Retrieval and Interpretation of Complex Images of Nanocrystals

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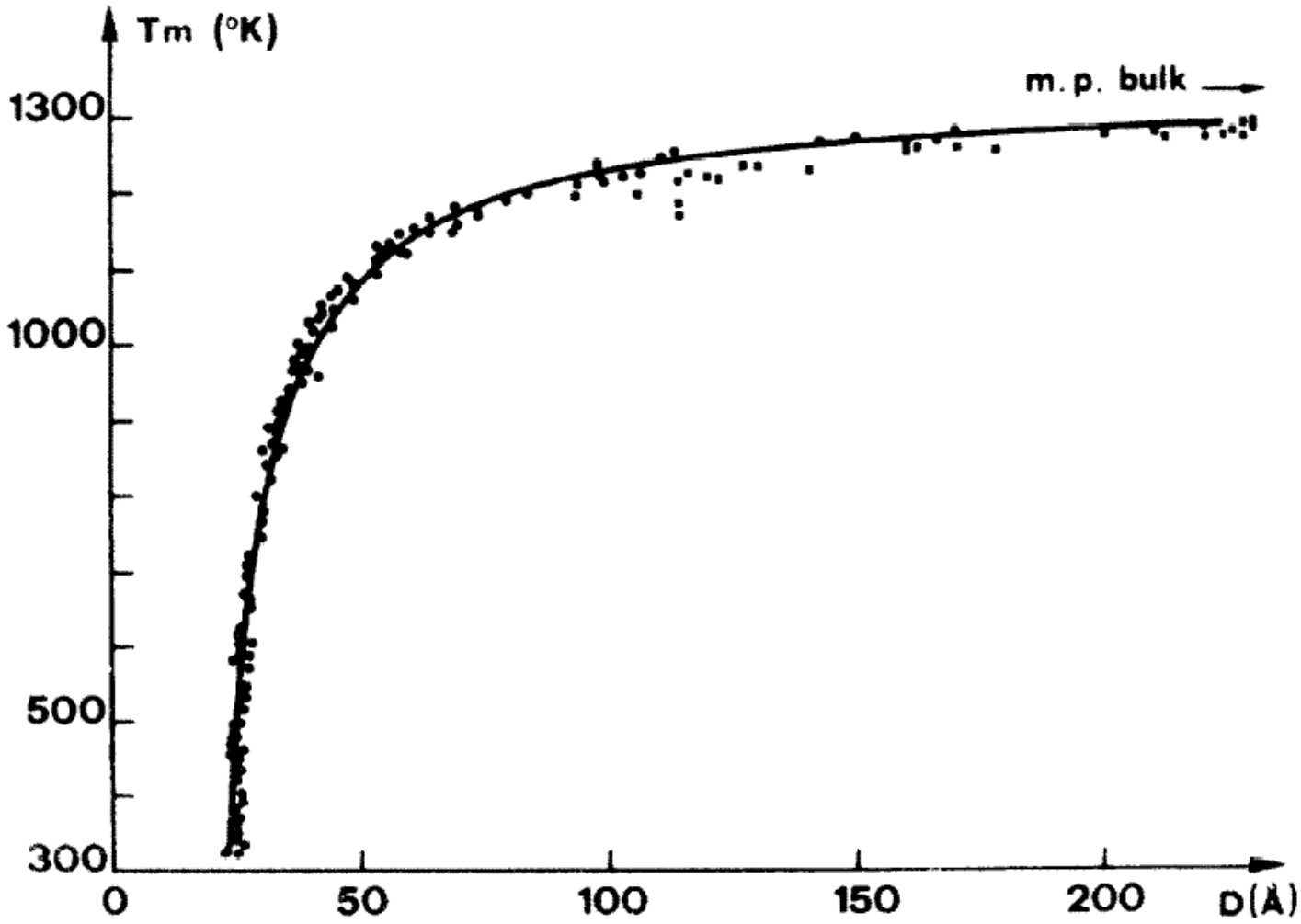
International Workshop on
Spectromicroscopy,
ICTP, Trieste, May 2006

Outline

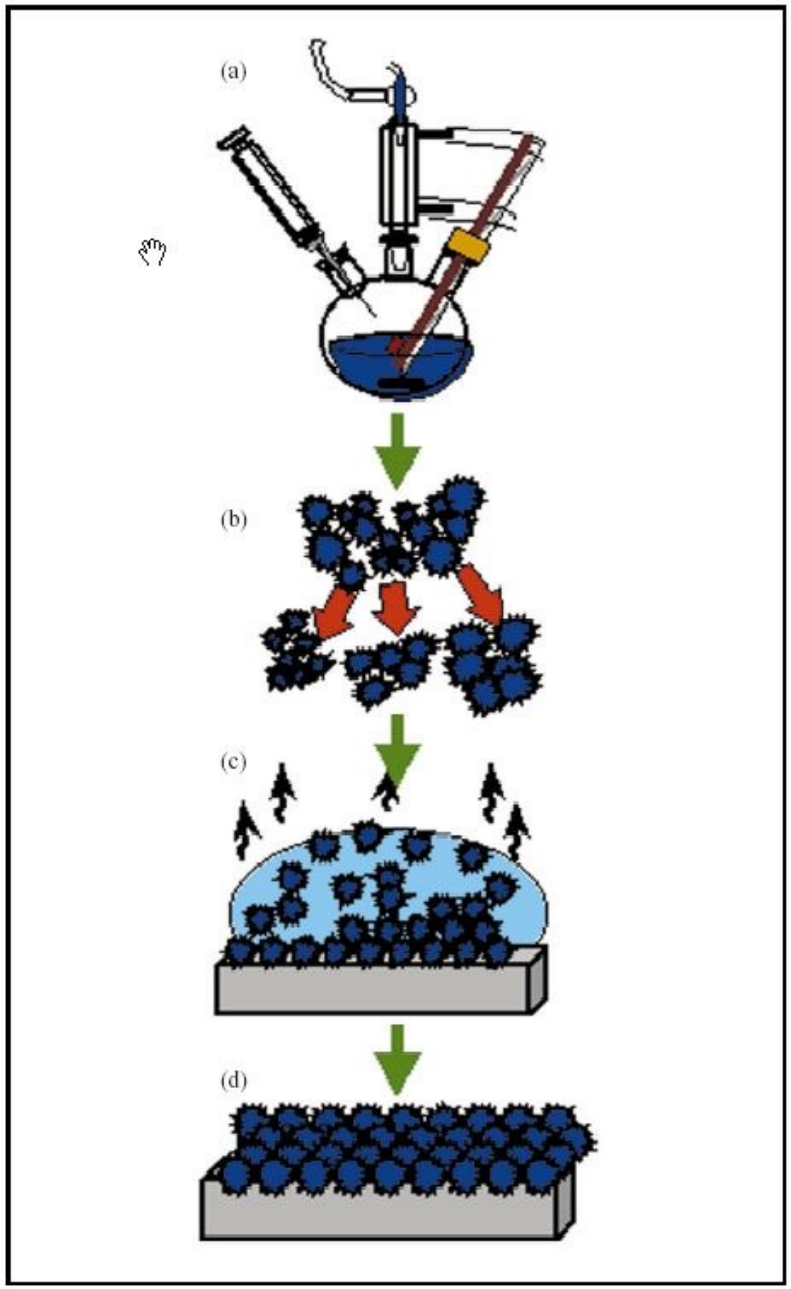
- Coherent X-ray Diffraction
- How to Solve the Phase Problem
- Nanocrystal Shapes
- Extension to Phase Objects

Size-dependent Melting of Au Particles

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

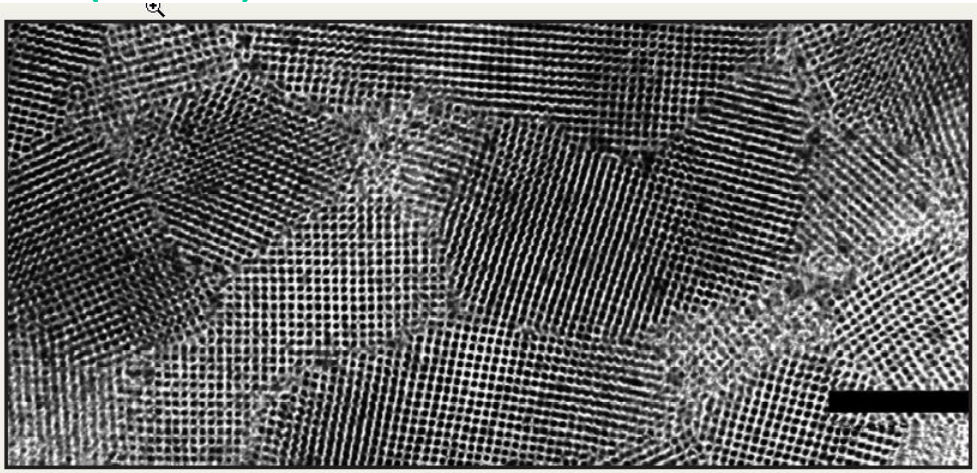


Chemical Synthesis of Nanocrystals

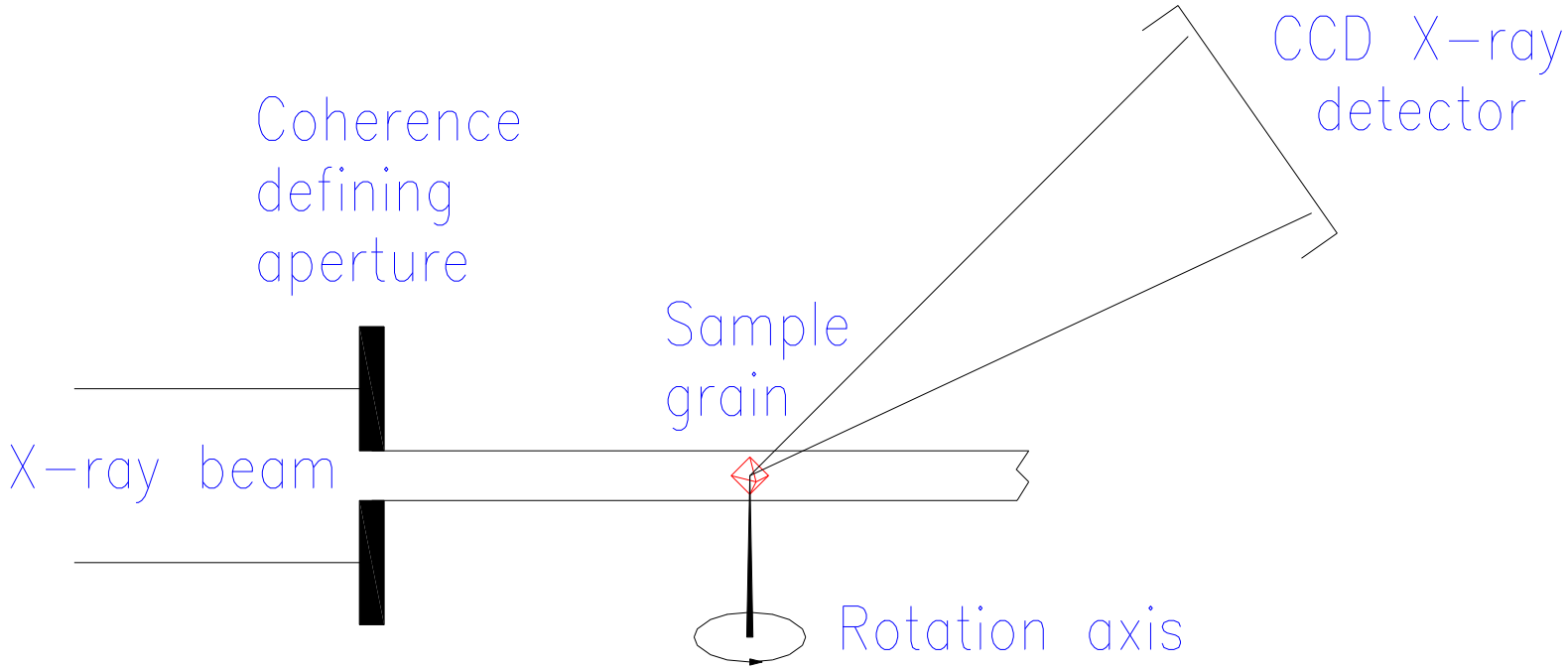


- Reactants introduced rapidly
- High temperature solvent
- Surfactant/organic capping agent
- Square superlattice (200nm scale)

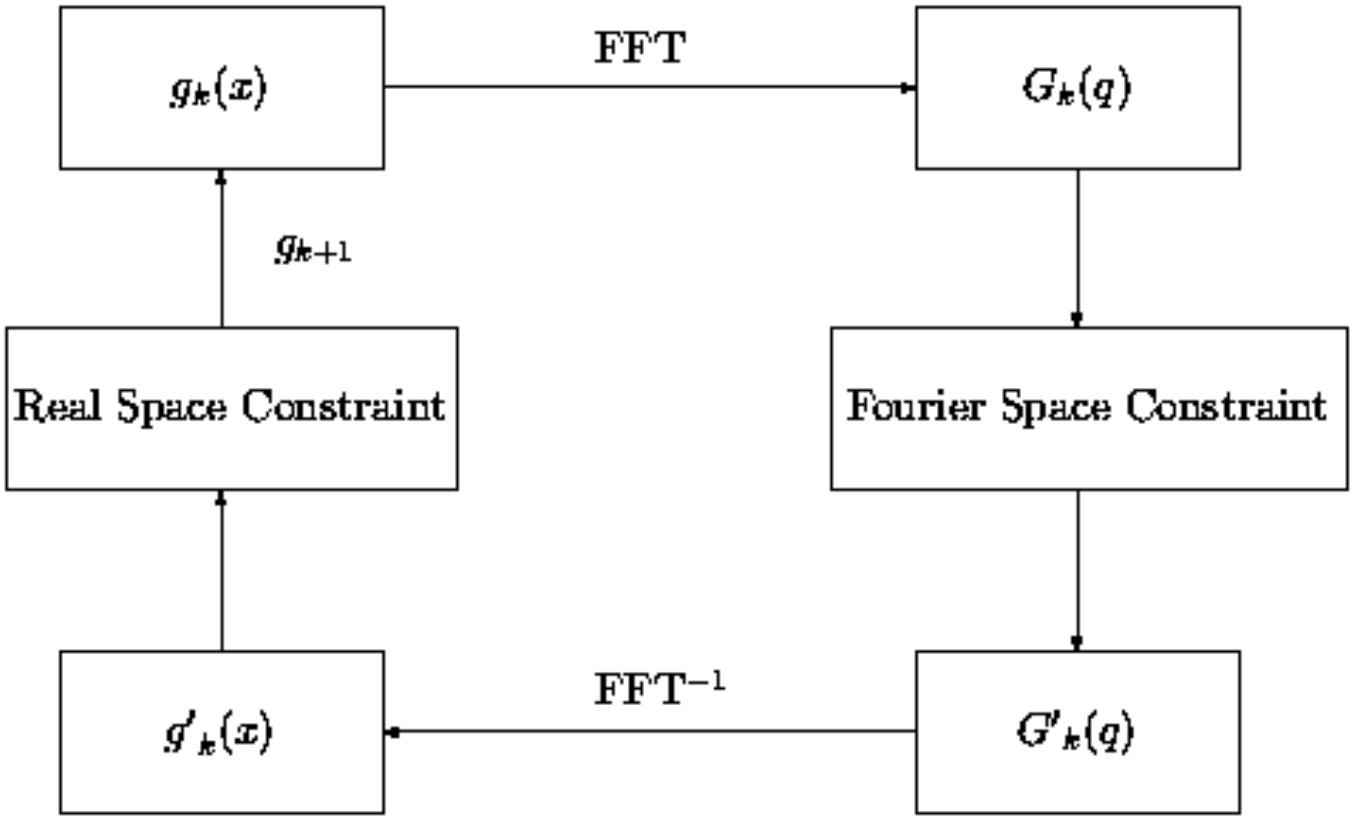
C. B. Murray, IBM J. Res. & Dev. **45** 47 (2001)



Lensless X-ray Microscope

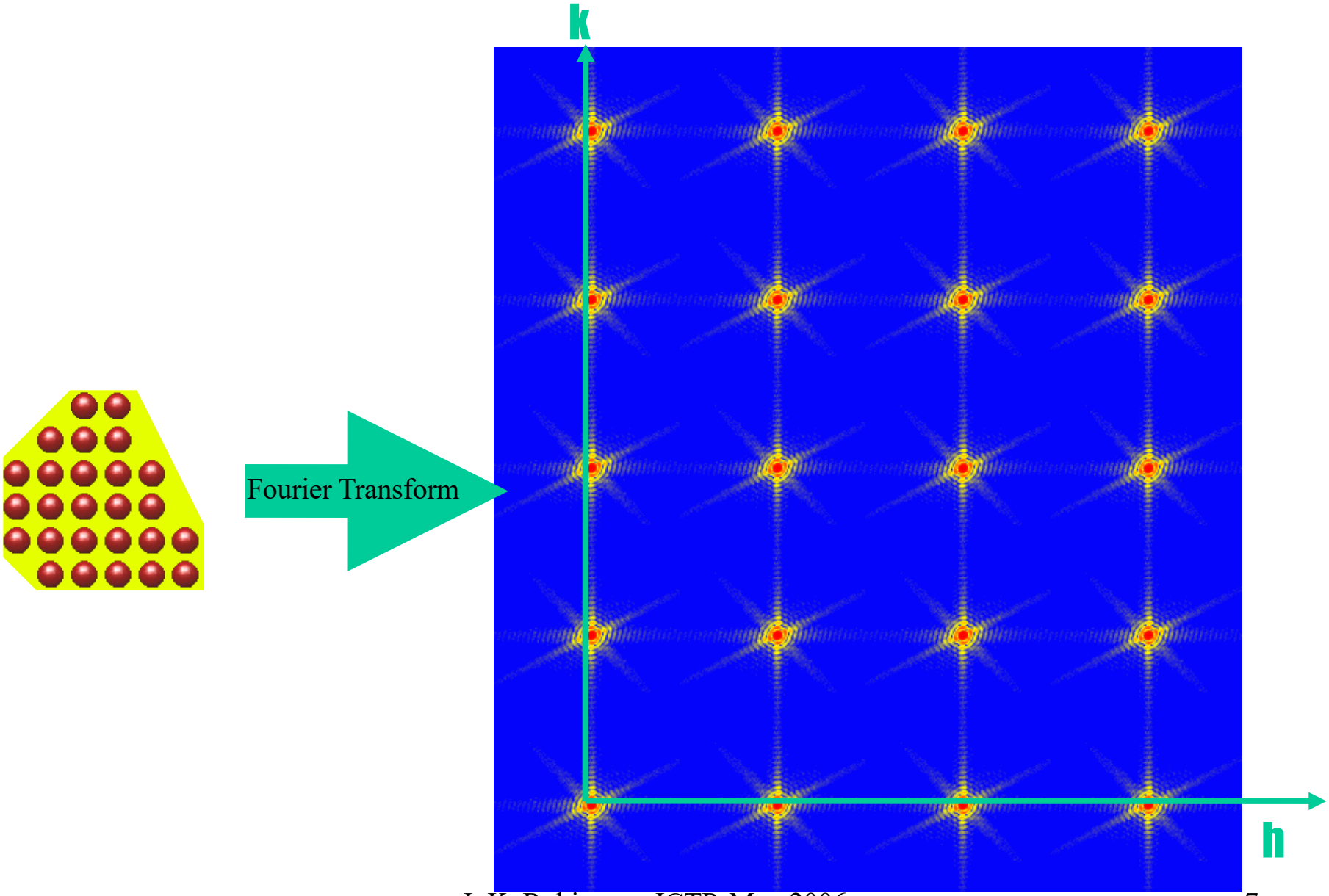


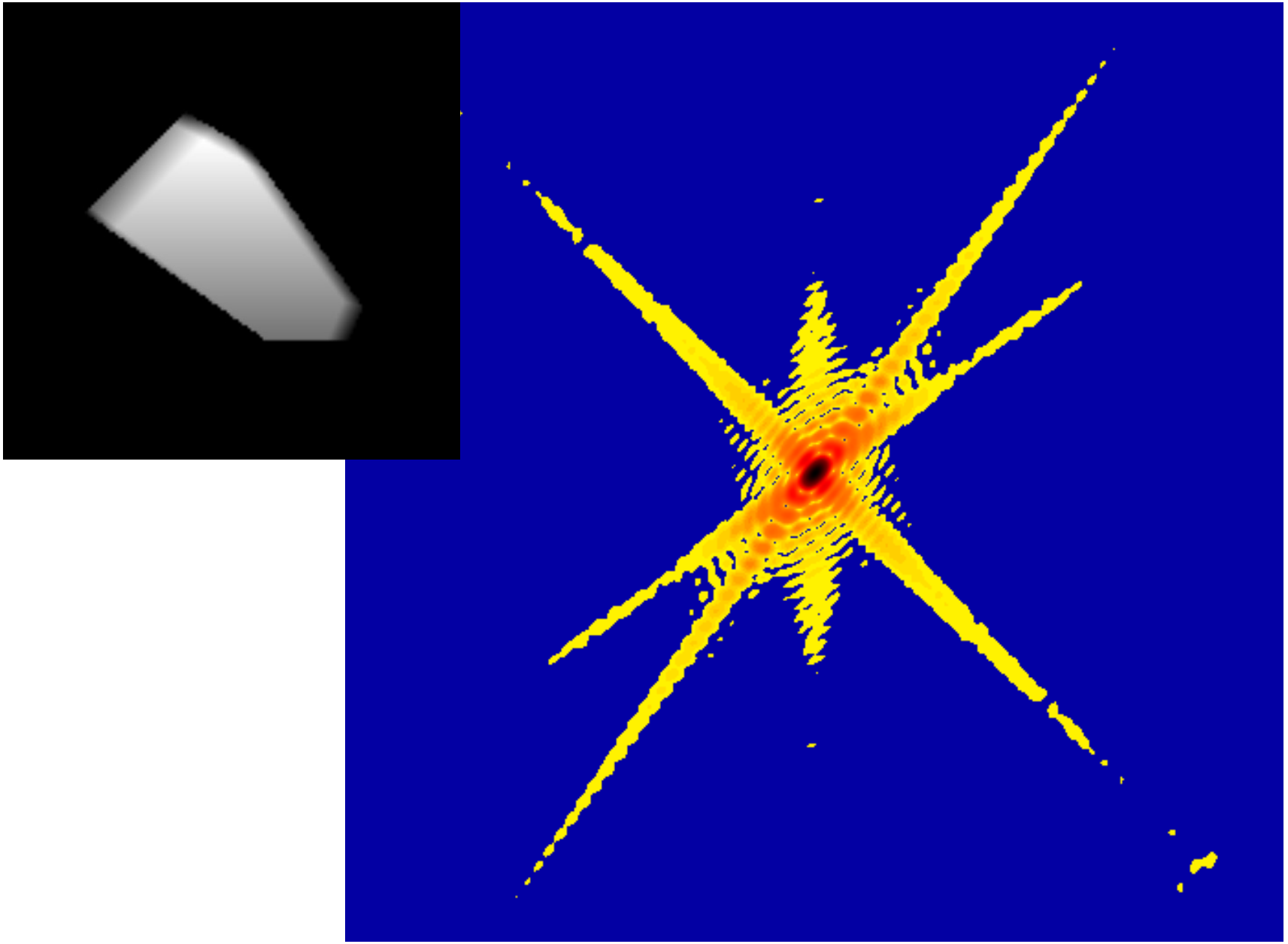
Generic "Error Reduction" method



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

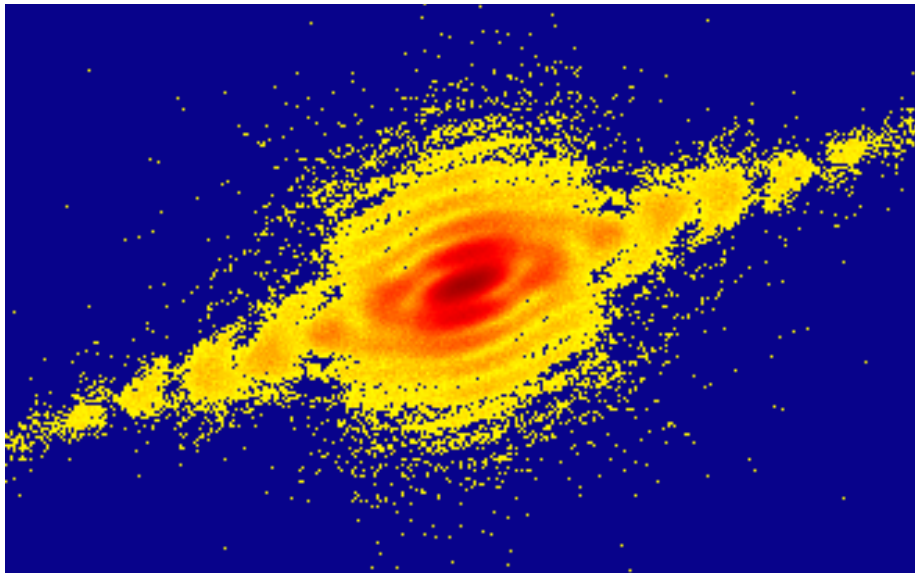
Coherent Diffraction from Crystals

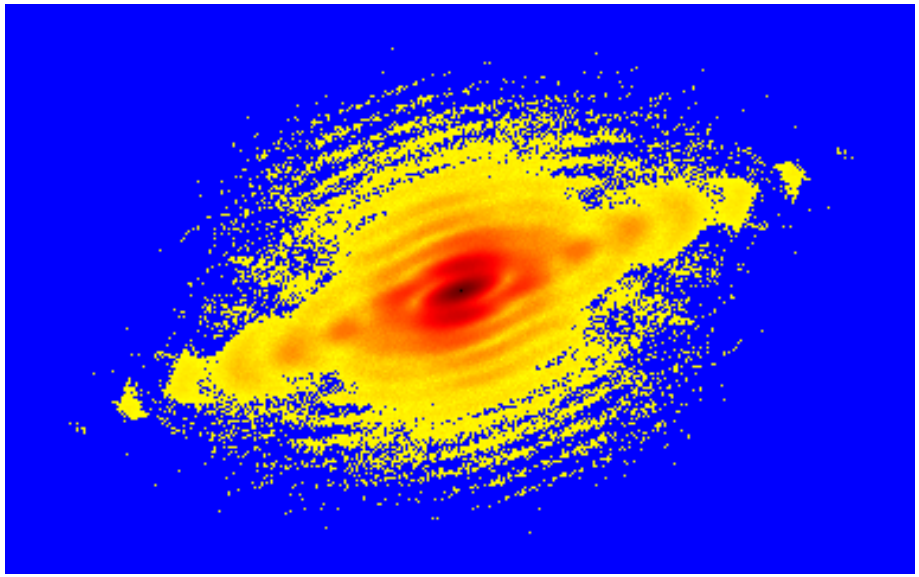


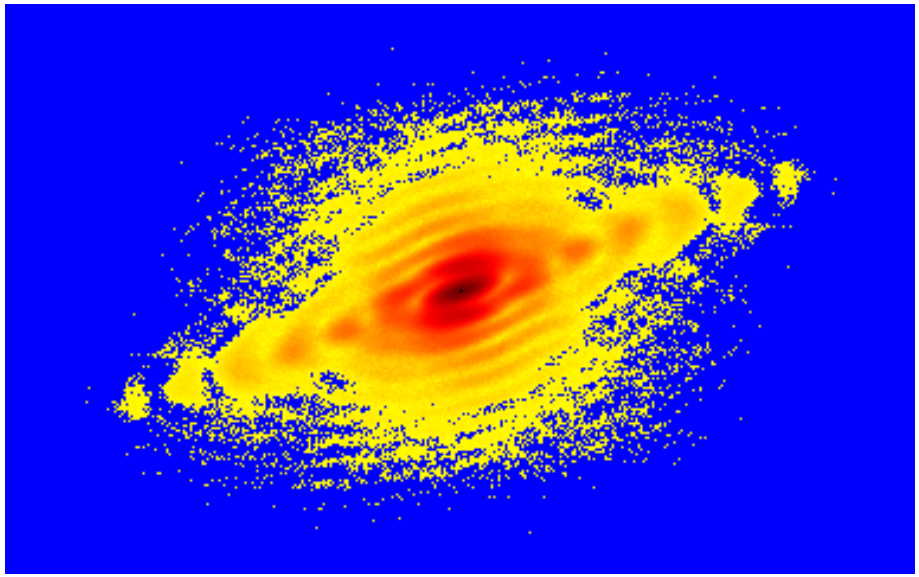


Symmetrized Data and two best fits

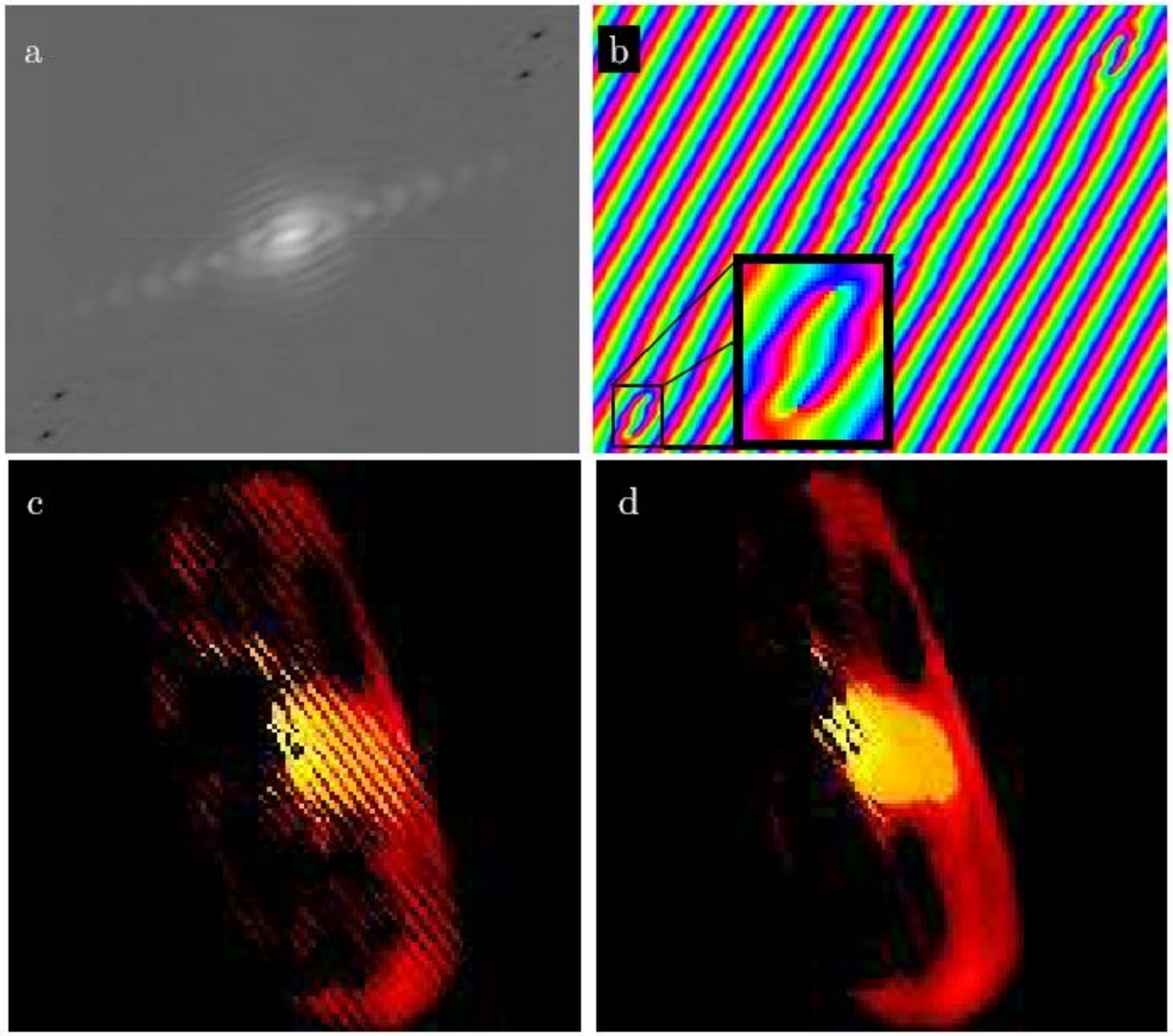
Chisq=0.0005



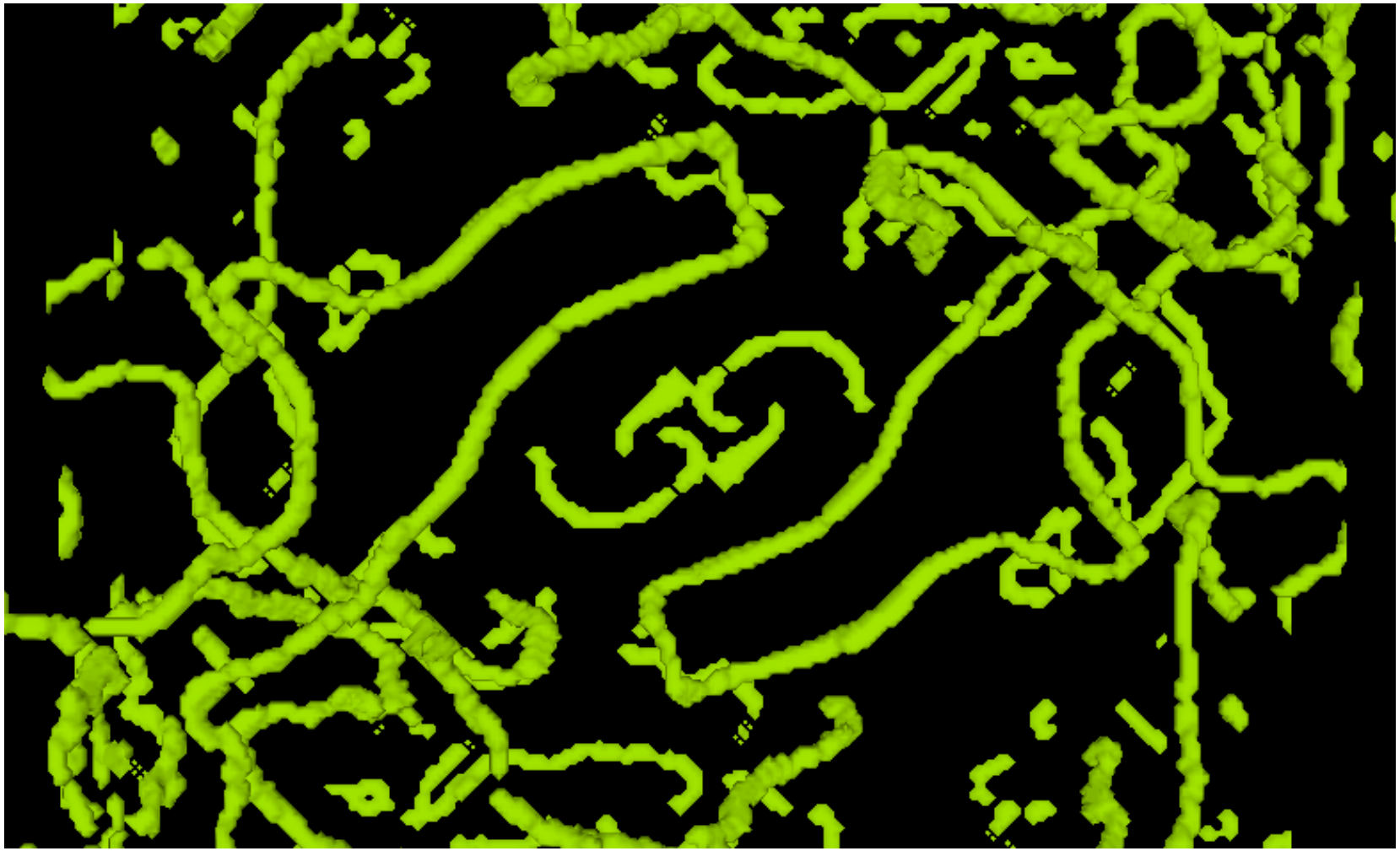




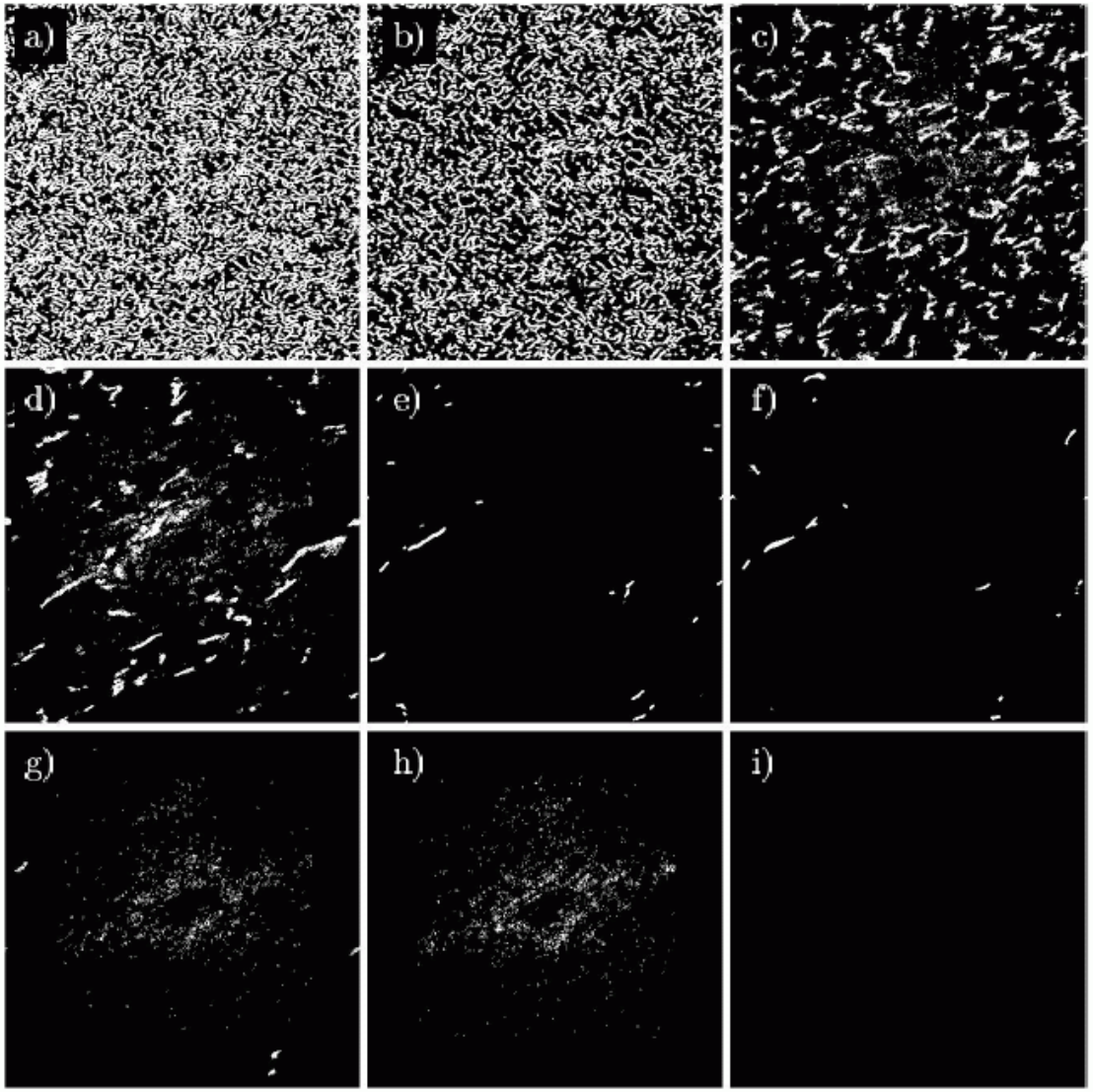
Phase Vortices and patching



‘Vortices’ Form Loops in 3D

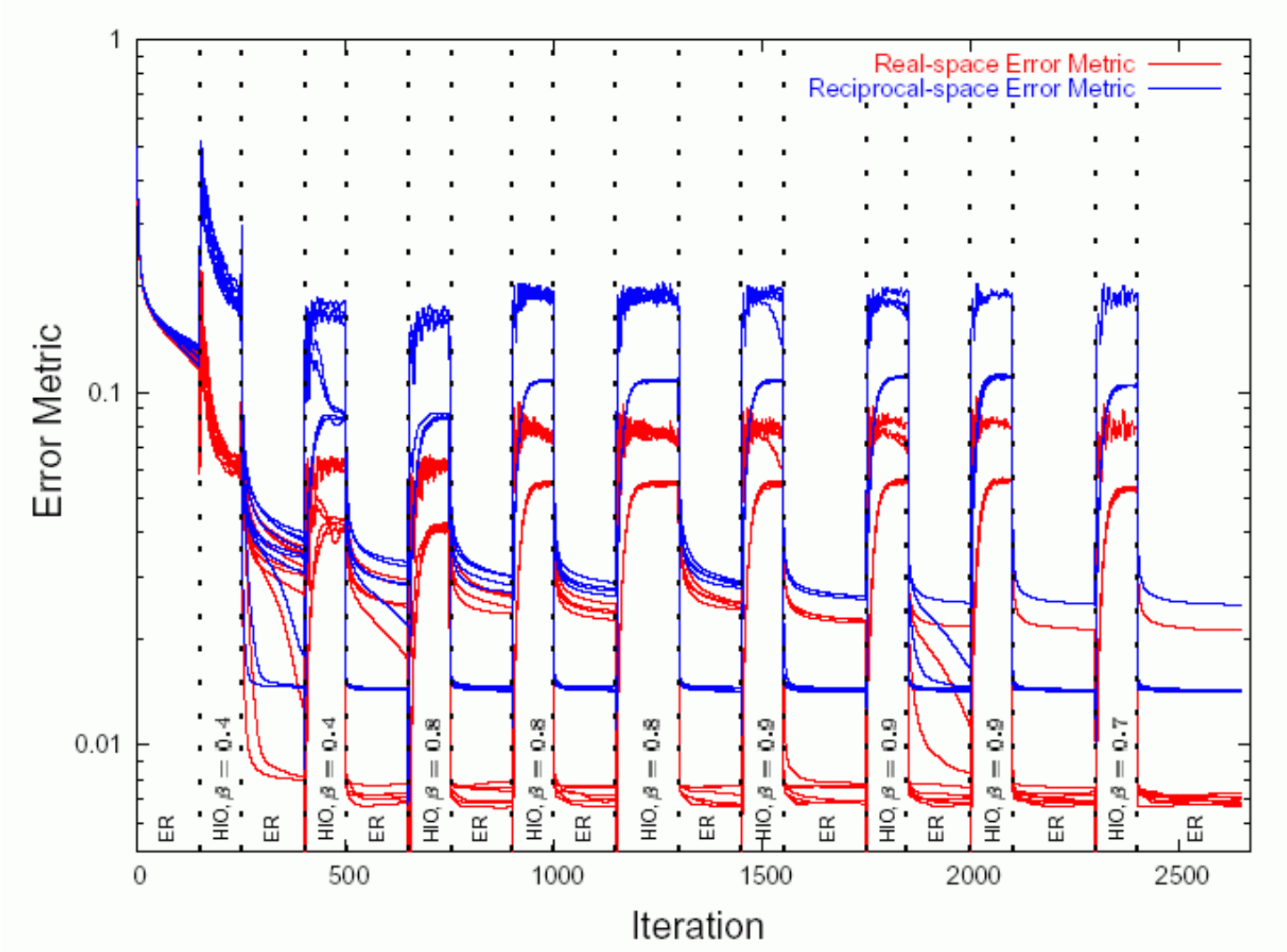


Clearing of Vortices during HIO

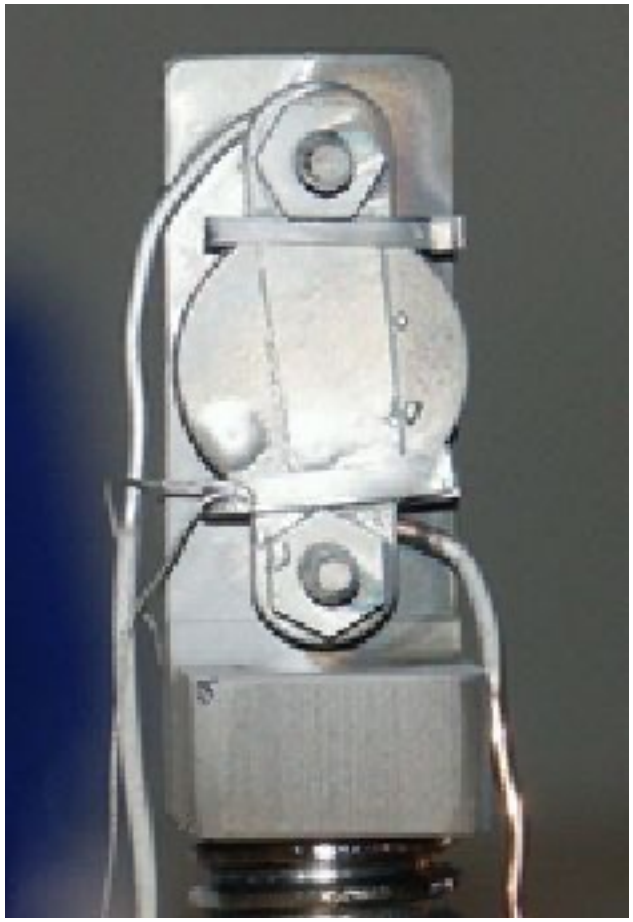


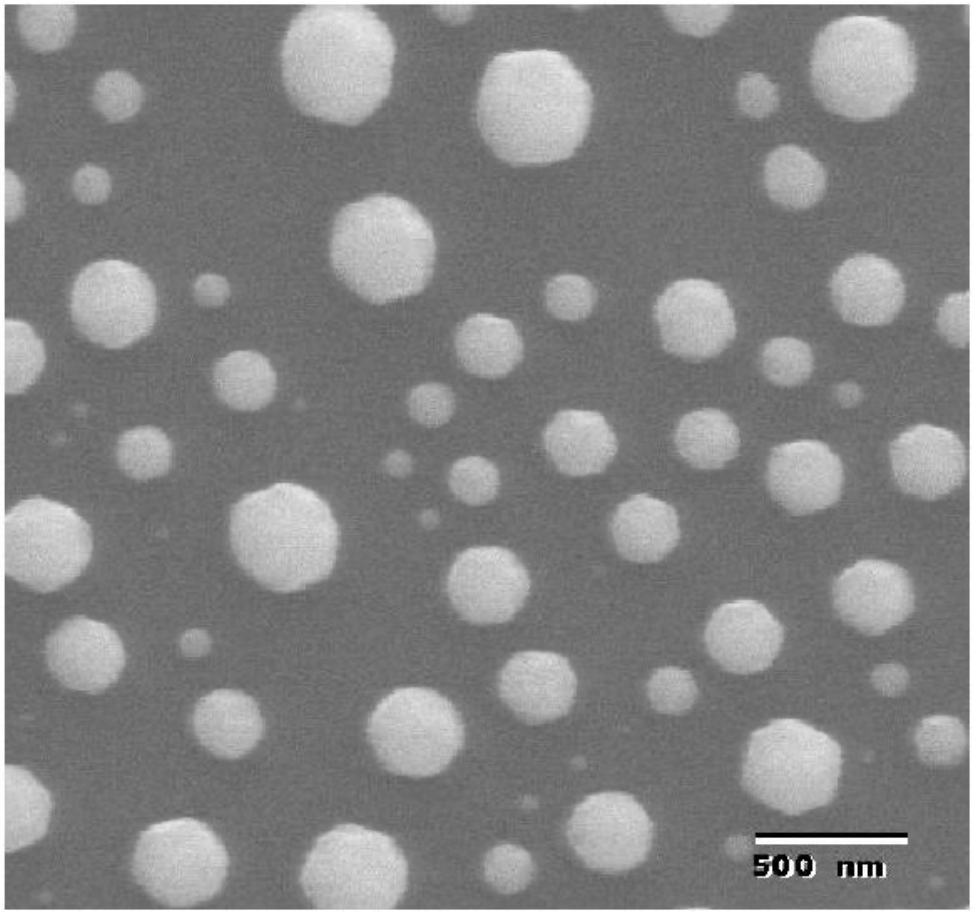
ER ER HIO
HIO ER ER
HIO HIO ER

Progress of Phase Retrieval

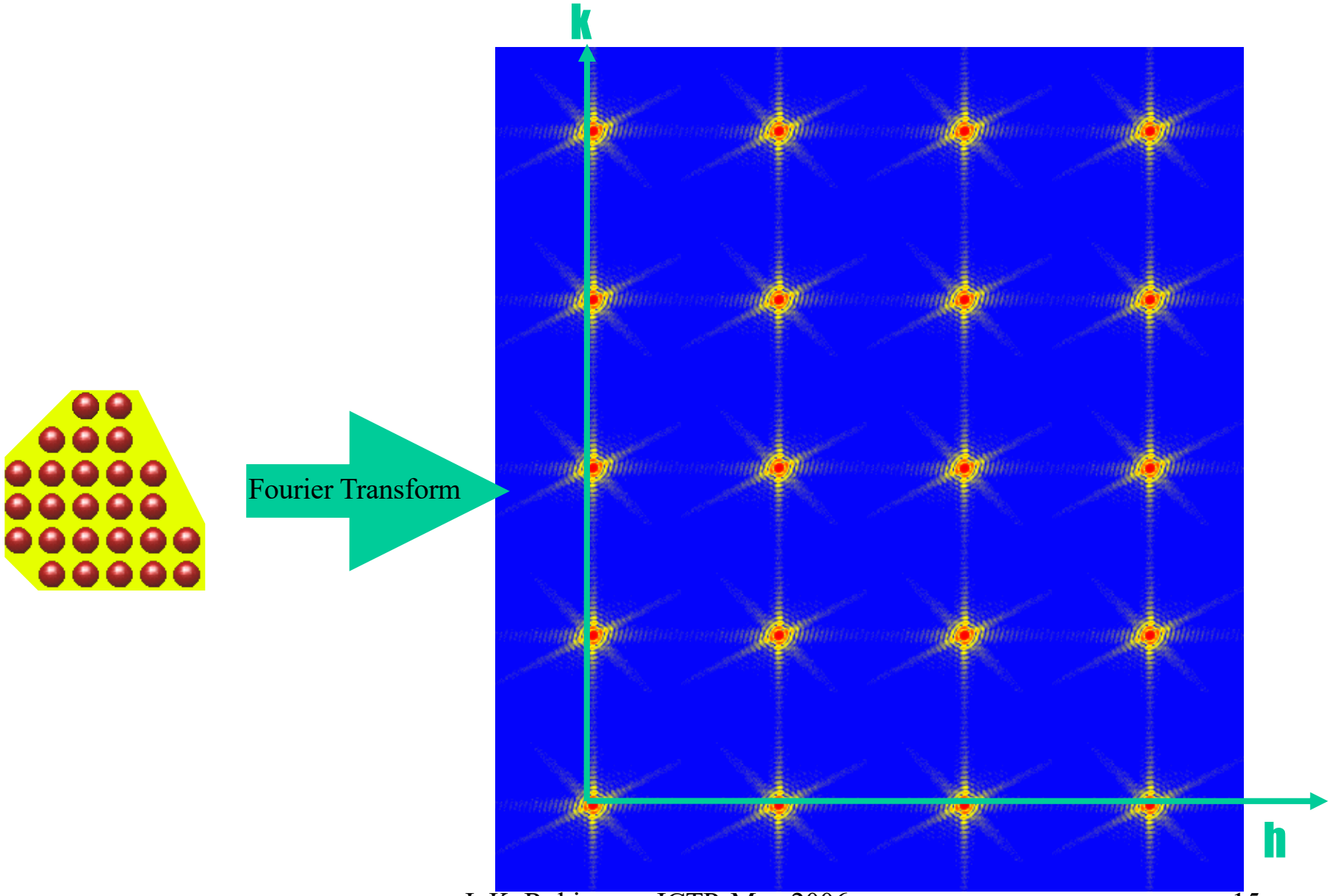


In situ growth of Pb crystals





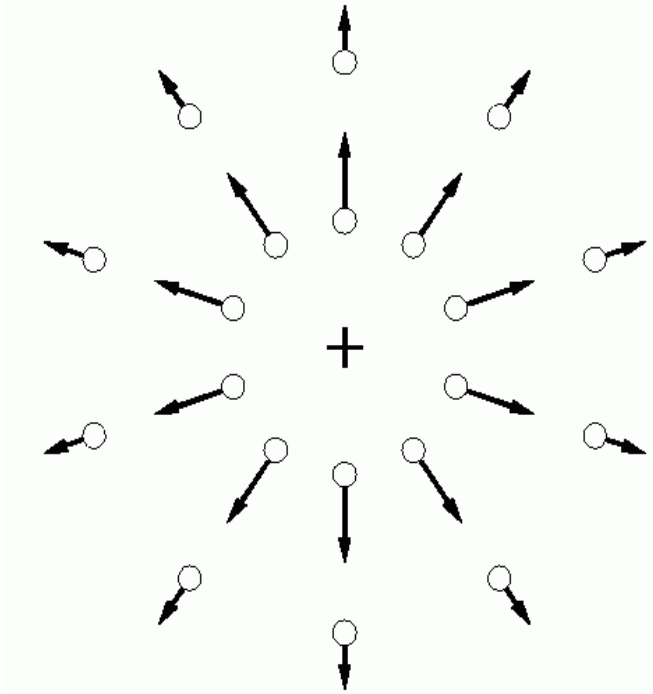
Coherent Diffraction from Crystals

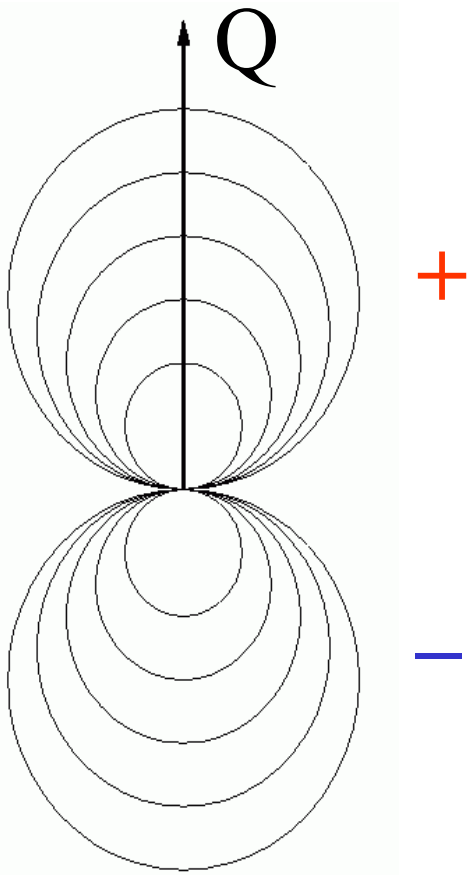


Diffraction by Strain of Point Defect

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

Imaginary density





Good statistics, 3D diffraction data

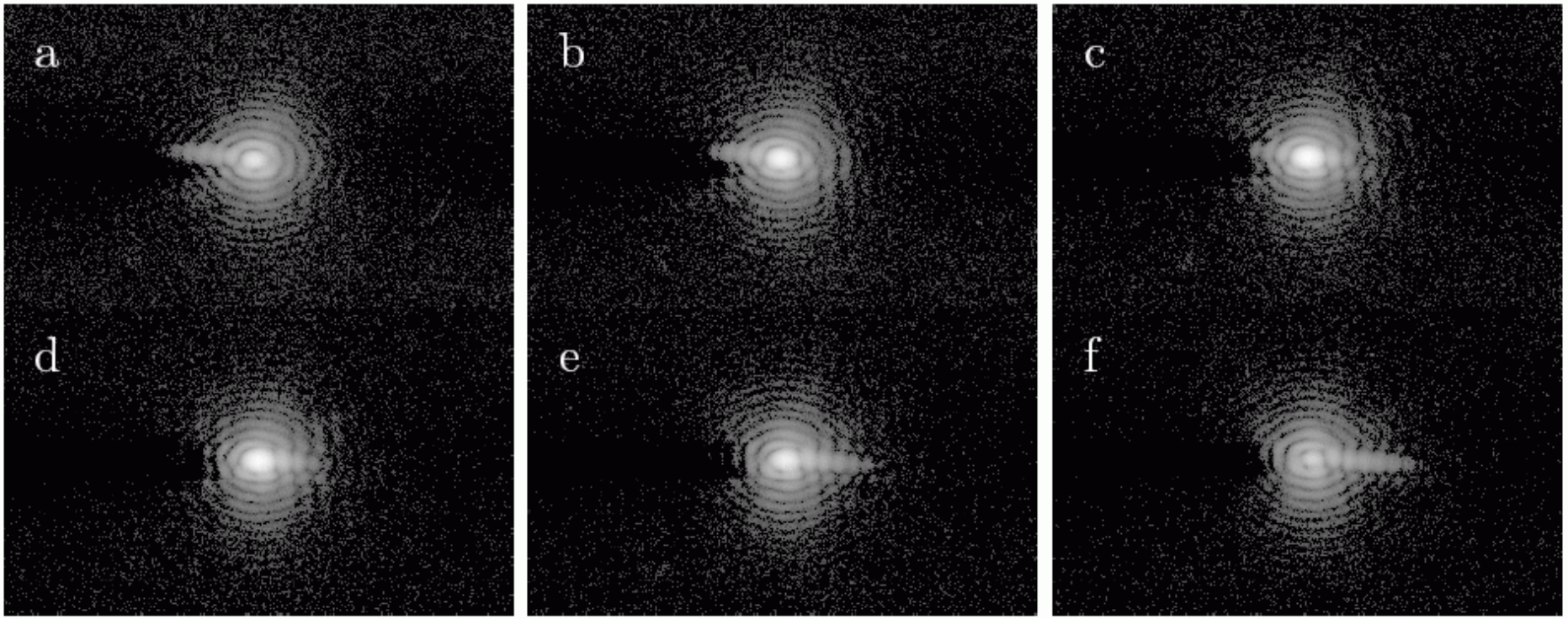
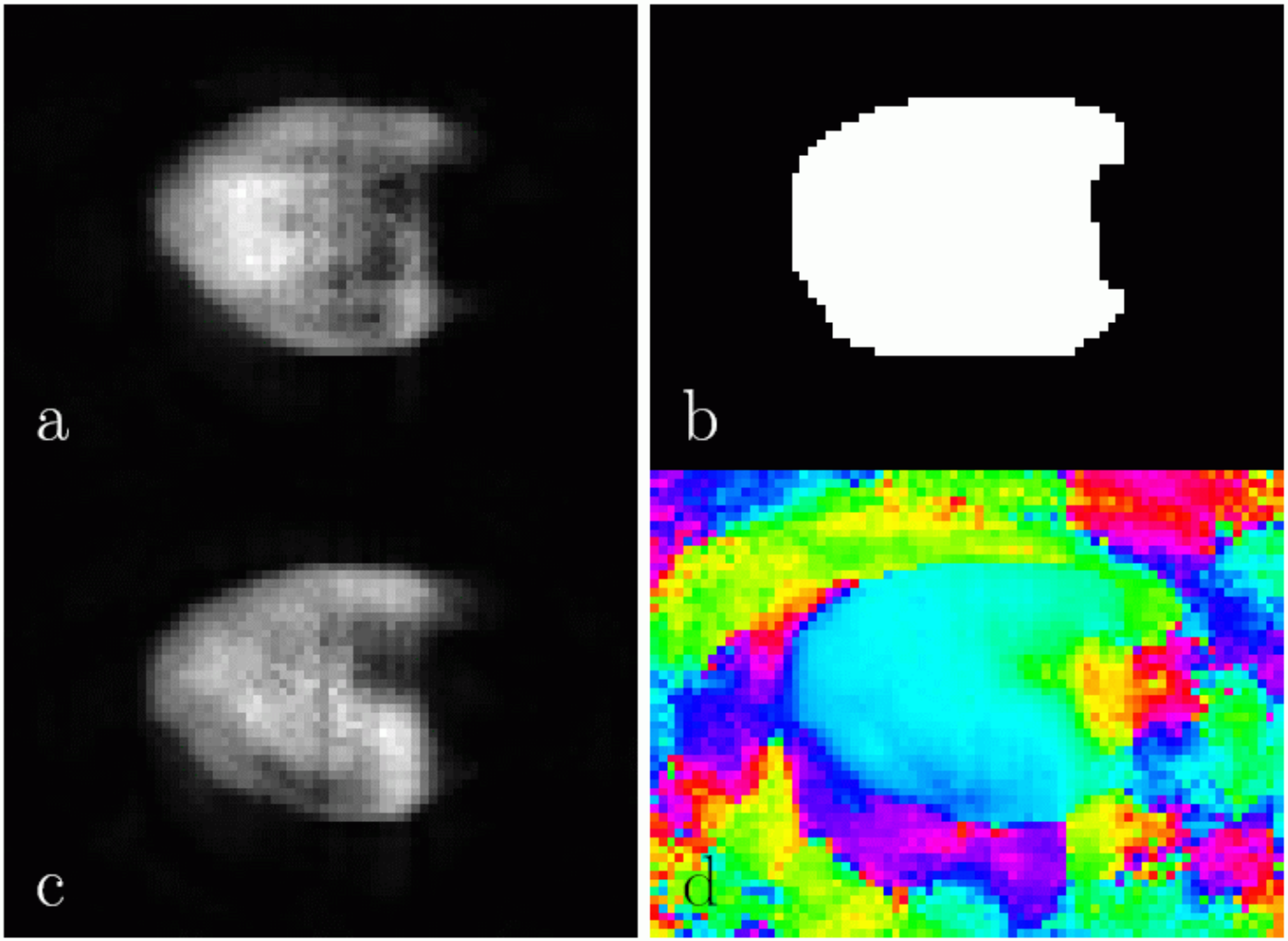
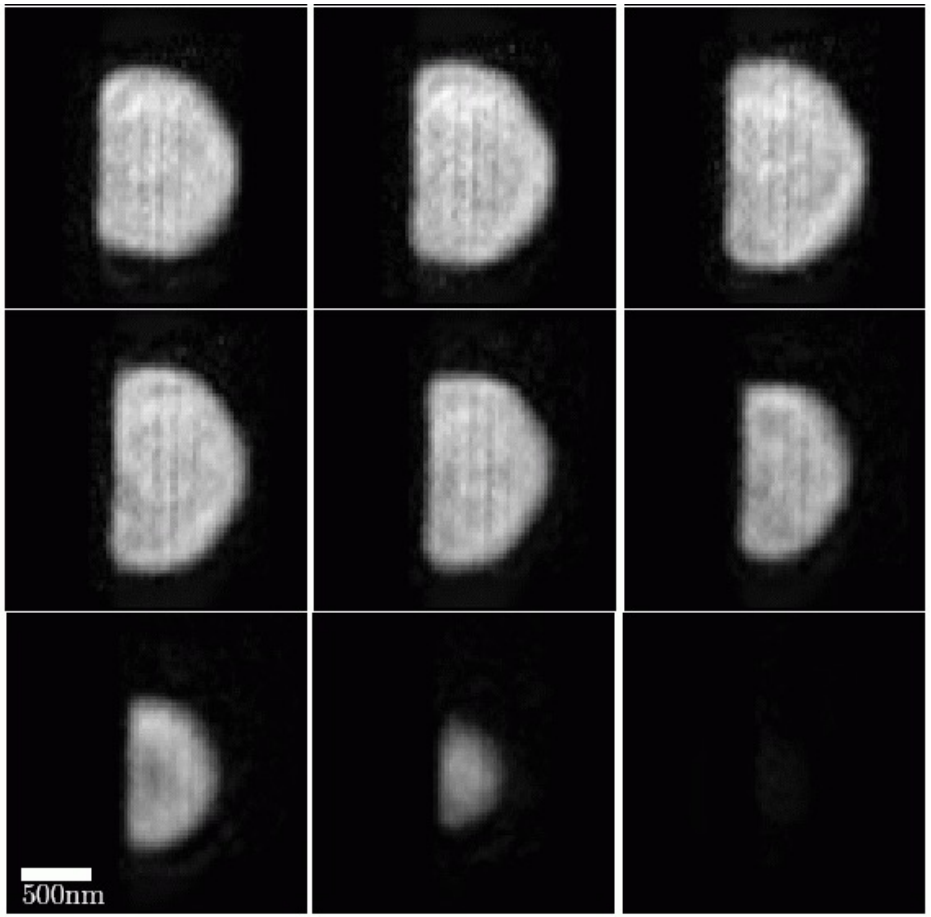


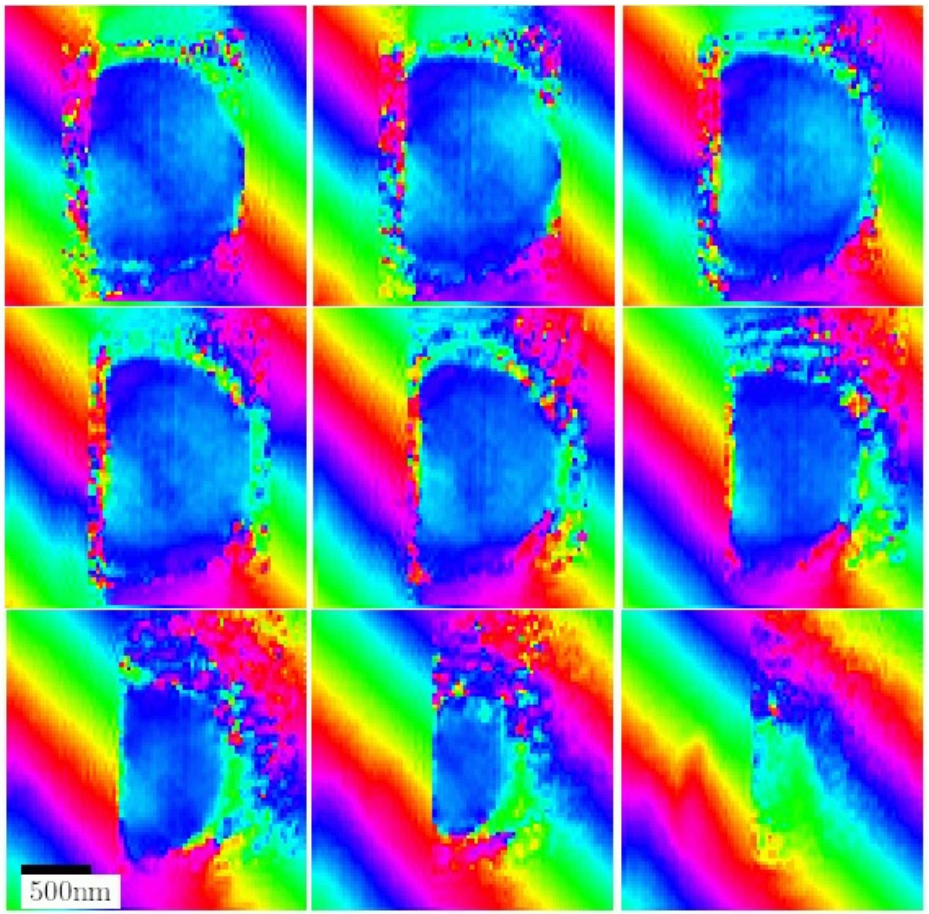
Figure 4.12: Center slices from 3D CXD pattern from Pb sample, on a log scale. Data file 296 from 10/03.

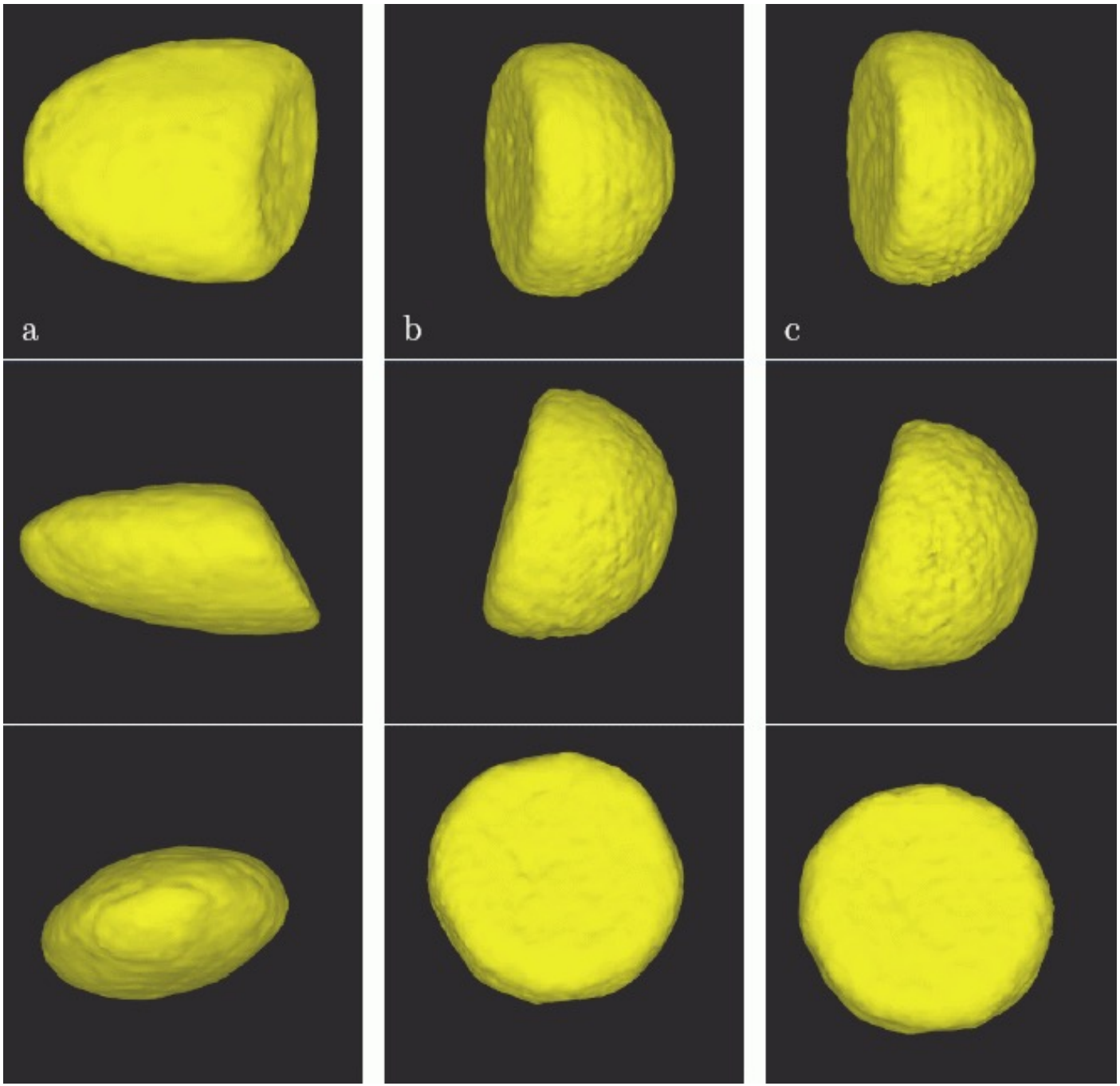
Learn shape of “tight” support



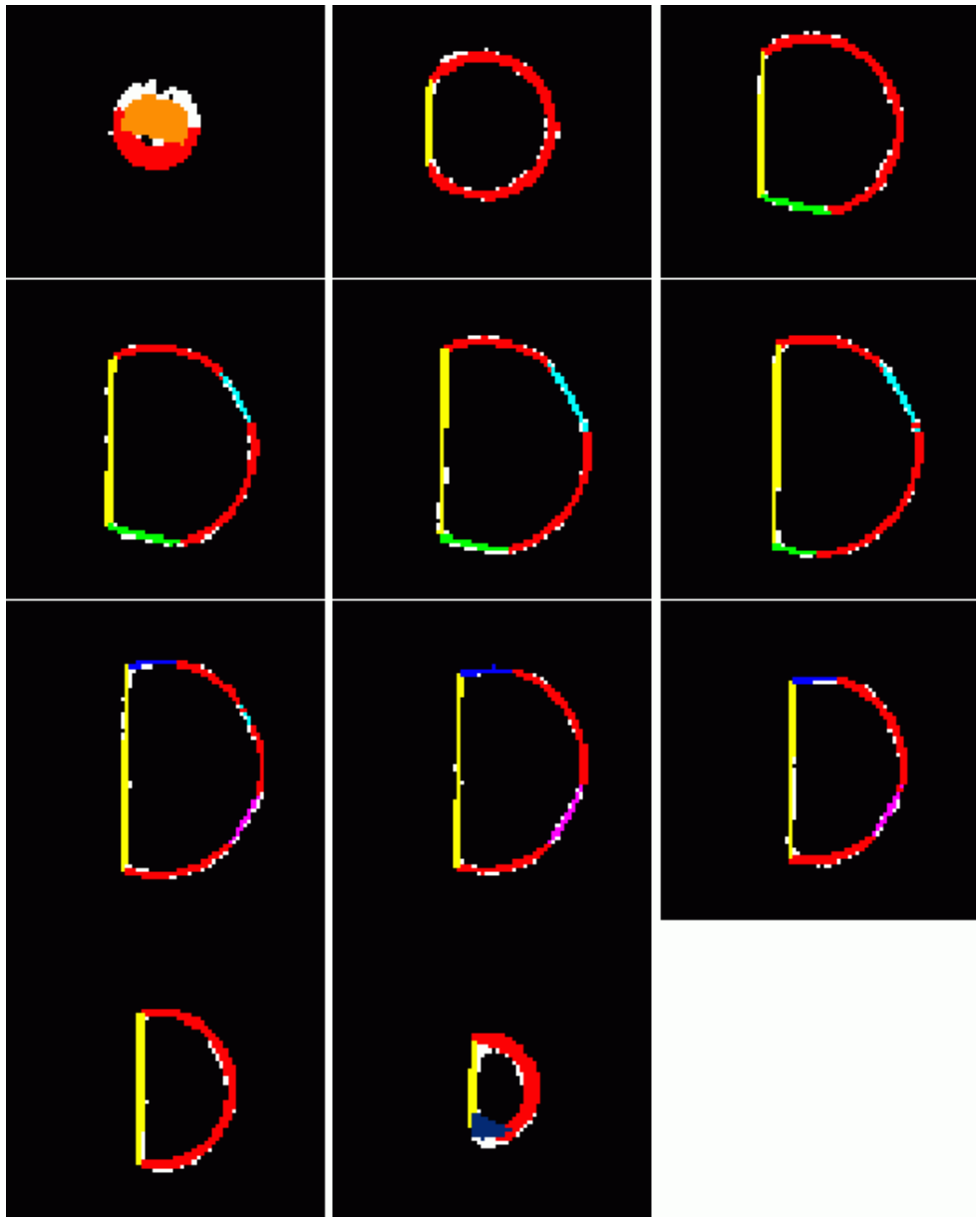
Then refine amplitude *and* phase





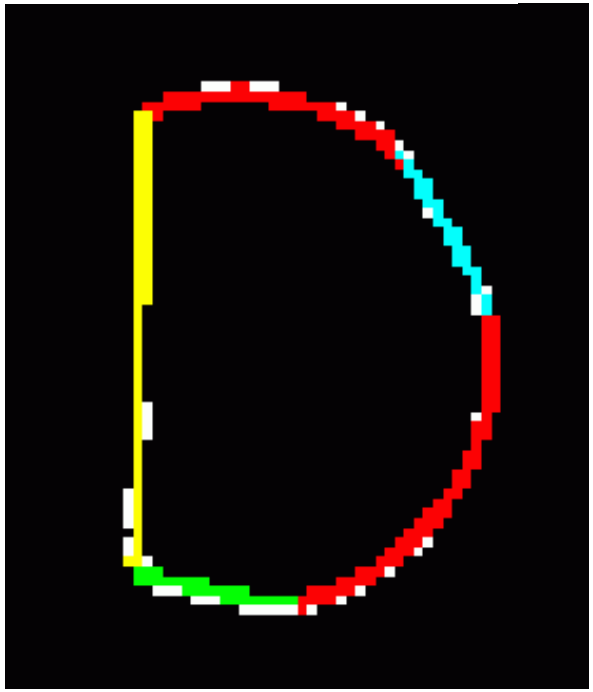

a
b
c

Fitting to facetted shape

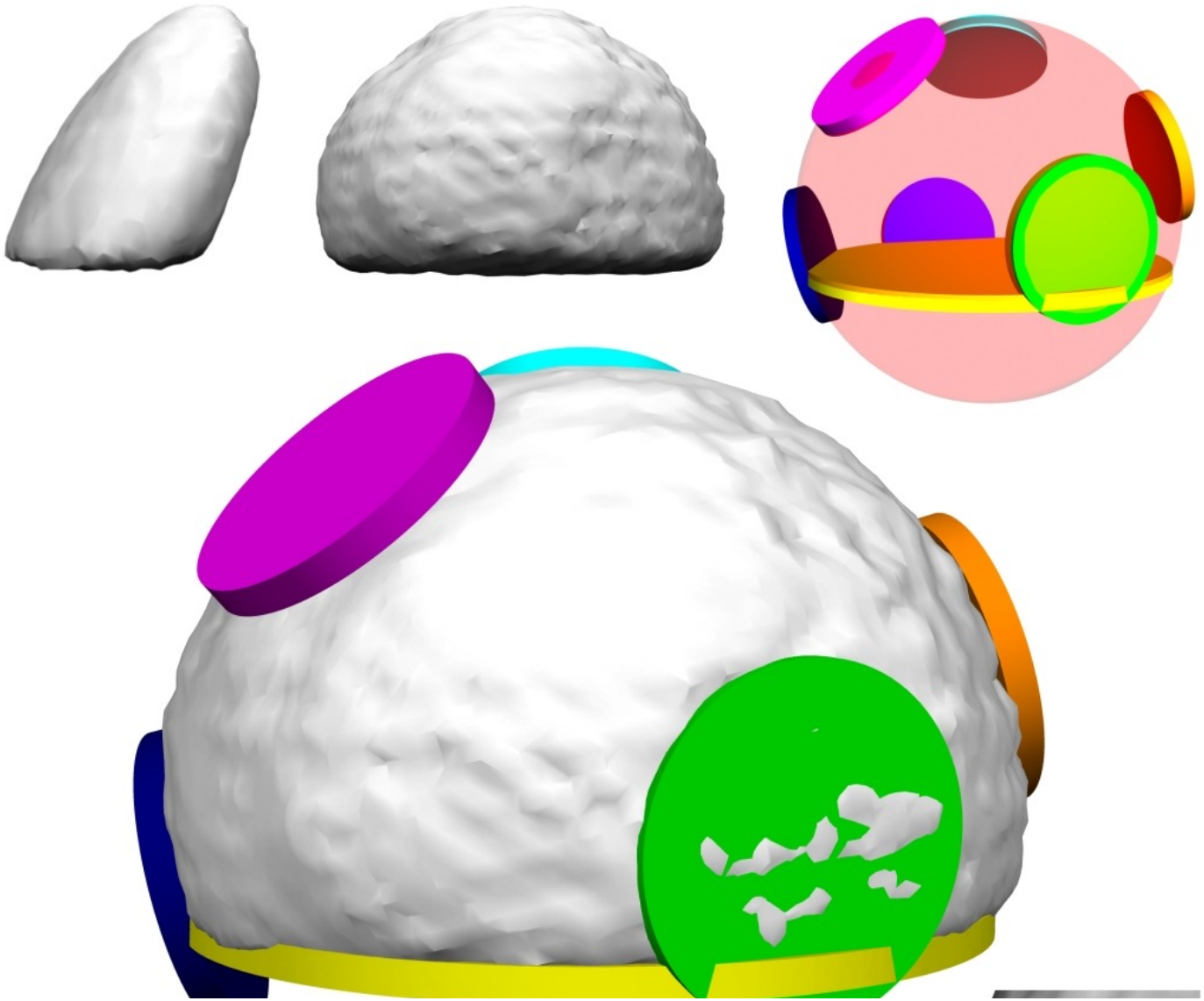


	$\|R\|$		P0	P1	P2	P3	P4	P5	P6
	9.4	P0	0	85	149	79	134	106	71
	25.7	P1		0	123	164	83	76	102
	25.1	P2			0	72	67	74	110
	25.9	P3				0	111	106	76
	25.4	P4					0	113	68
	25.4	P5						0	176
	26.0	P6							0 0

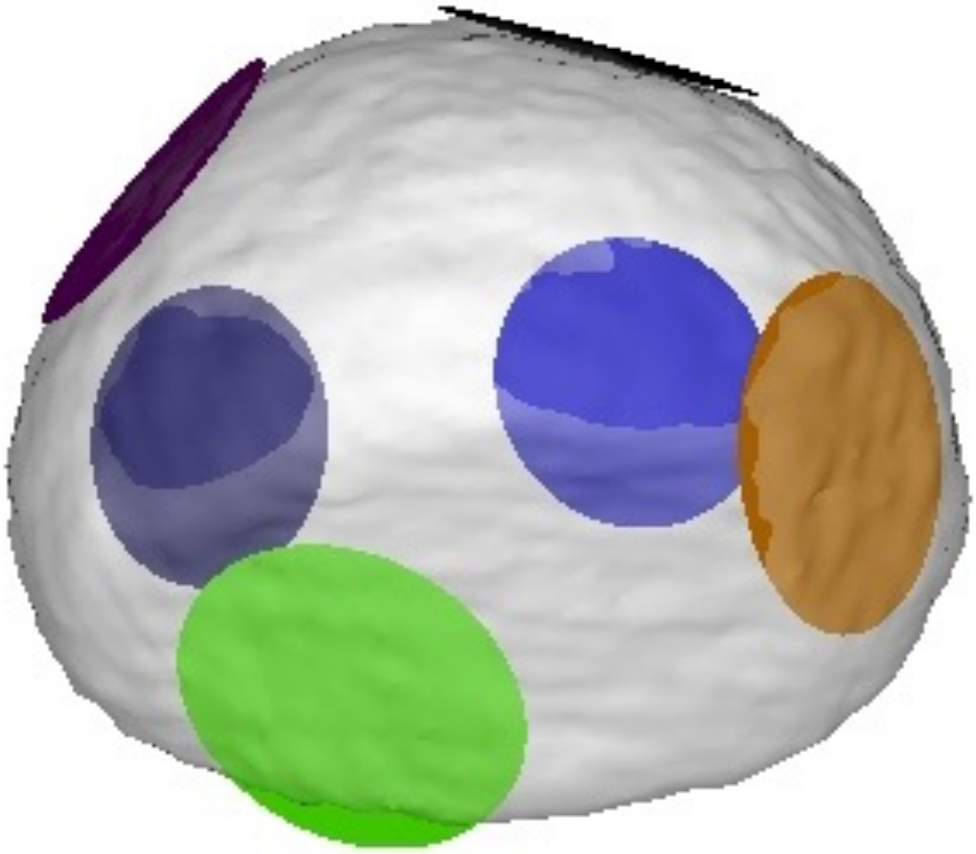
Angles between facets

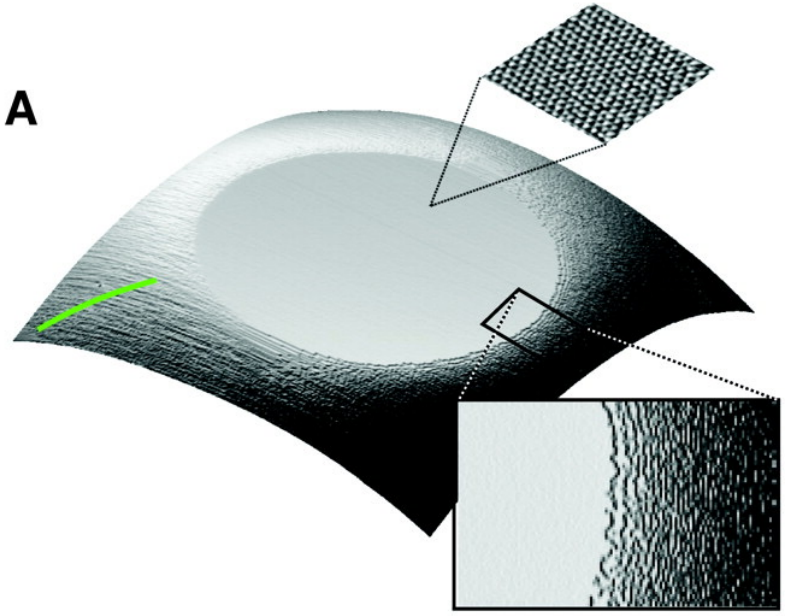


Fitting of crystal shape



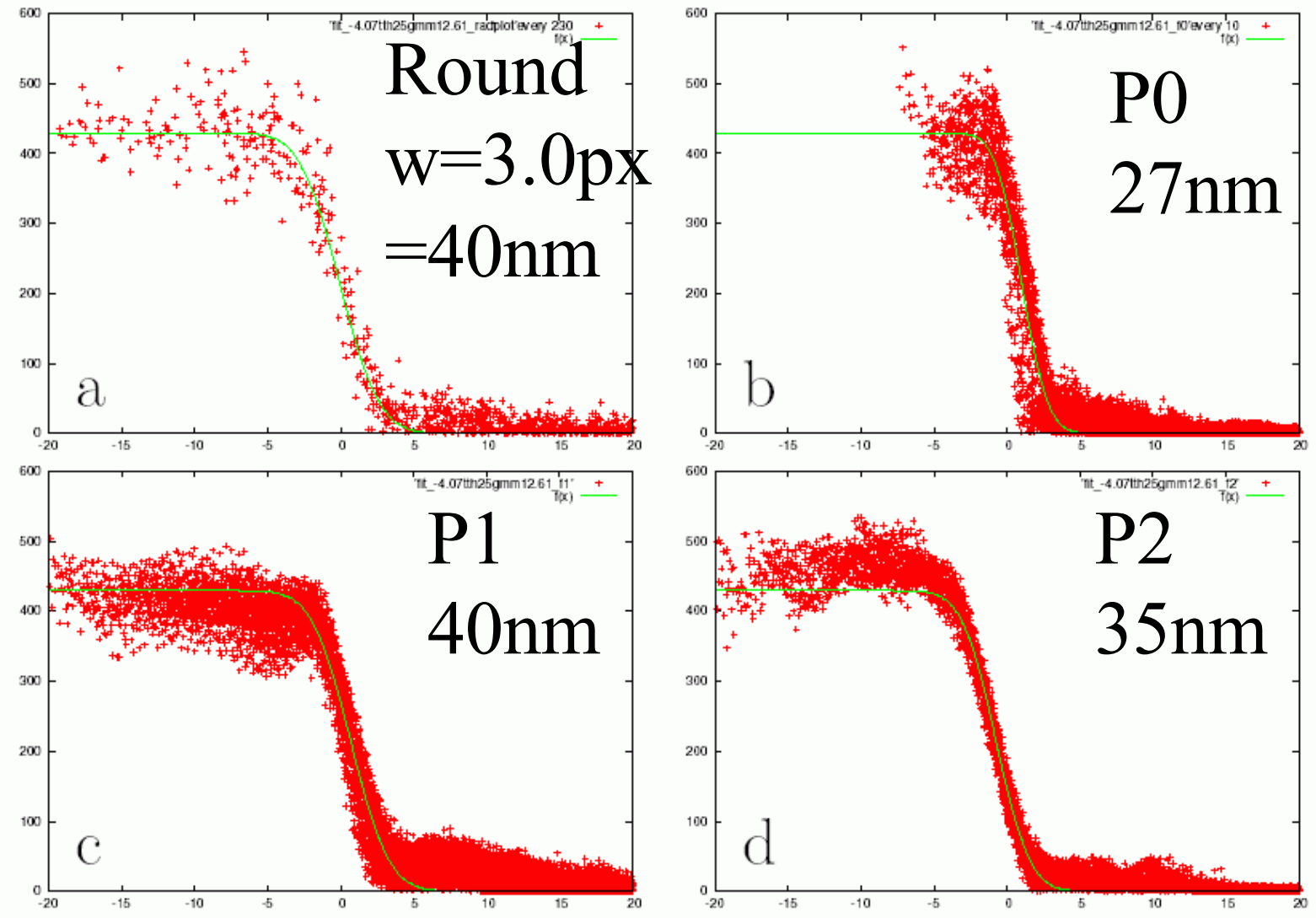
Facets of Equilibrium Crystal Shape



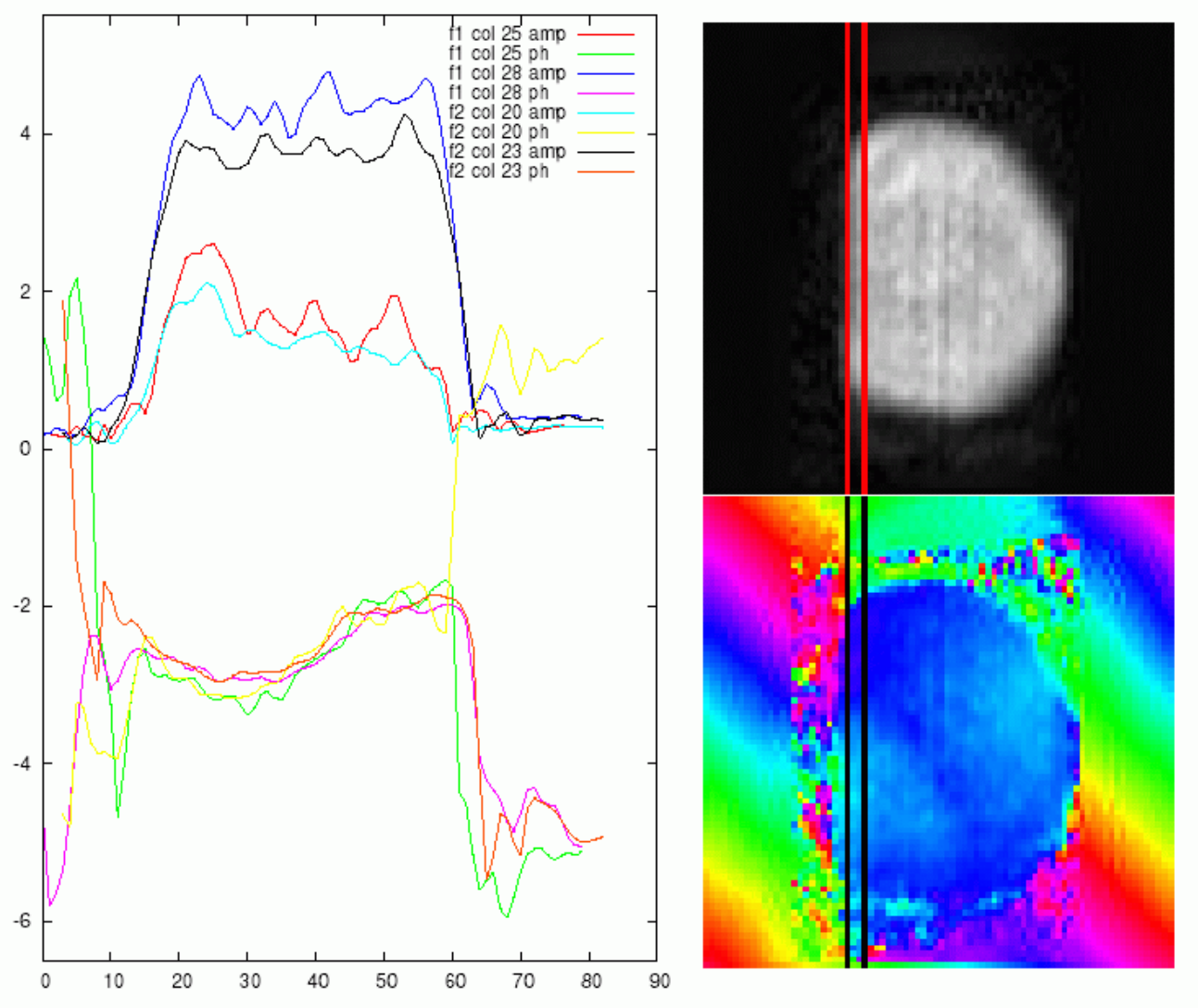


Thurmer K, Williams E, Reutt-Robey J
Science **297** 2033 (2002)

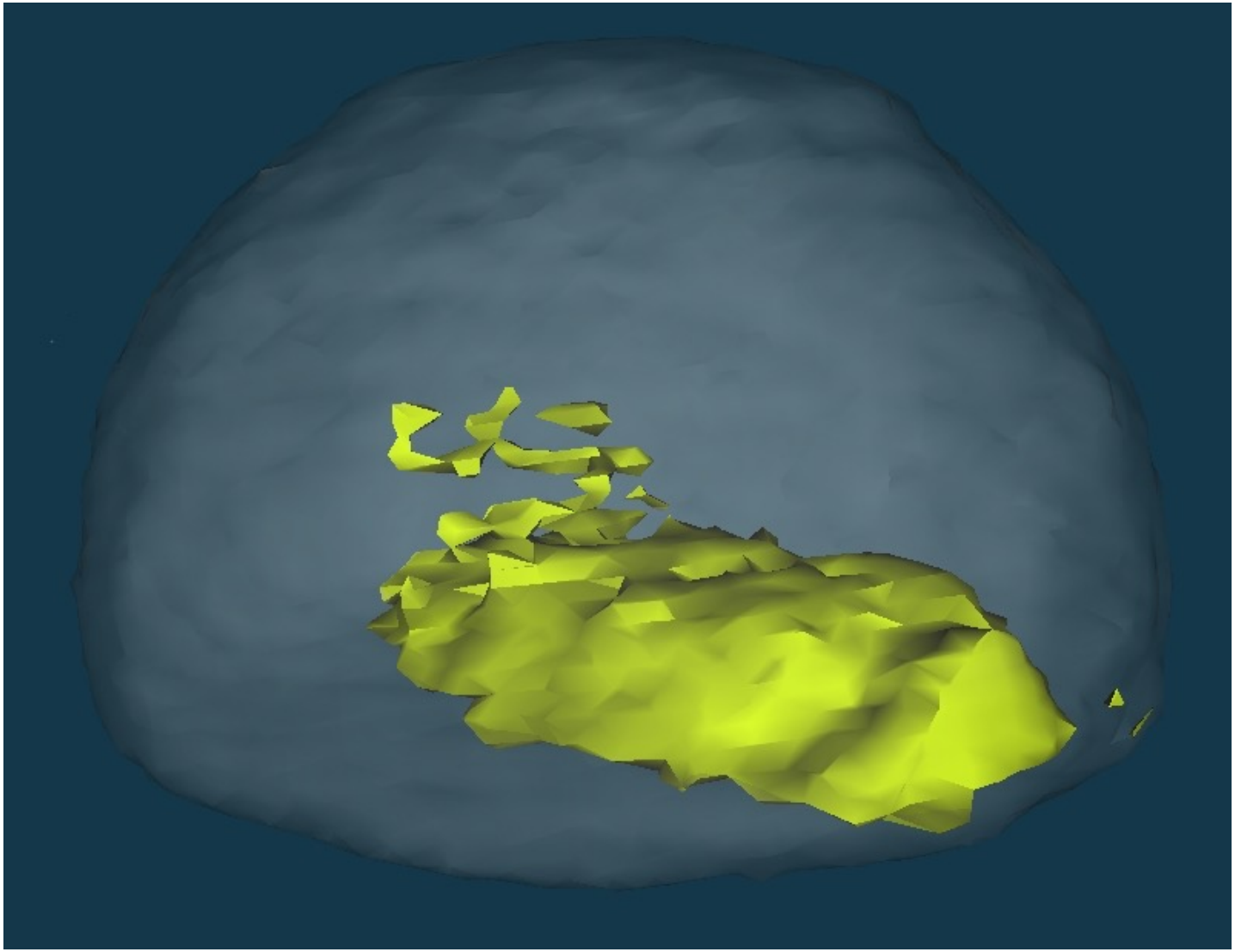
Density distribution across surface



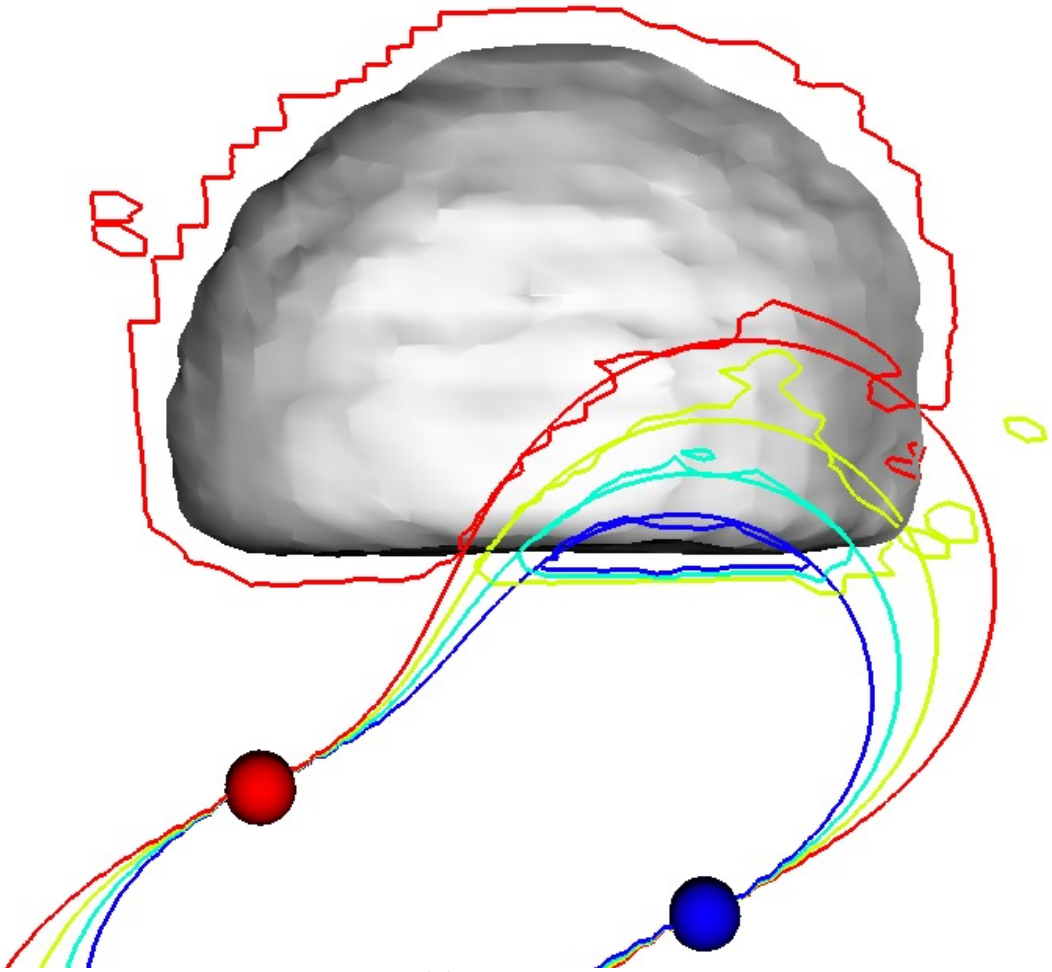
Phase structure near substrate interface

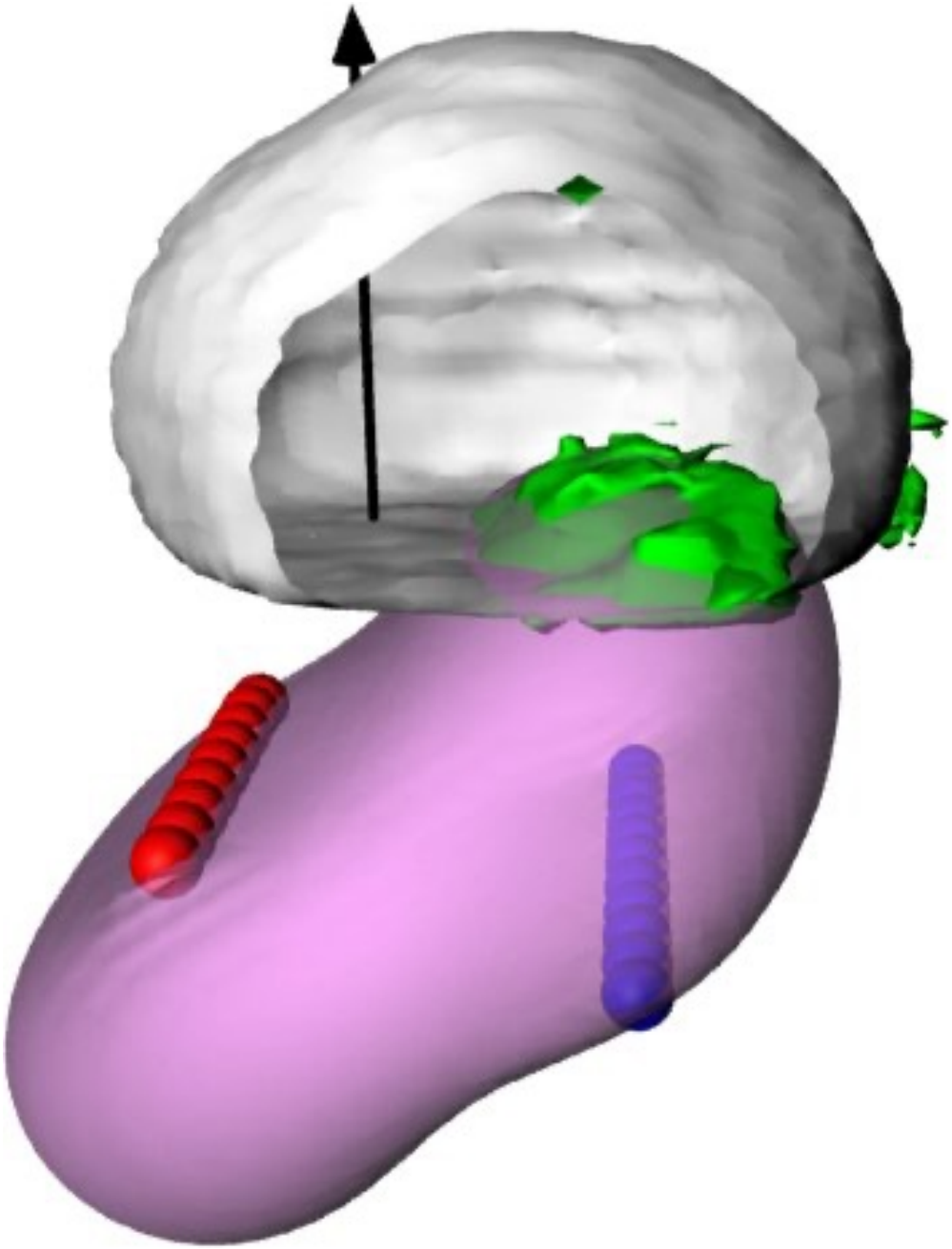


Modeling of 3D Phase Bump



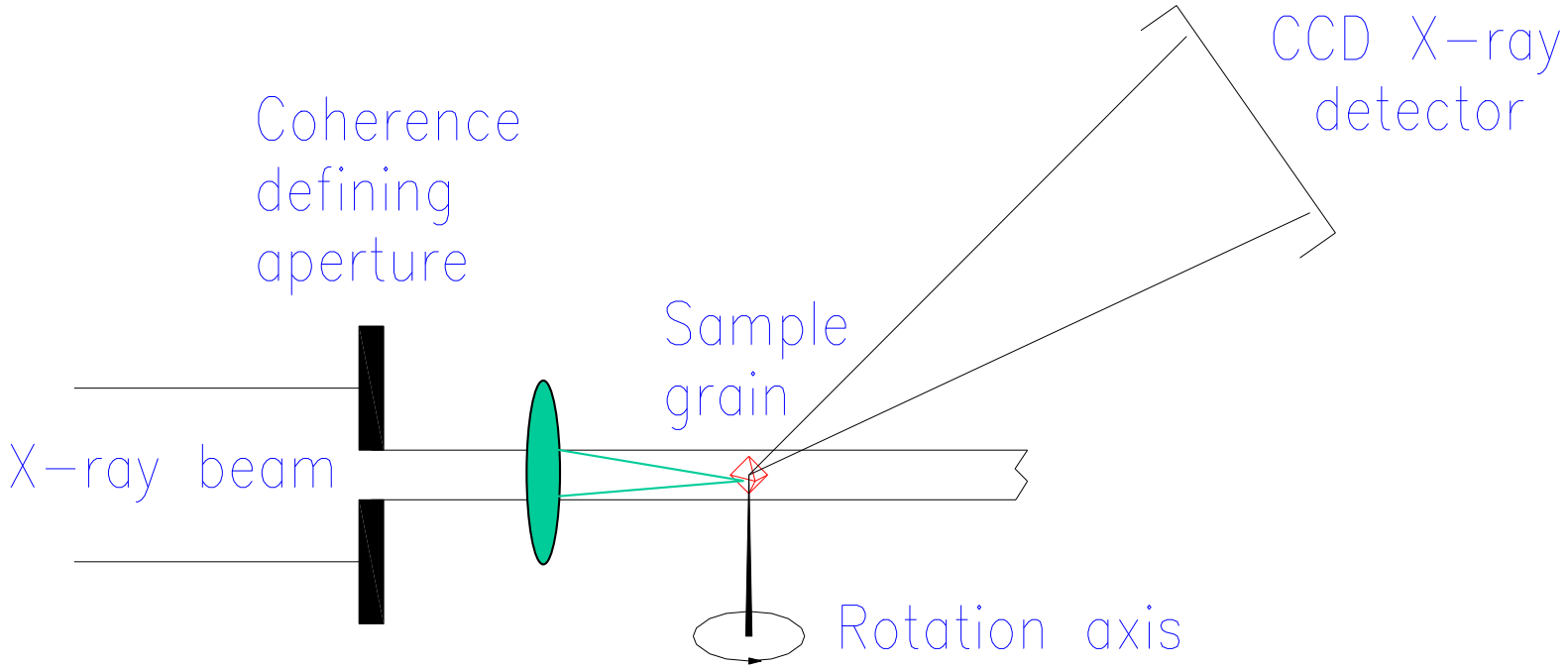
Field lines of Point Charges



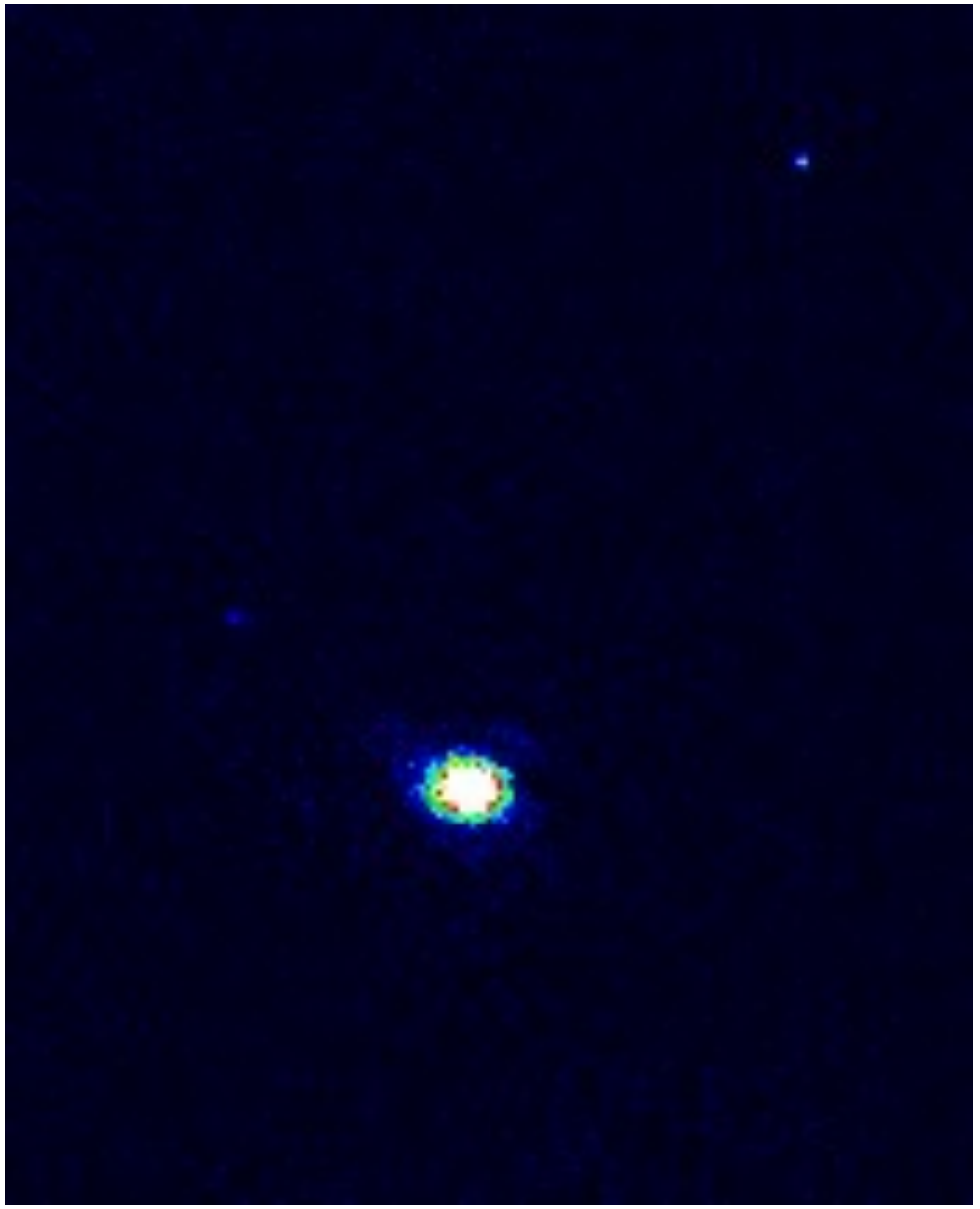


Future: Optimise using Optics

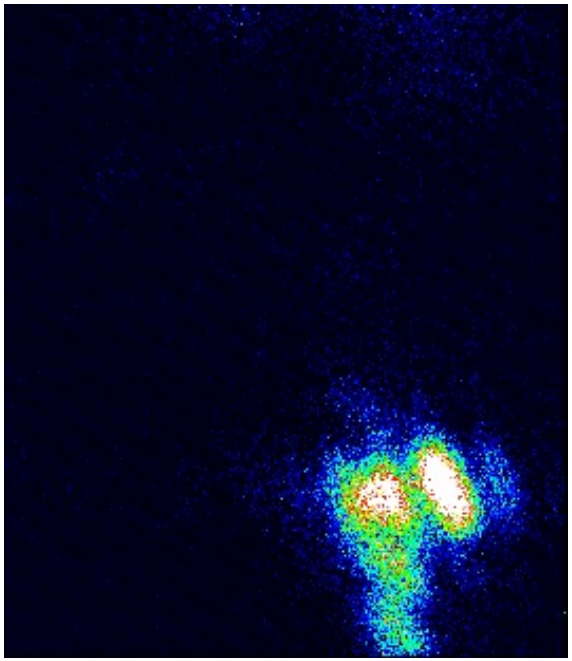
match available coherence to sample size



Rocking scan of Ag cubes with 0.01° steps



Move beam on to sample....



Conclusions and Outlook

- Internal structure of Pb Nanocrystals
- 3D imaging of individual nanocrystals
- Phasing by computation instead of lens
- Strain fields imaged from asymmetric patterns
- Consistency with elasticity theory