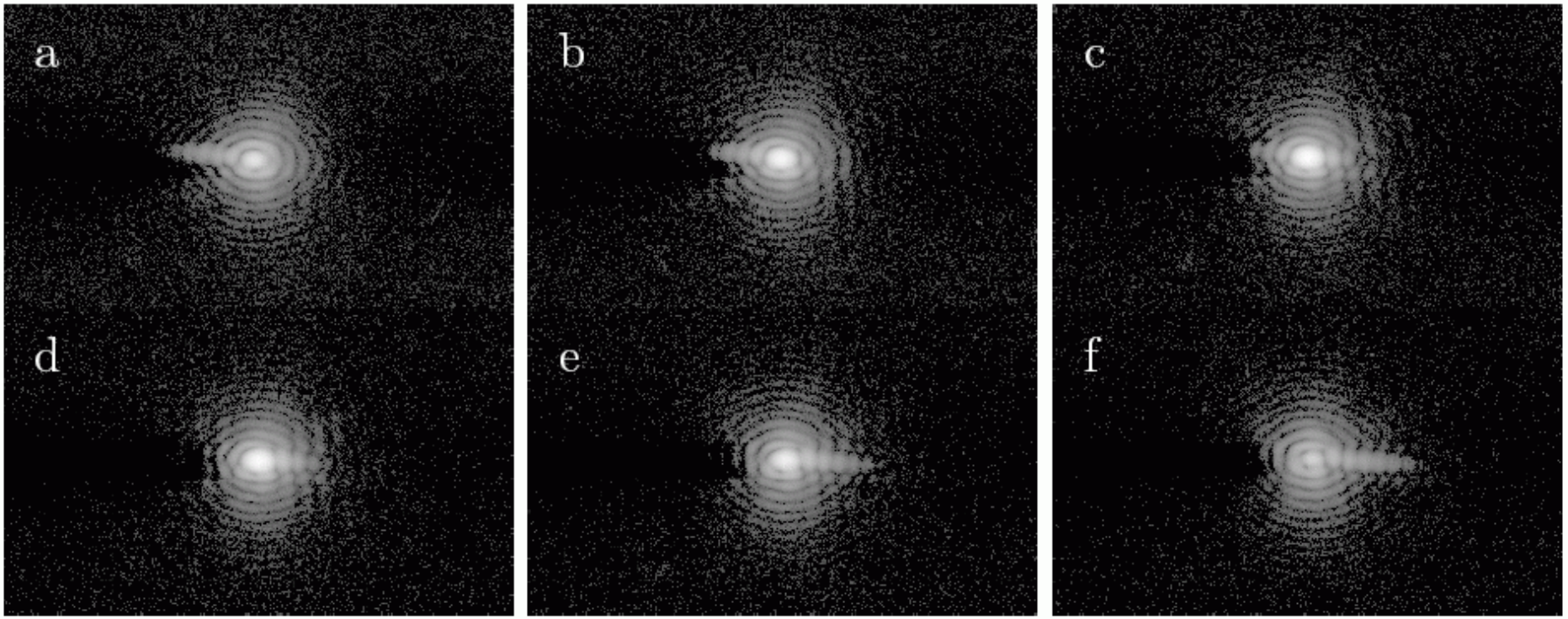
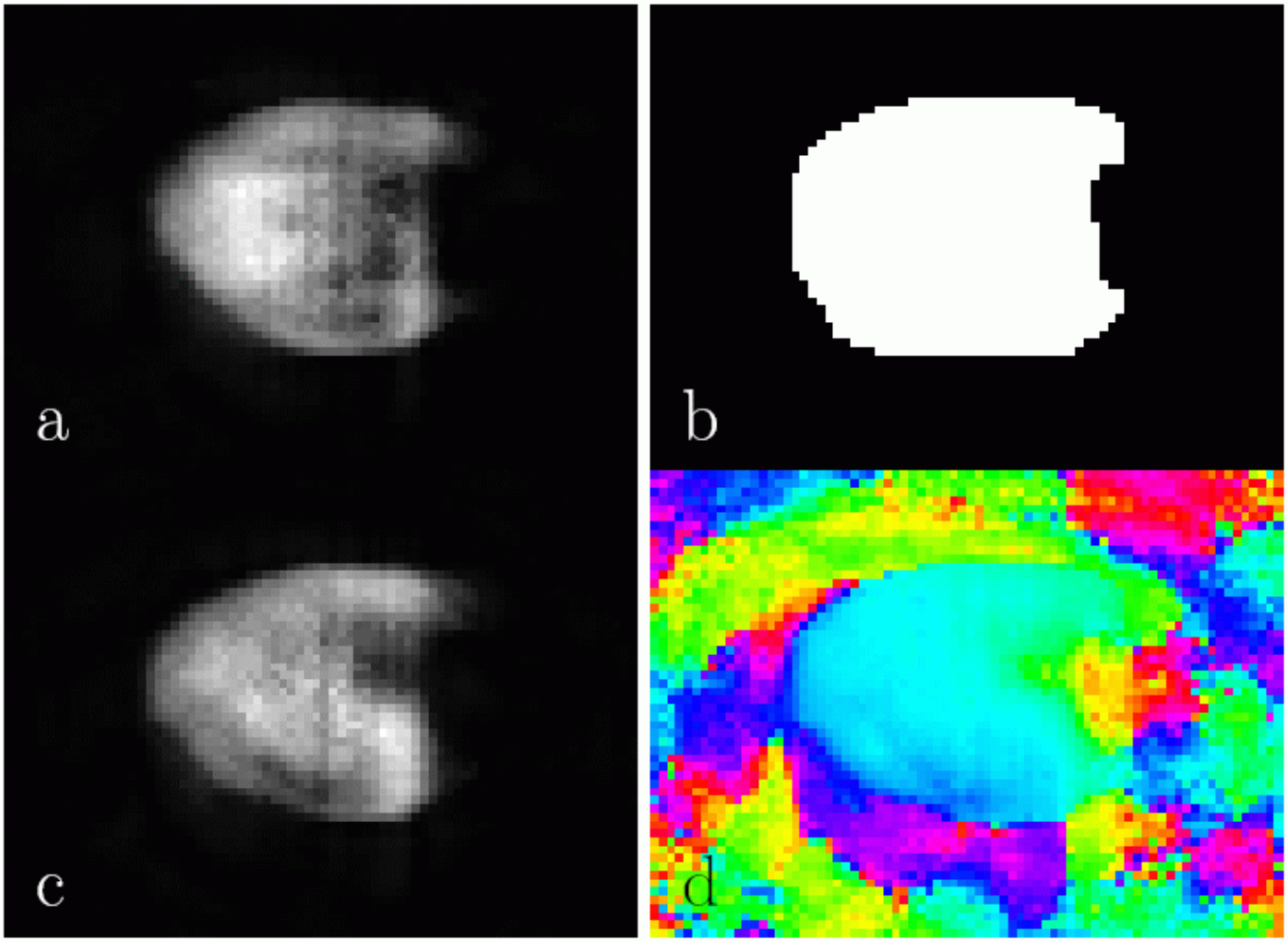
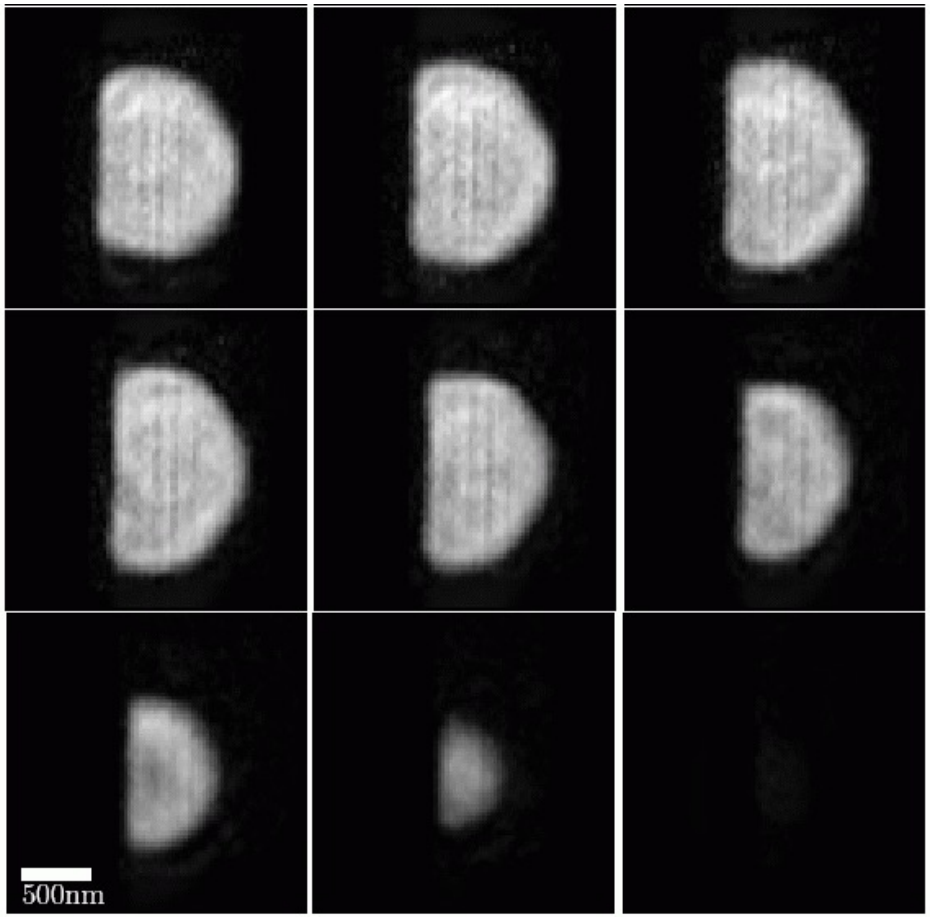


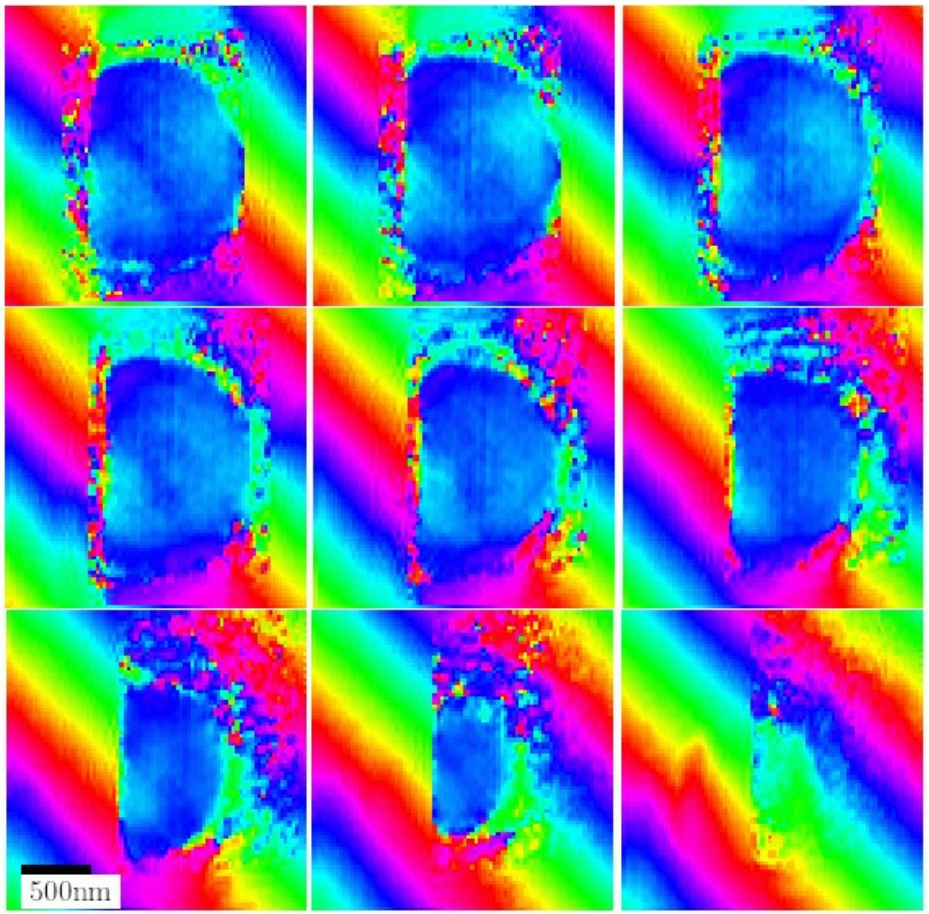
Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

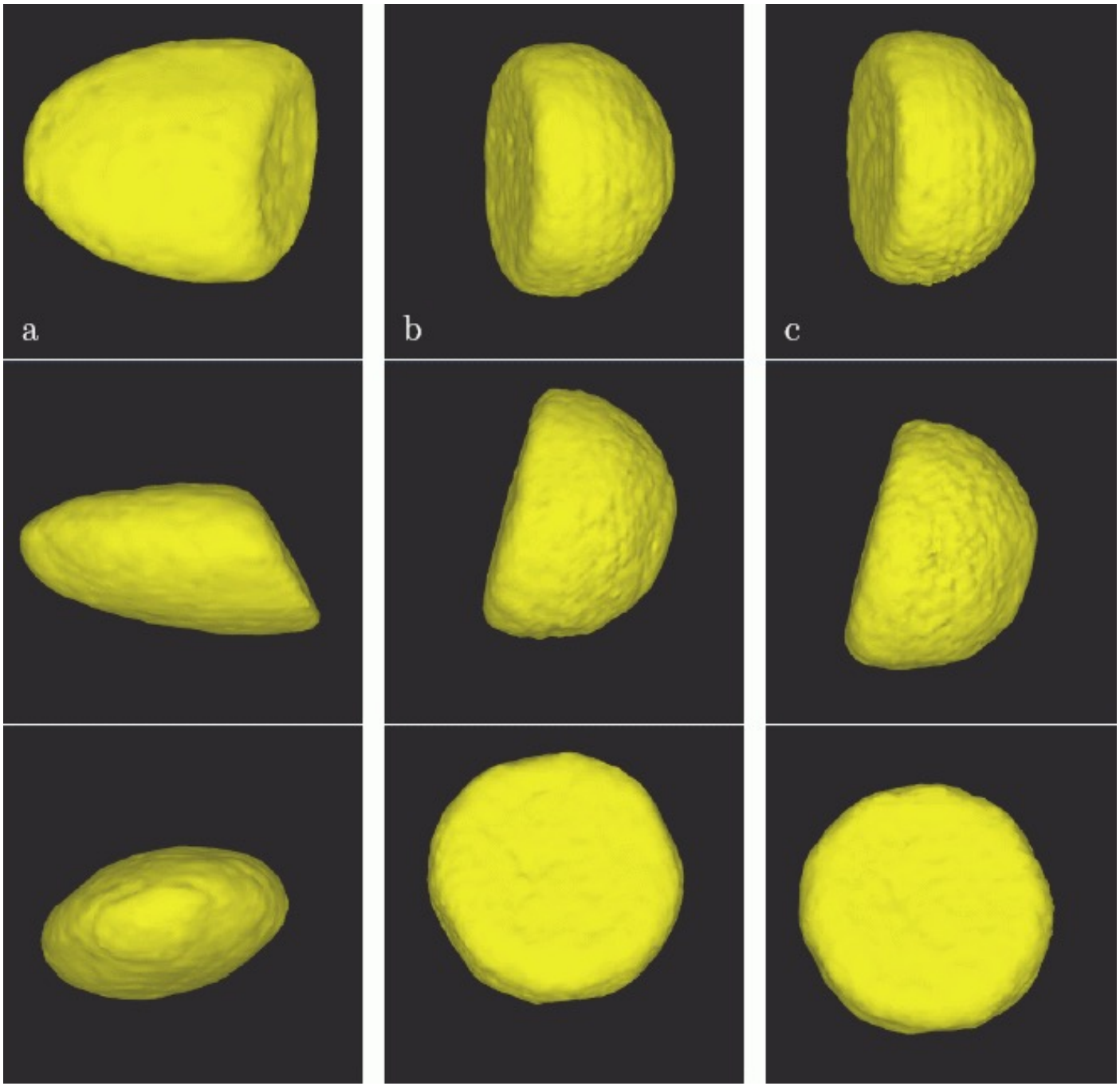
Learn shape of “tight” support



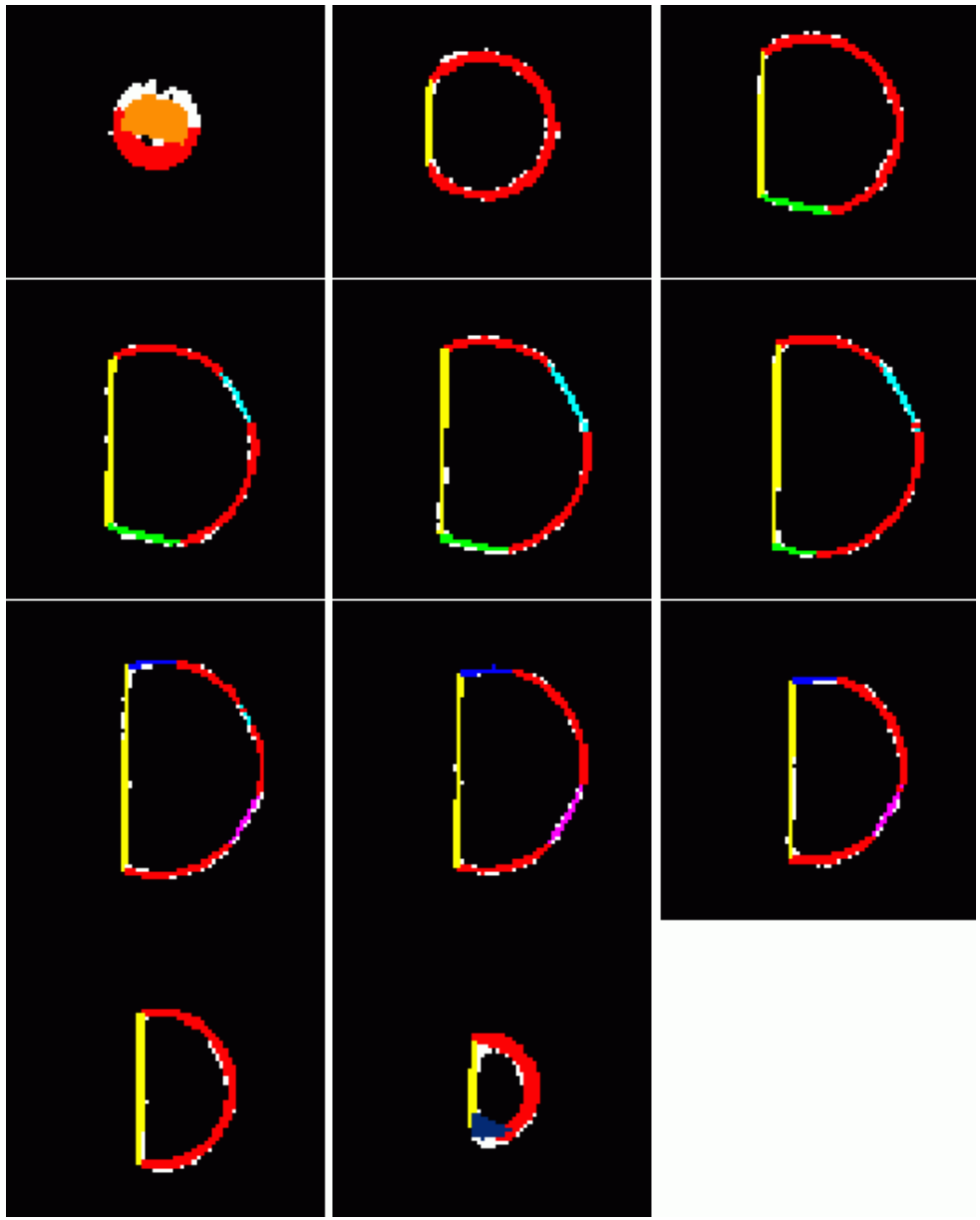
Then refine amplitude *and* phase





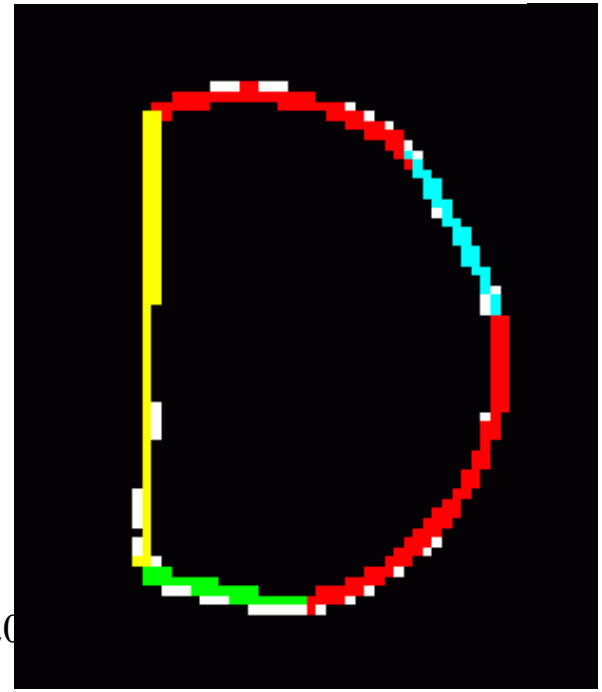

a
b
c

Fitting to facetted shape

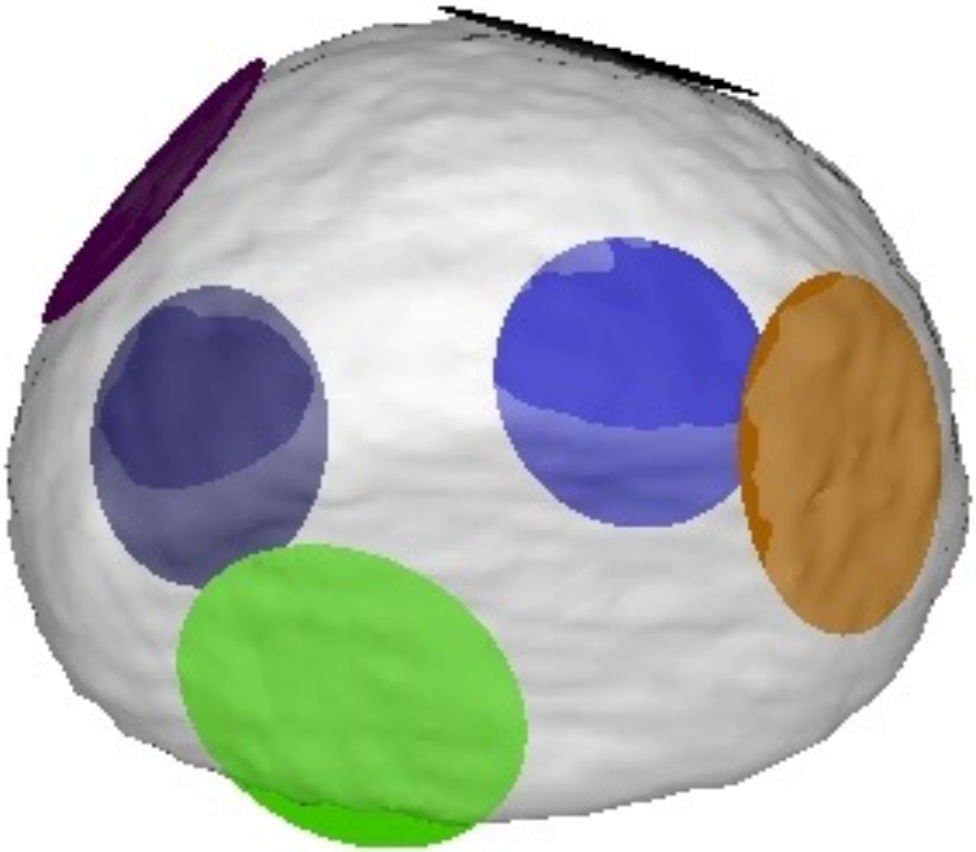


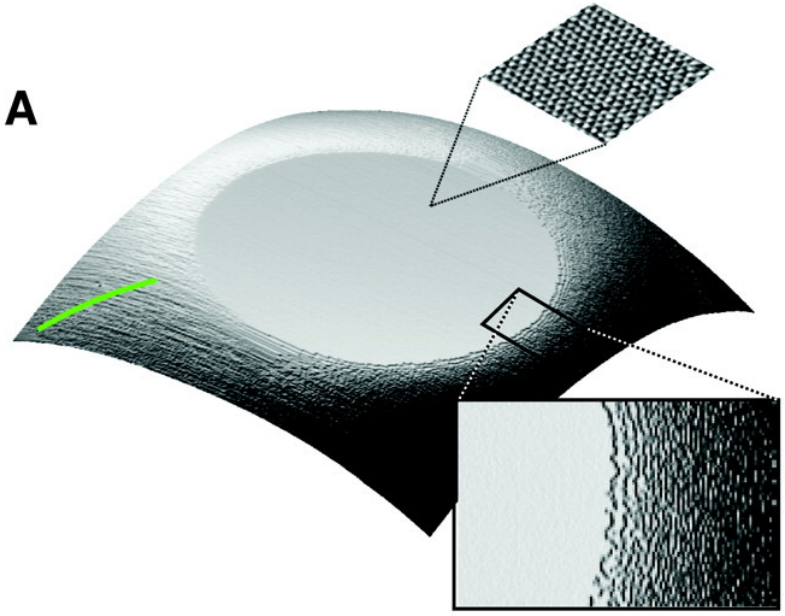
	$\|R\|$		P0	P1	P2	P3	P4	P5	P6
	9.4	P0	0	85	149	79	134	106	71
	25.7	P1		0	123	164	83	76	102
	25.1	P2			0	72	67	74	110
	25.9	P3				0	111	106	76
	25.4	P4					0	113	68
	25.4	P5						0	176
	26.0	P6							0 0

Angles between facets



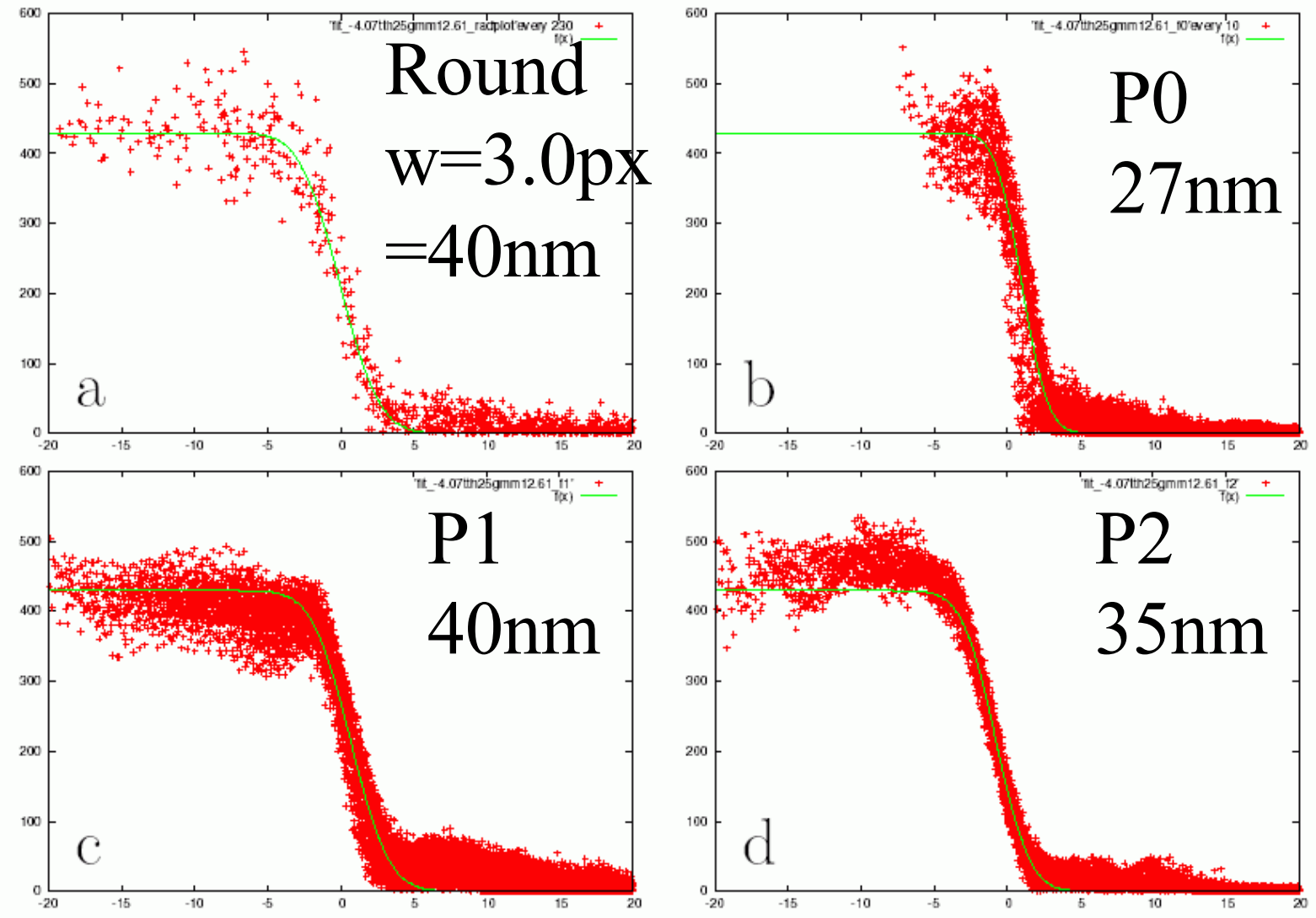
Facets of Equilibrium Crystal Shape



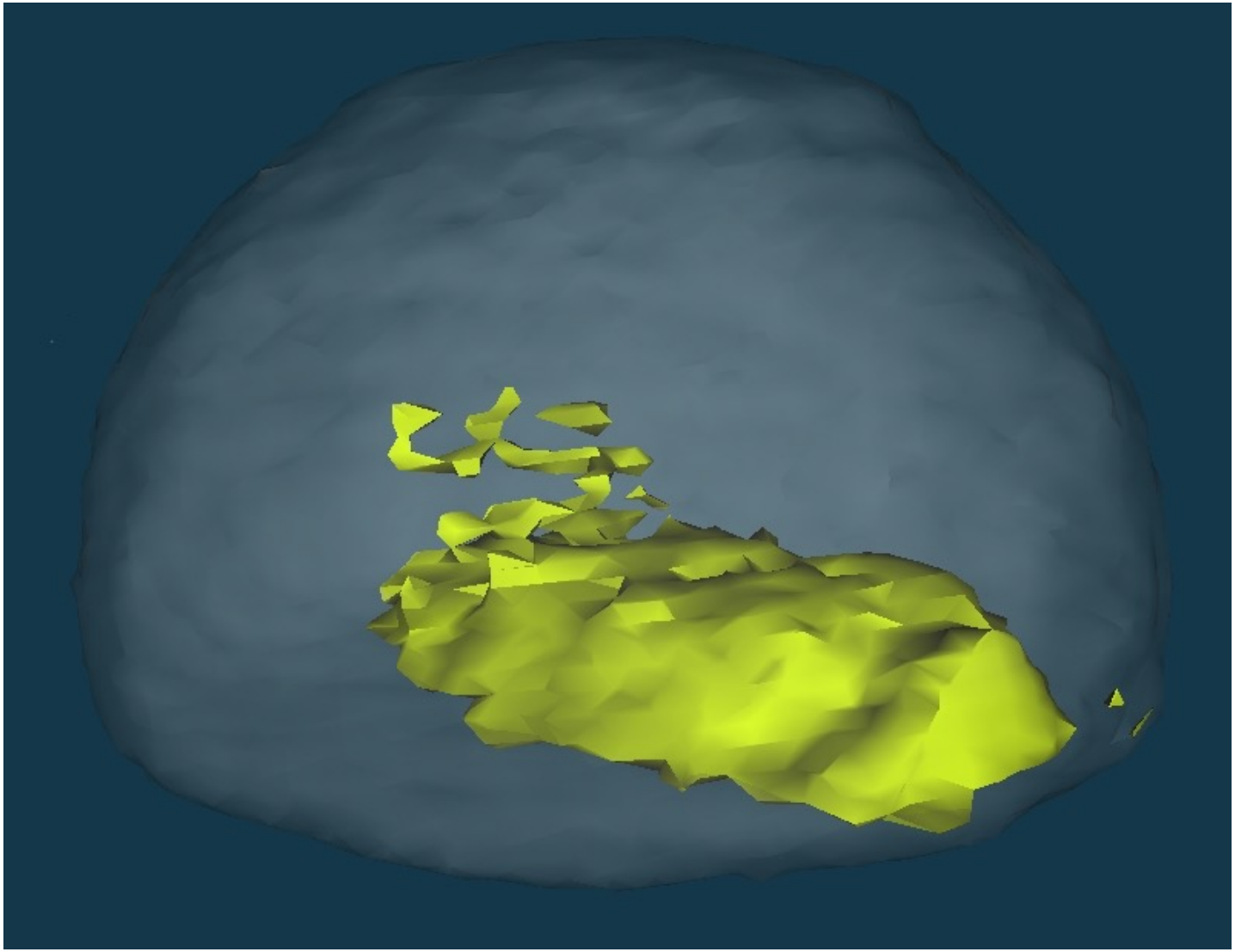


Thurmer K, Williams E, Reutt-Robey J
Science **297** 2033 (2002)

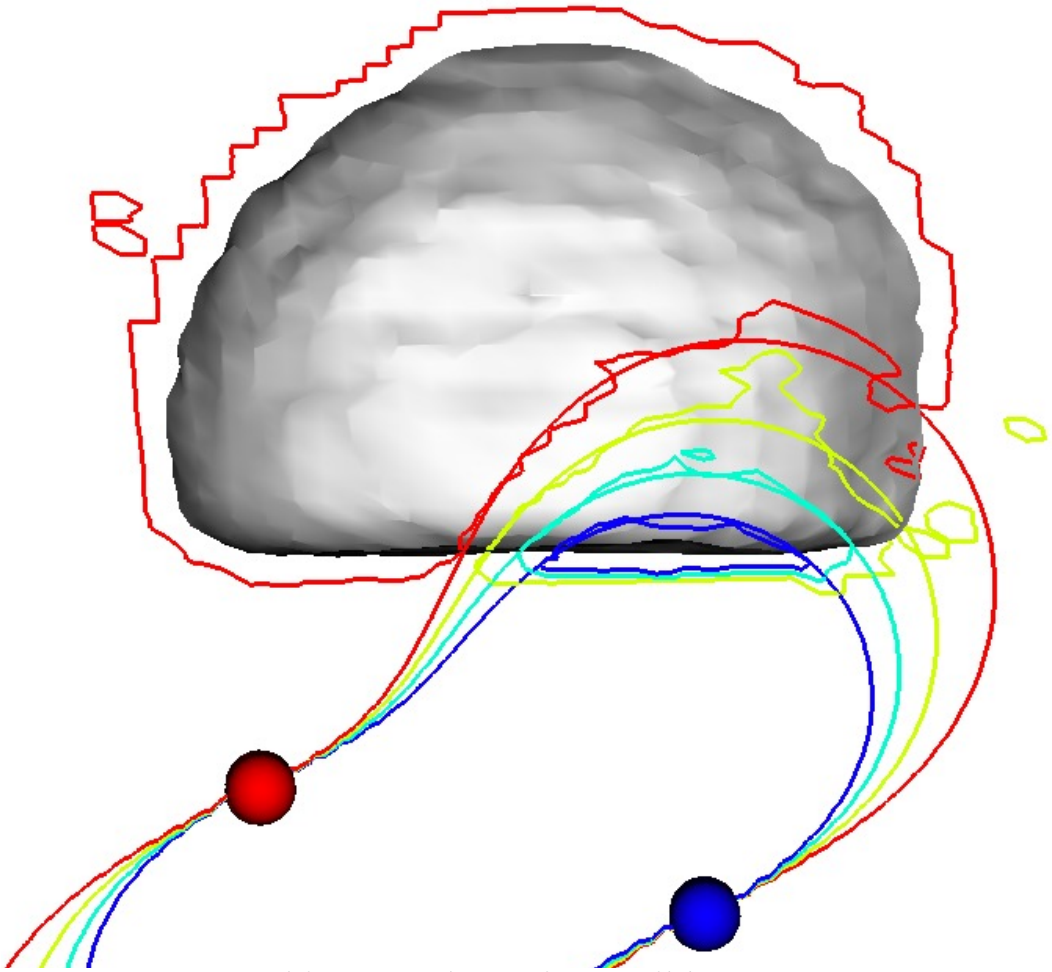
Density distribution across surface

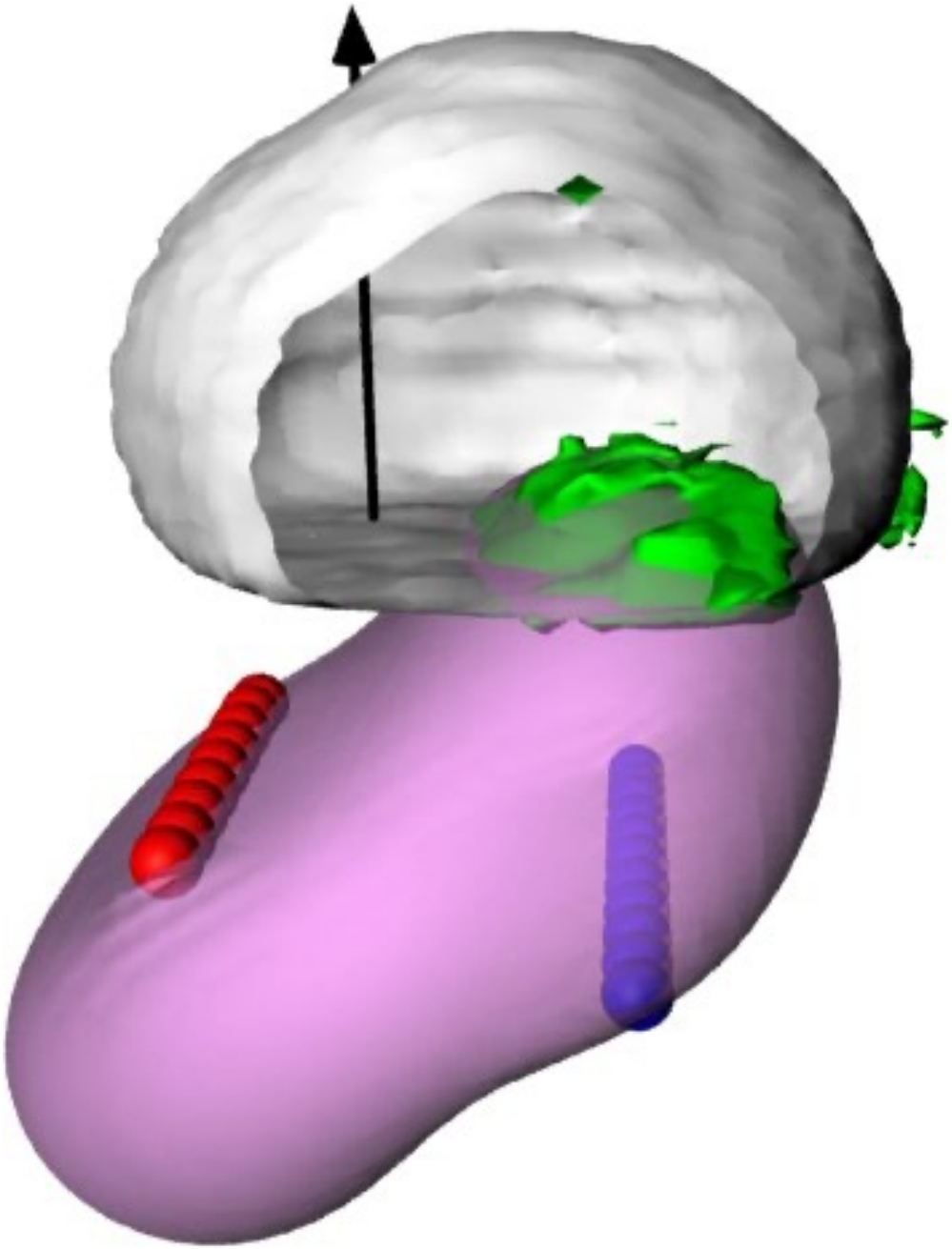


Modeling of 3D Phase Bump



Field lines of Point Charges

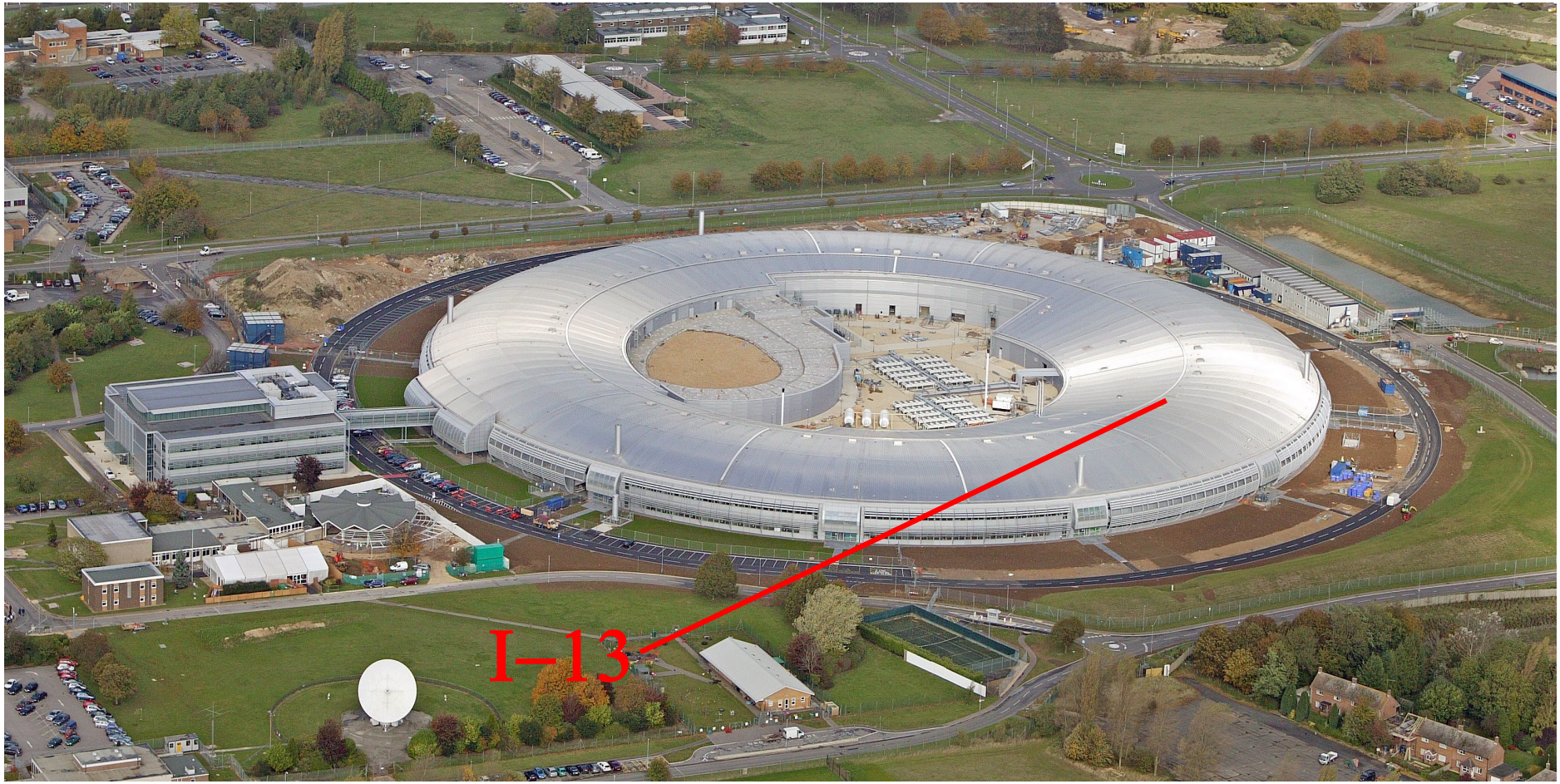




New Beamline Opportunities

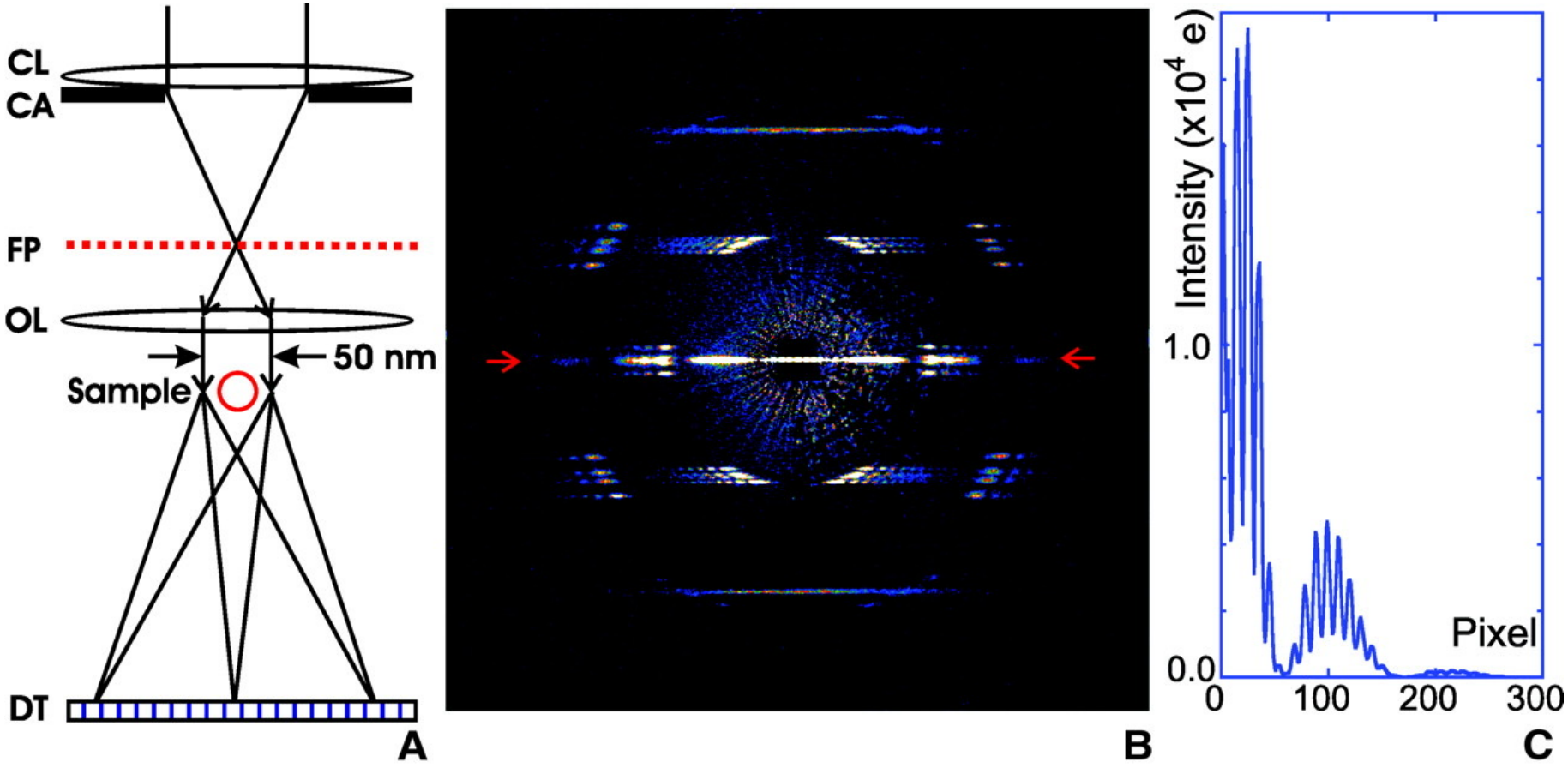
- I-13 phase 2 “Coherence” beamline at Diamond
- Principal Beamline Scientist in Aug 2006
- First Users in 2010-11
- Three branches on canted undulators:
  - USAXS and XPCS
  - Coherent Diffraction, lensless imaging
  - Full-field Imaging with hard X-rays

Diamond Light Source, Oct 2005



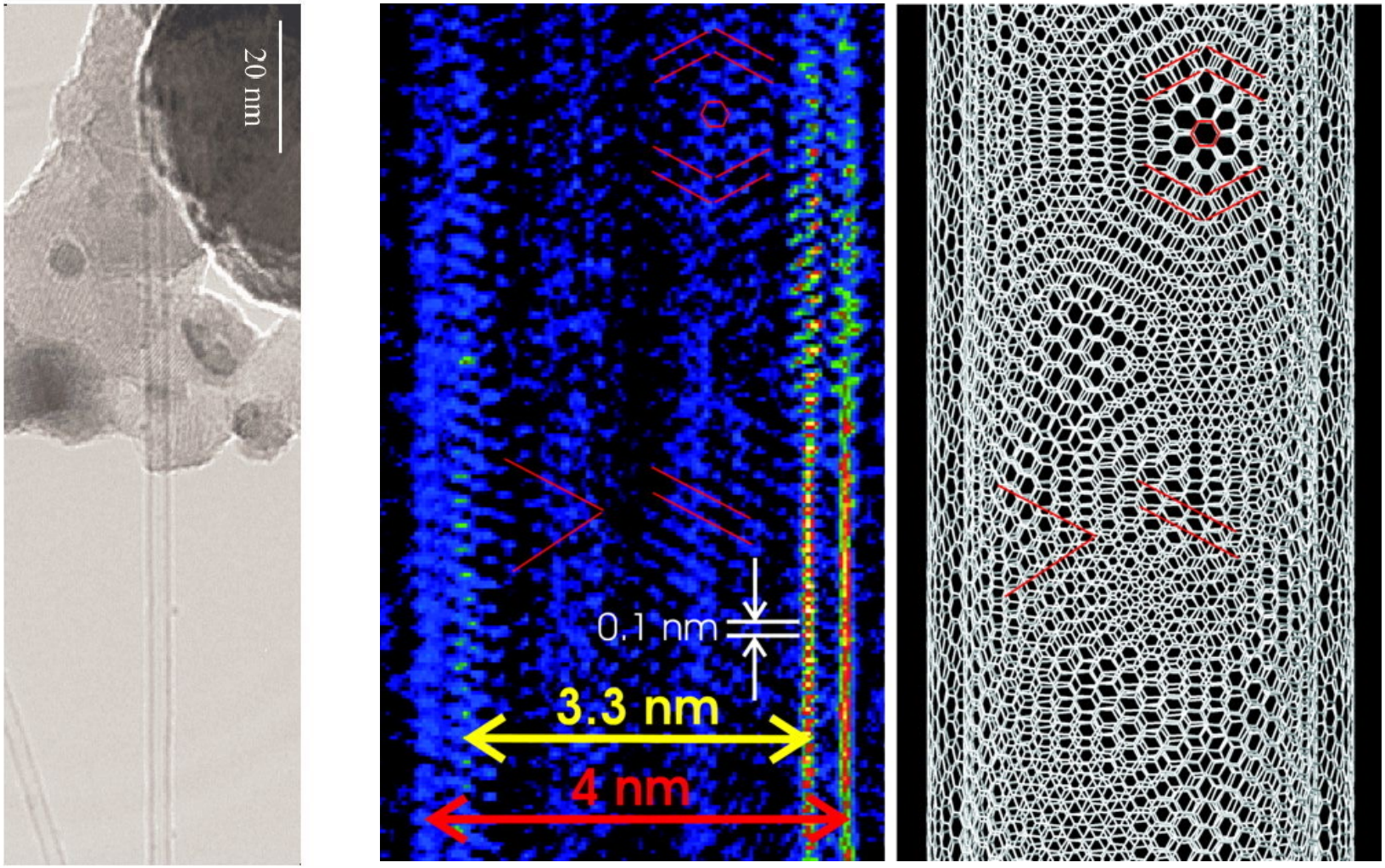
Electron Diffraction from C-nanotube

Jim Zuo et. al. Science 300 1419 (2003)

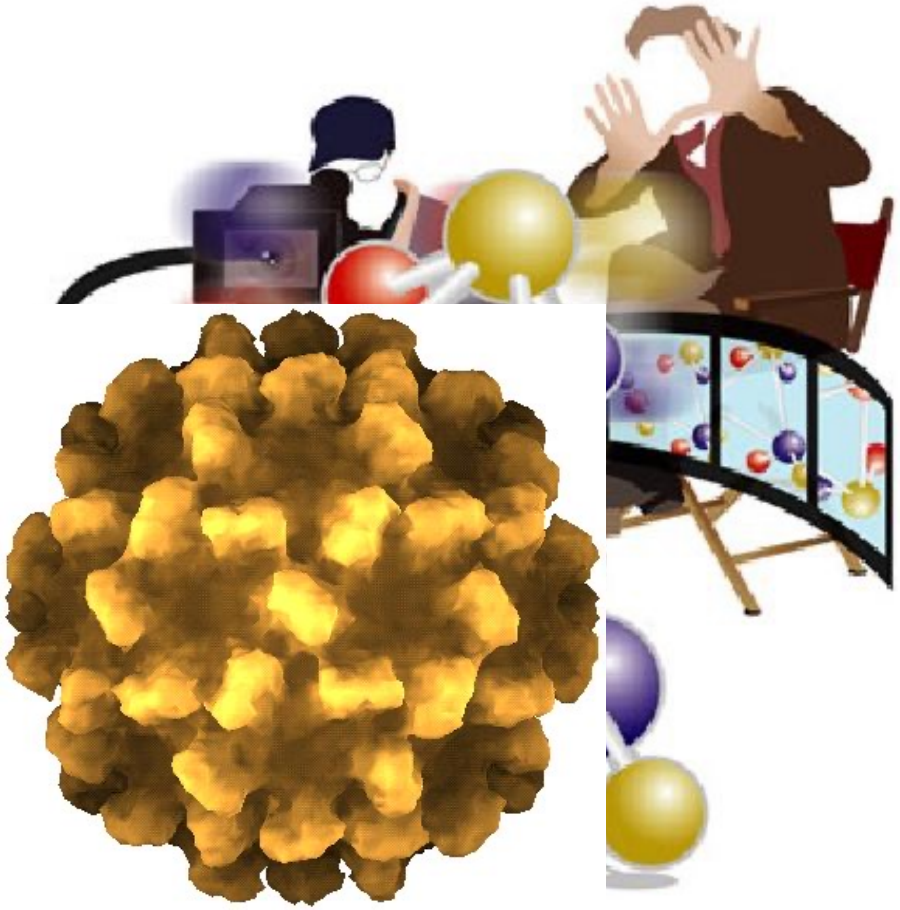


Images of DW C-nanotube

Jim Zuo et. al. Science 300 1419 (2003)



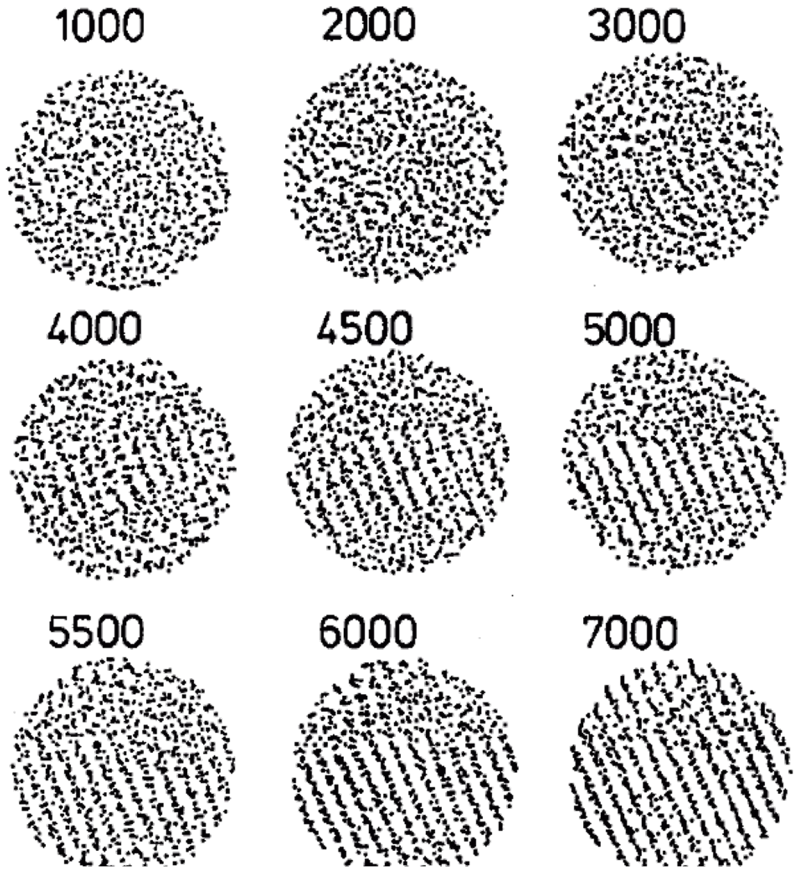
Molecular Movies using XFEL

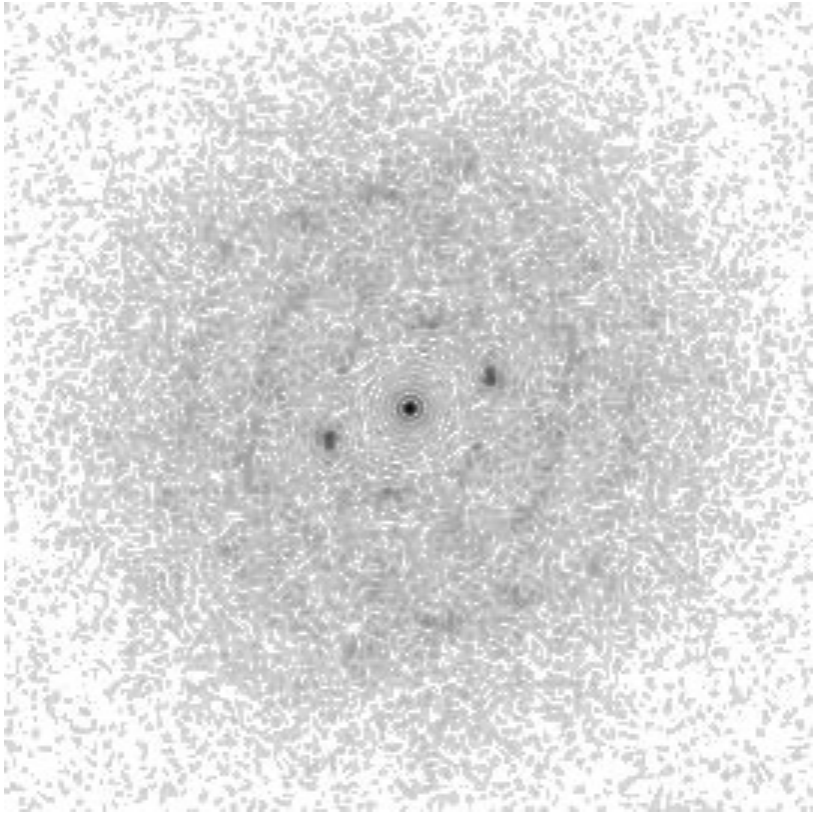


MD simulation of freezing

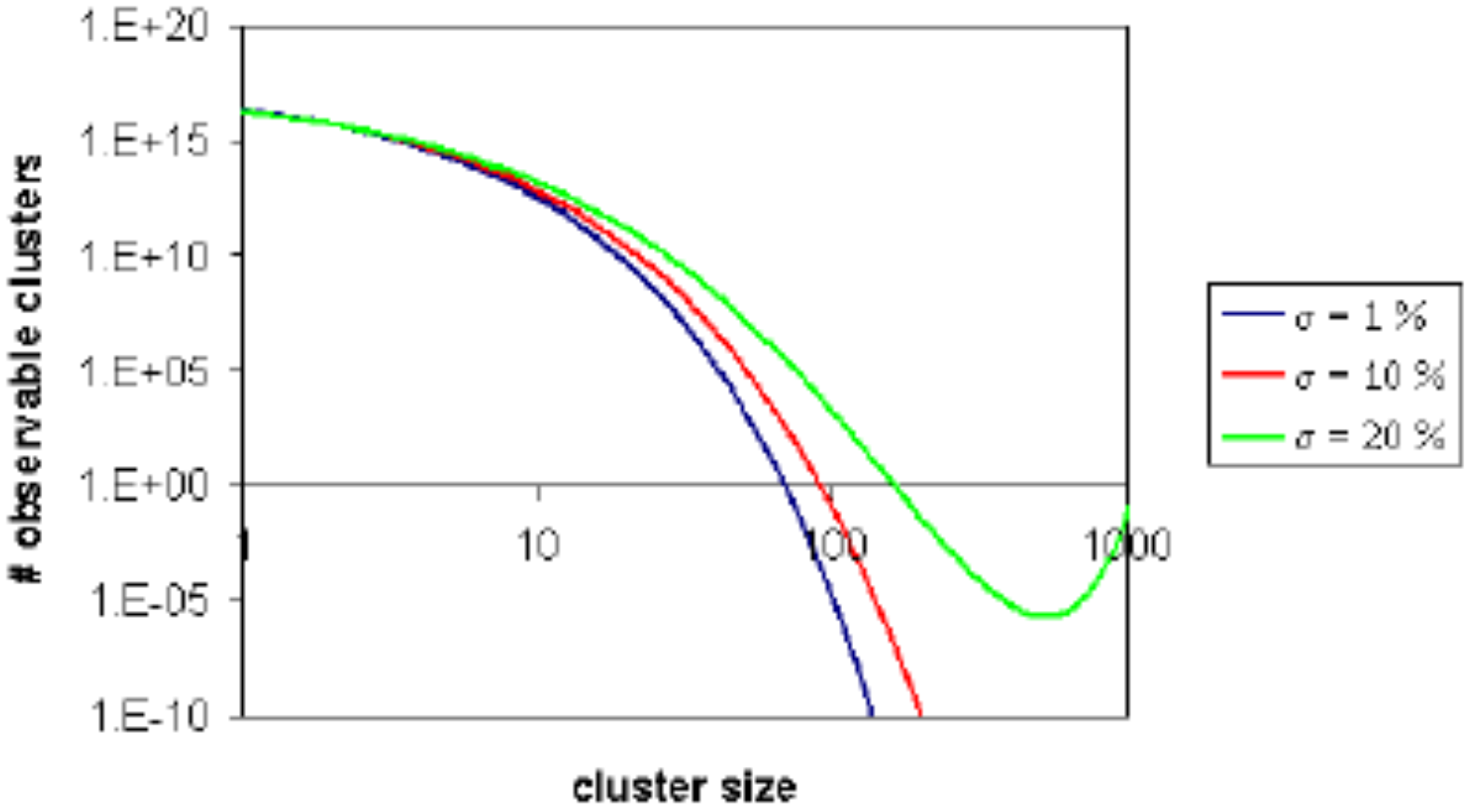
LJ liquid of 864 atoms. Time steps after T-Jump

S. Nose and F. Yonezawa, JCP 84 1893 (1986)





Nucleation cluster size distribution



Conclusions and Outlook

- Internal structure of Au Nanocrystals
- 3D imaging practical for nanocrystals
- Phasing by computation instead of lens
- Strain fields in Pb imaged from pattern asymmetry
- Atomic resolution with electron diffraction
- Structure of fluctuations using ERL