Imaging of Nanocrystals by Inversion of Coherent X-ray Diffraction

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- Mark Pfeifer
- Garth Williams

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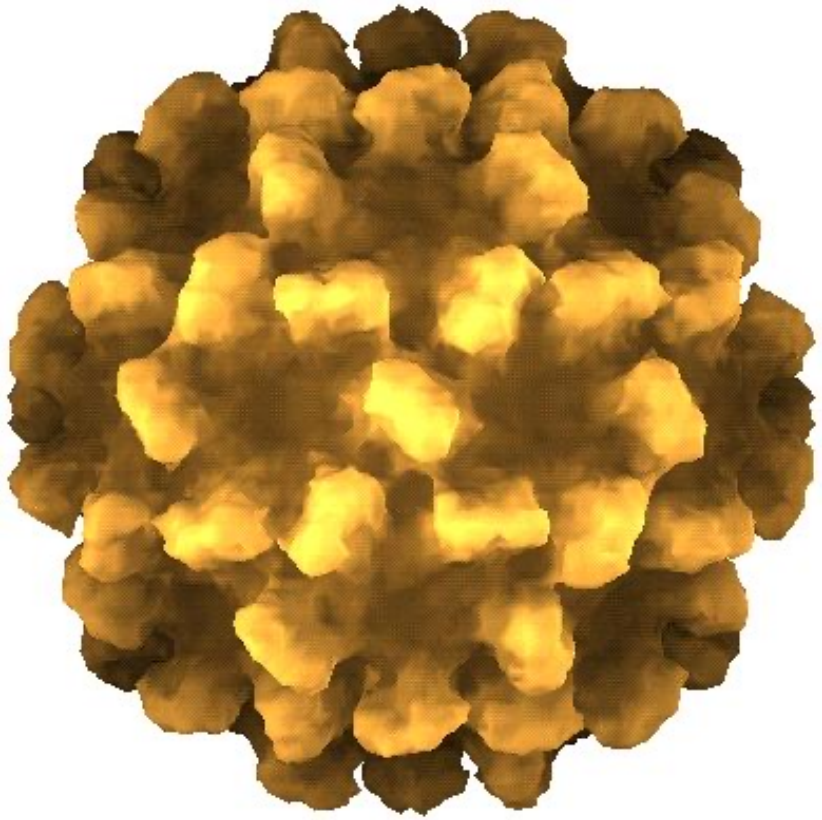
ICTP Advanced X-ray Imaging, June 2005

Tomato Bushy Stunt Virus
1980



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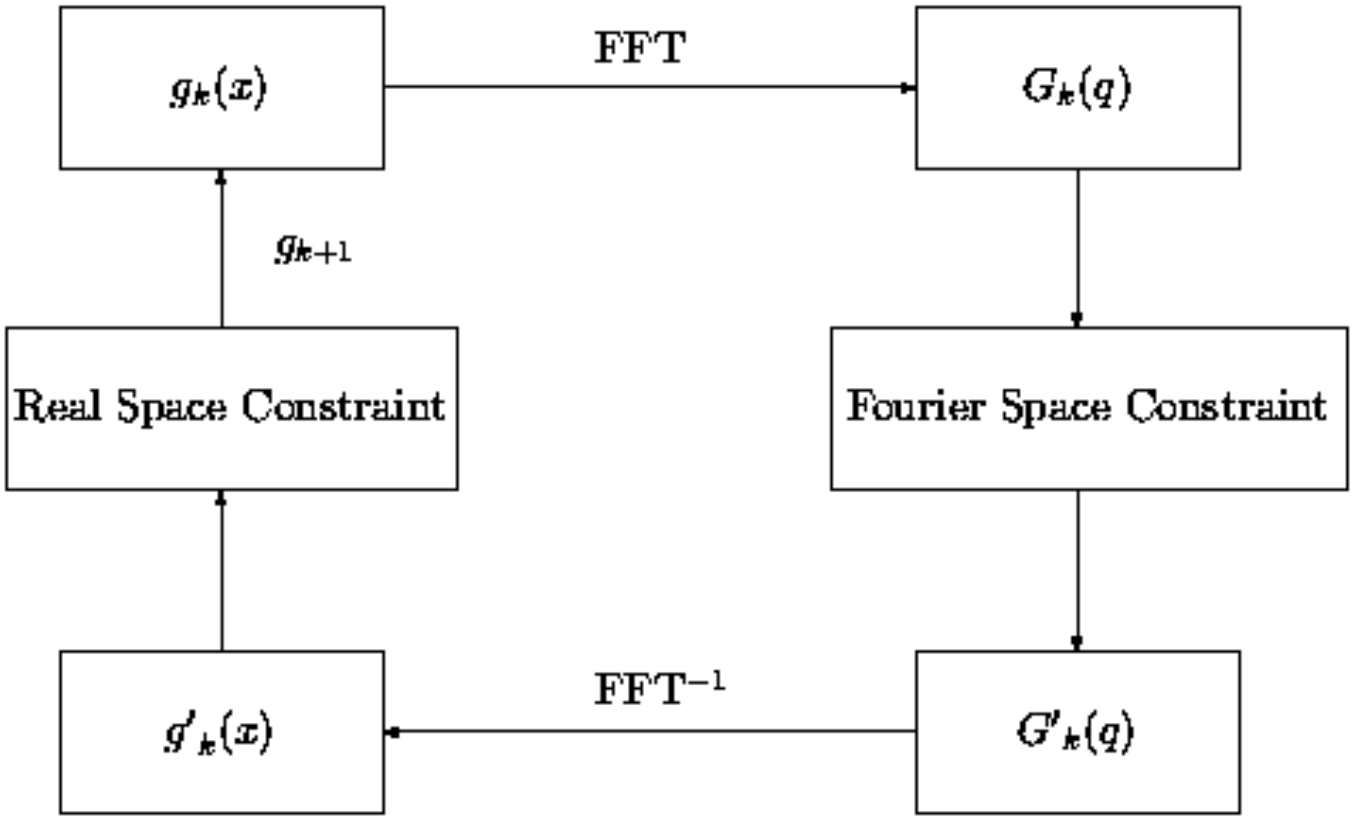
Outline

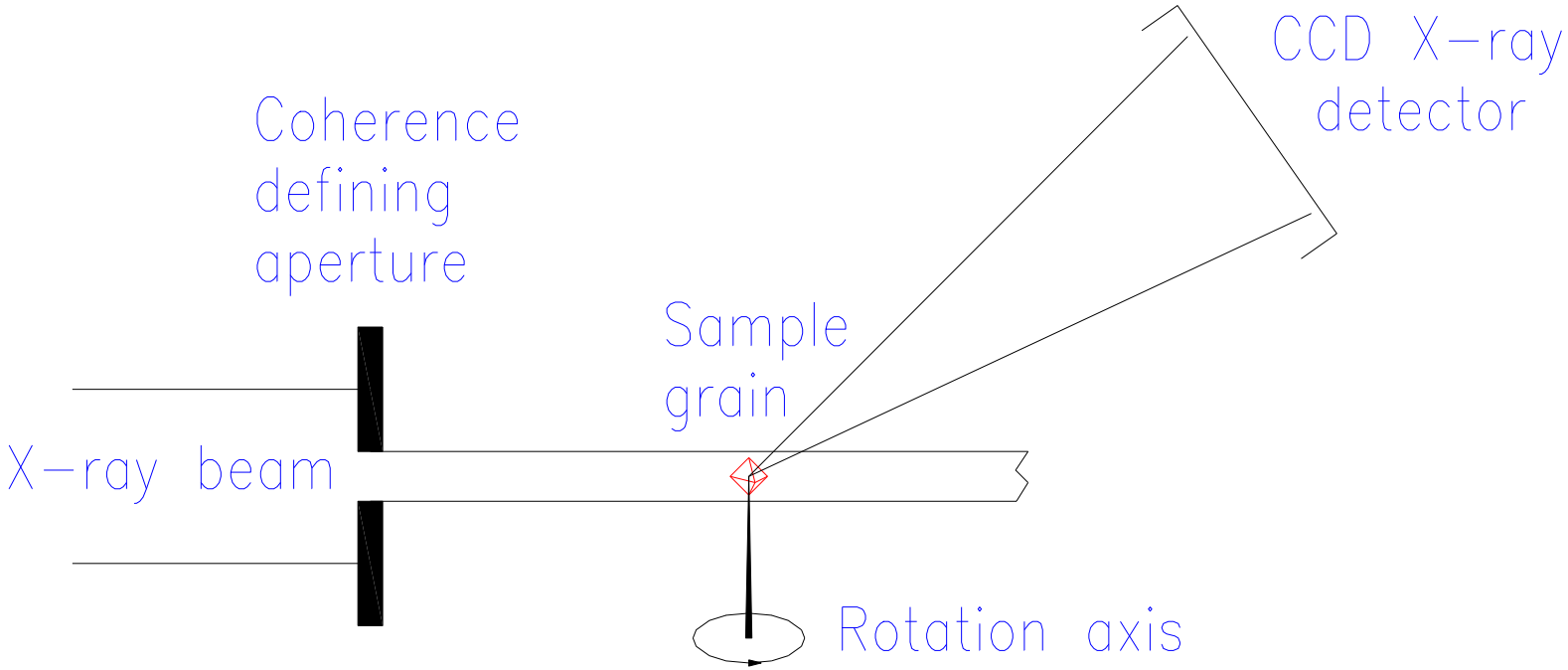
- Coherent X-rays can Image Structure in 3D
- Solve Phase Problem by Phase Retrieval
- Internal structure of Nanocrystals
- Imaging of Phase Objects
- How small can we go?

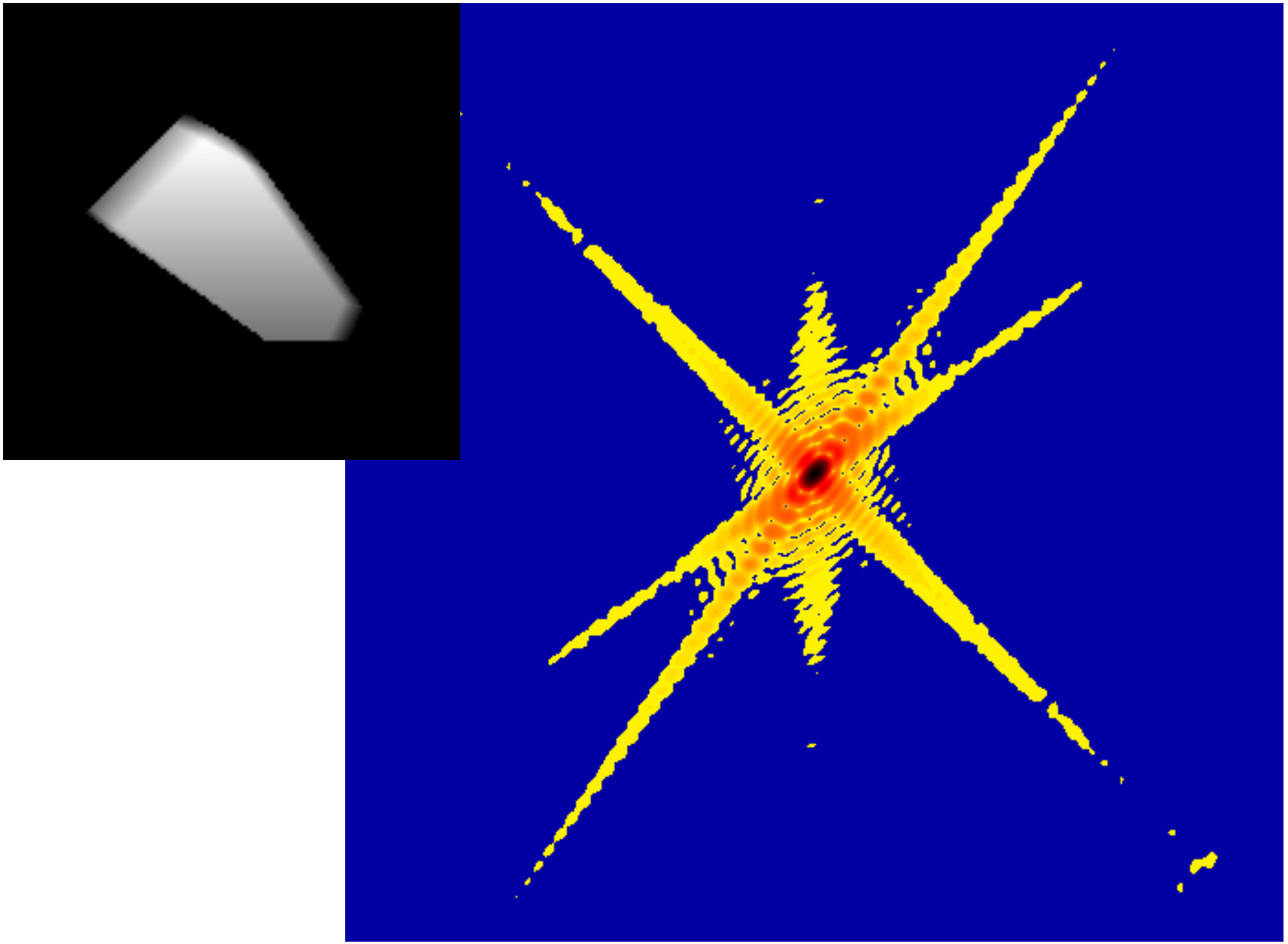
Generic "Error Reduction" method



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

Lensless X-ray Microscope





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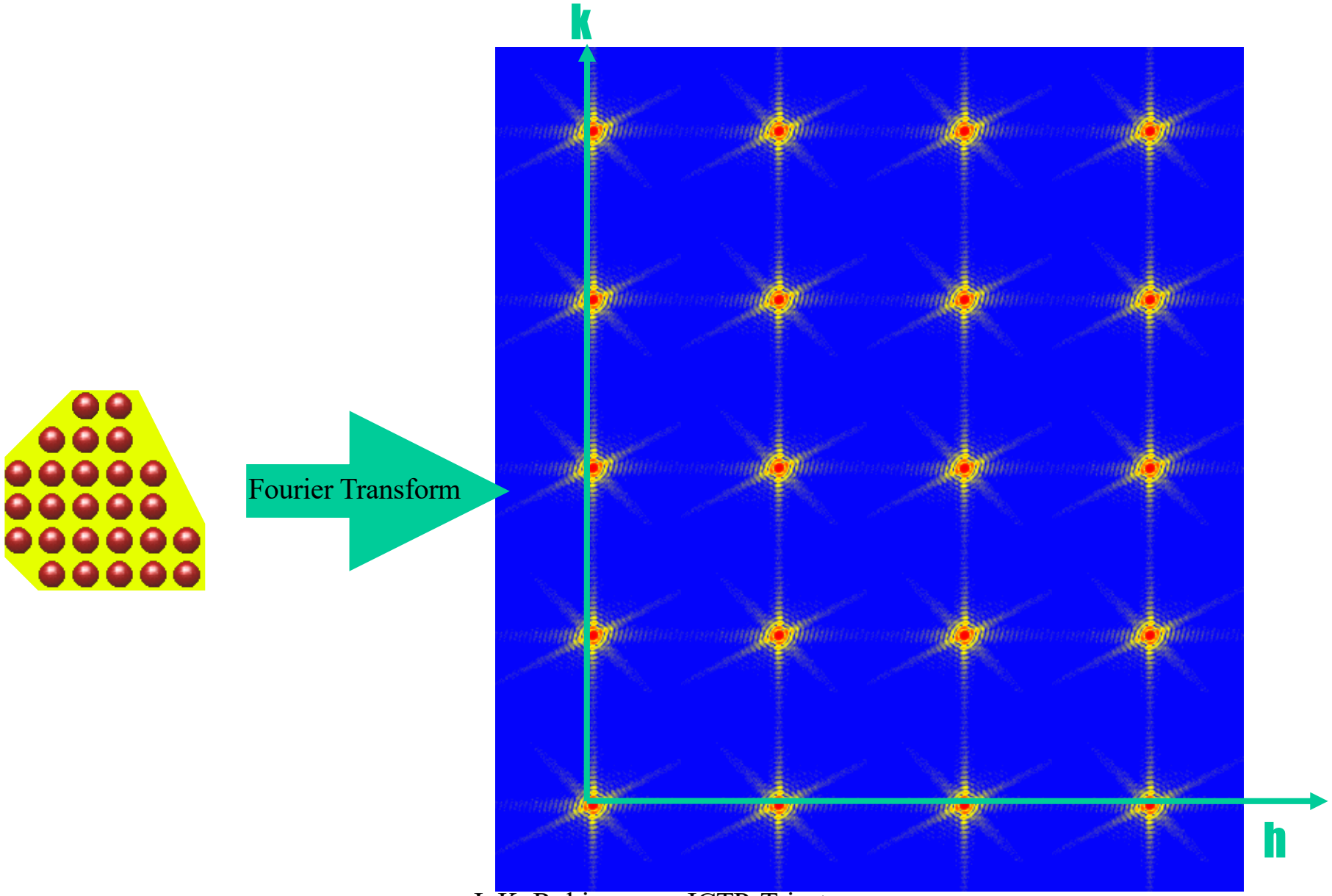
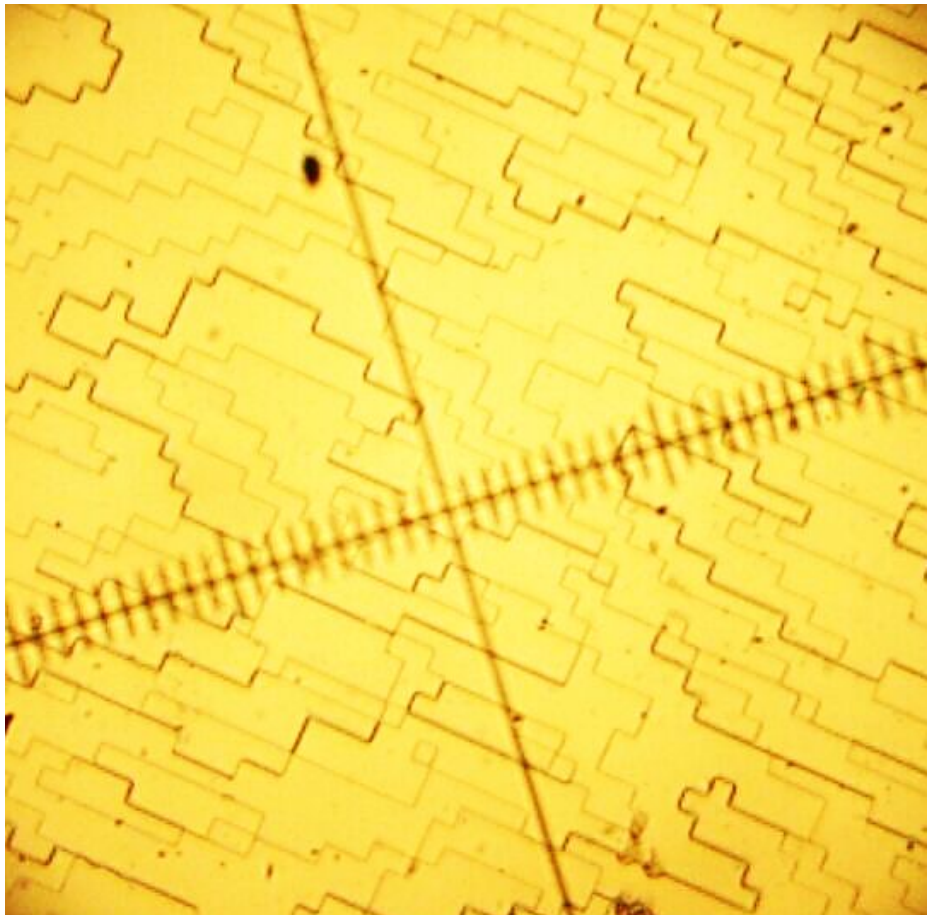
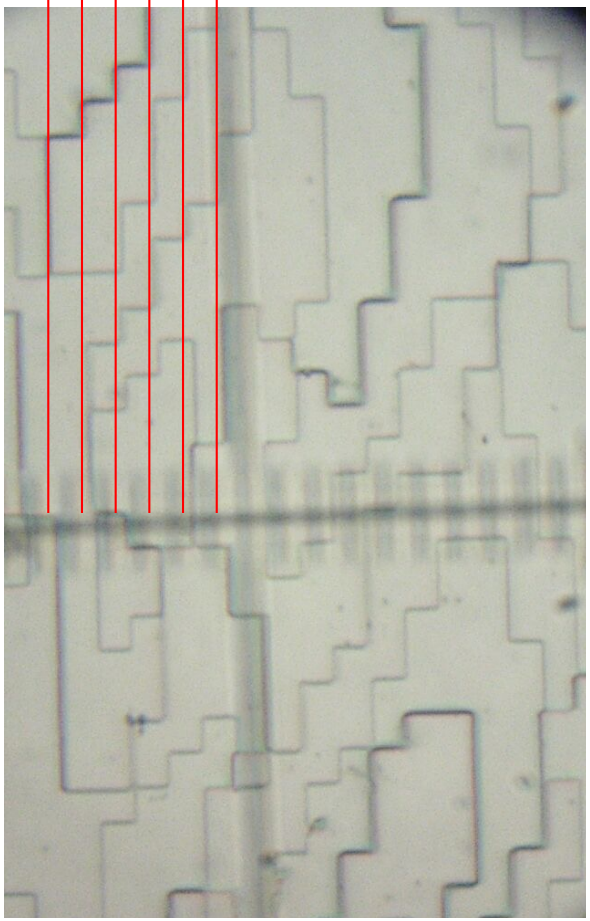
Coherent Diffraction from Crystals



Microscope Images of Gratings

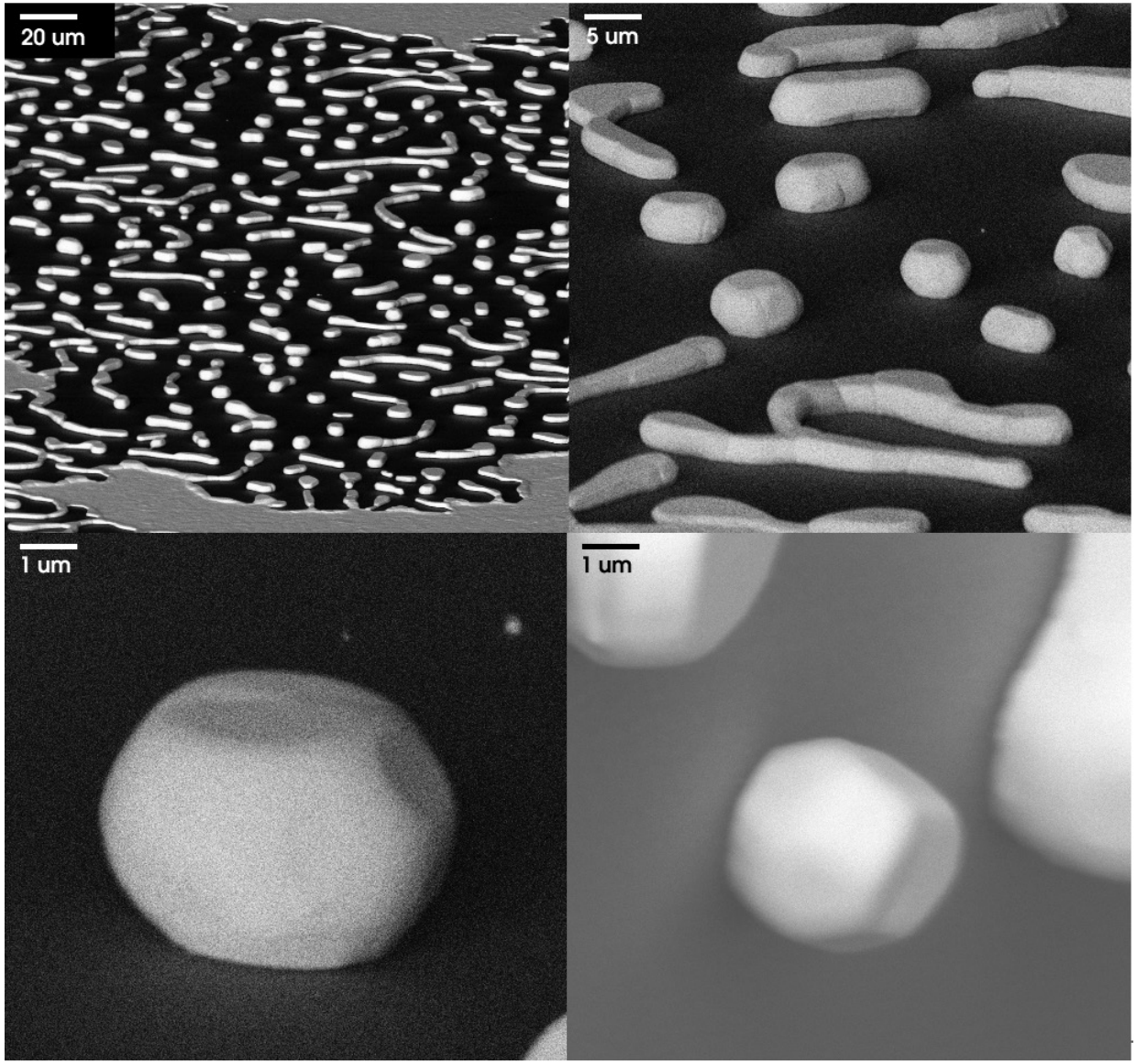


5μm grid lines



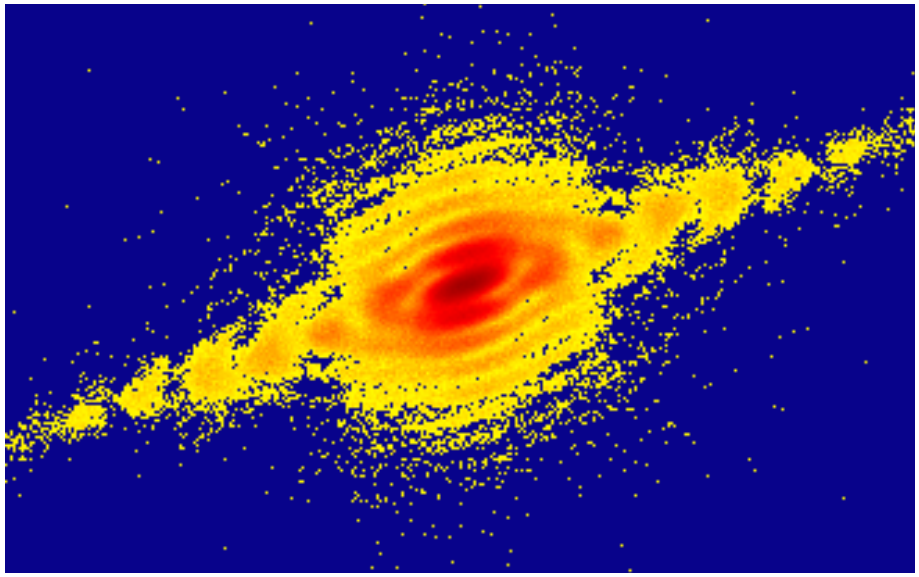
SEMS

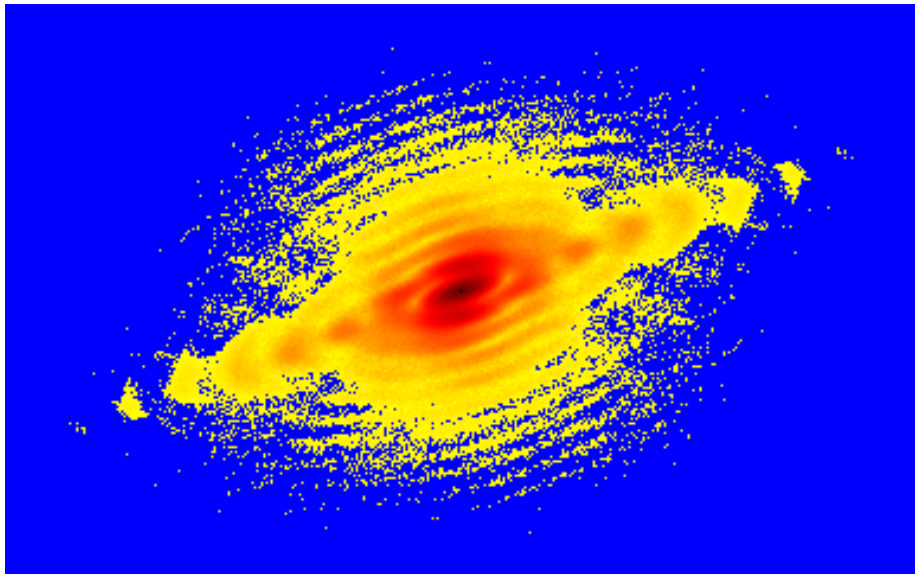
- Au blanket film
- Quartz substrate
- Annealed at 950°C for 70 hrs.

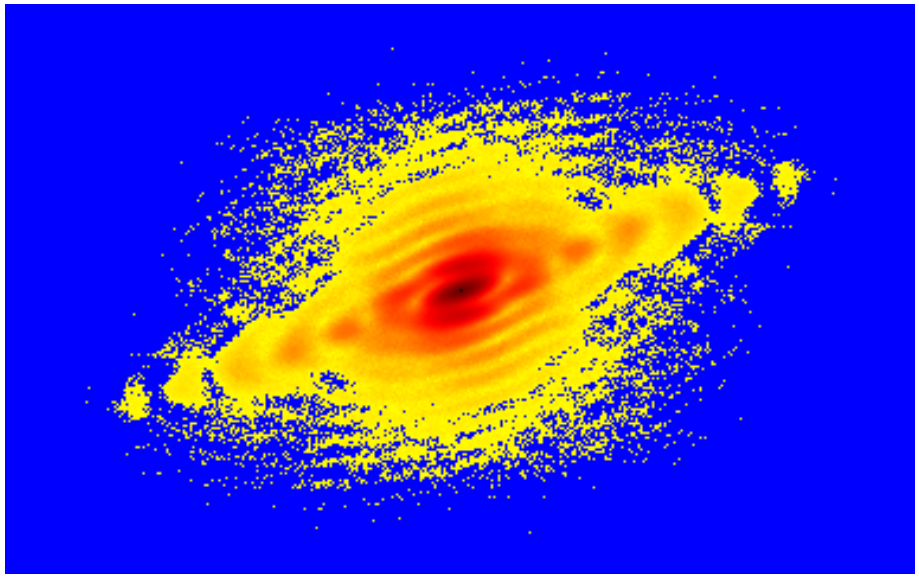


Symmetrized Data and two best fits

Chisq=0.0005







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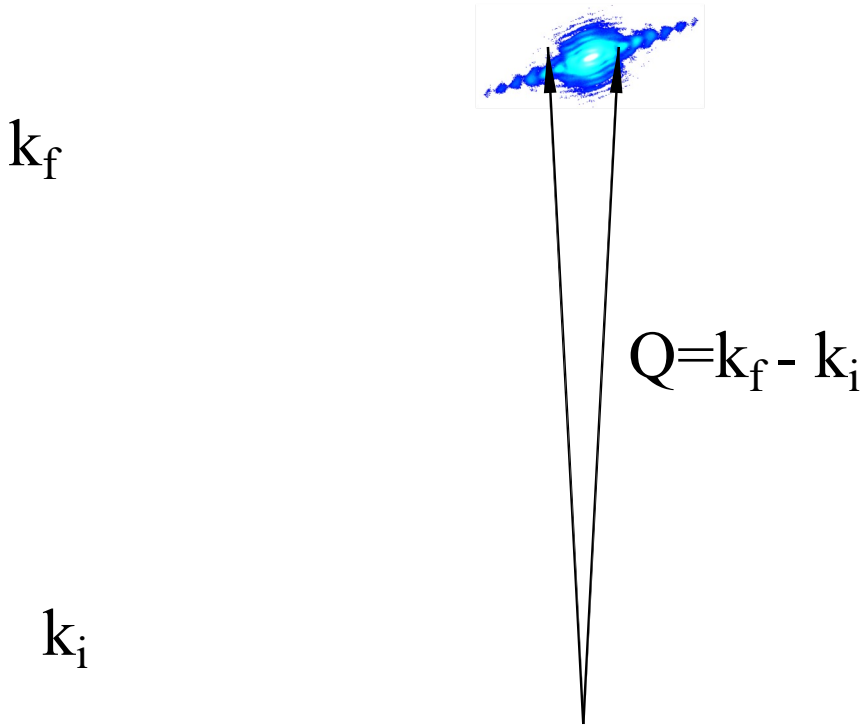
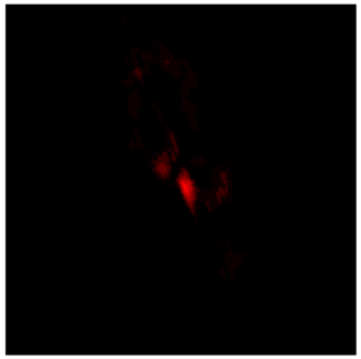
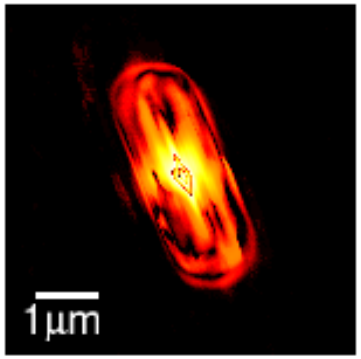
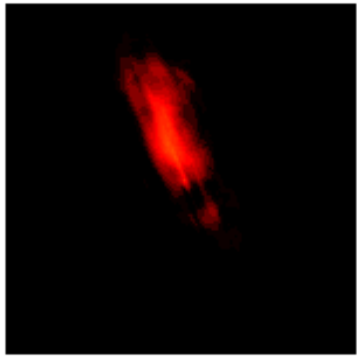
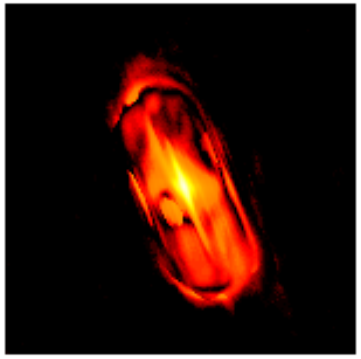
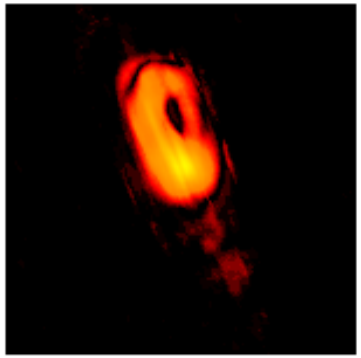
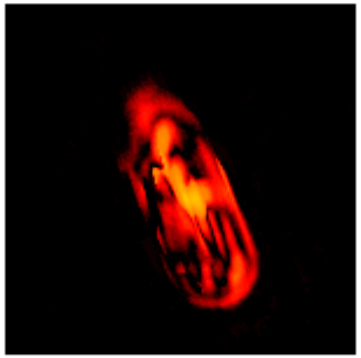
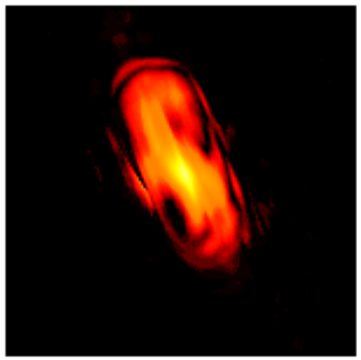
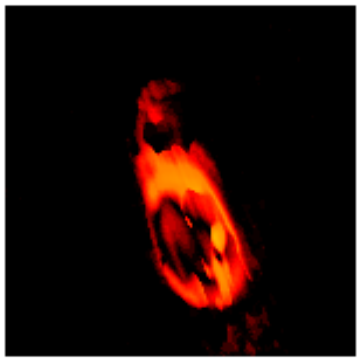
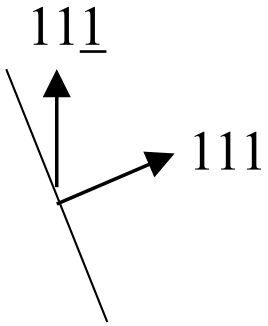
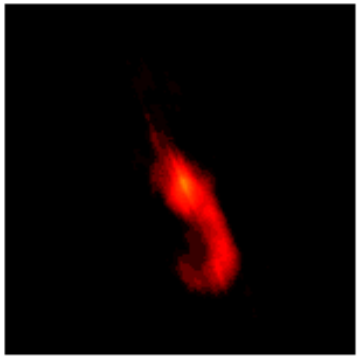
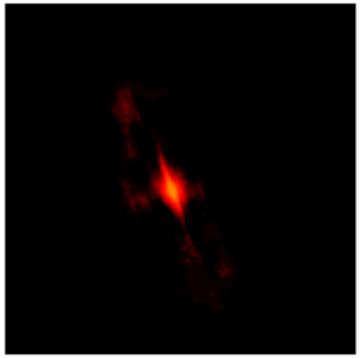
3D Diffraction Method

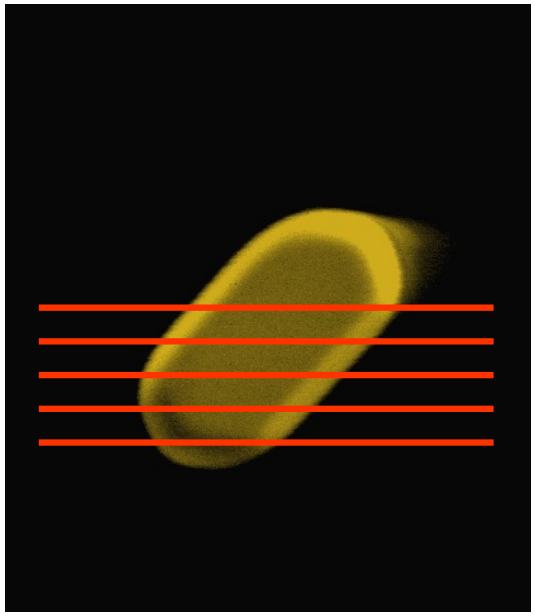


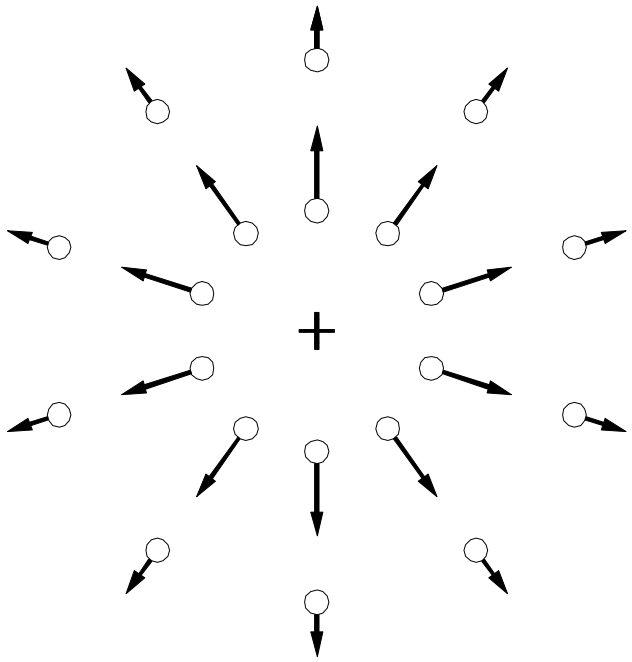
Slices through plan view SEM:

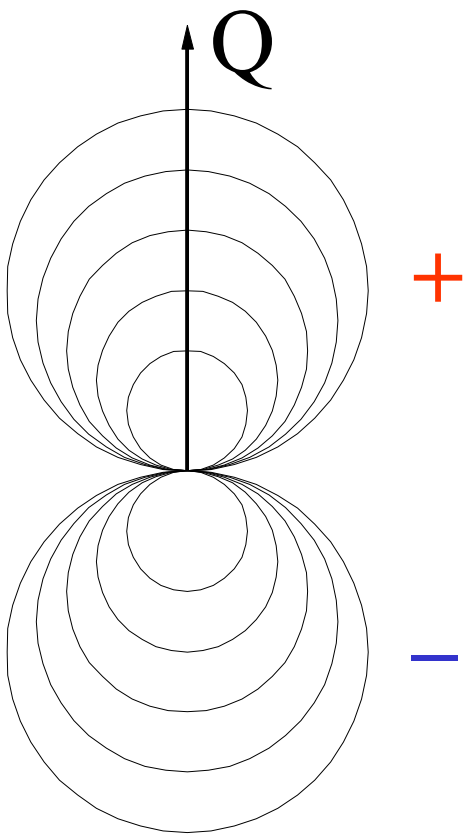


Diffraction by Strain of Point Defect

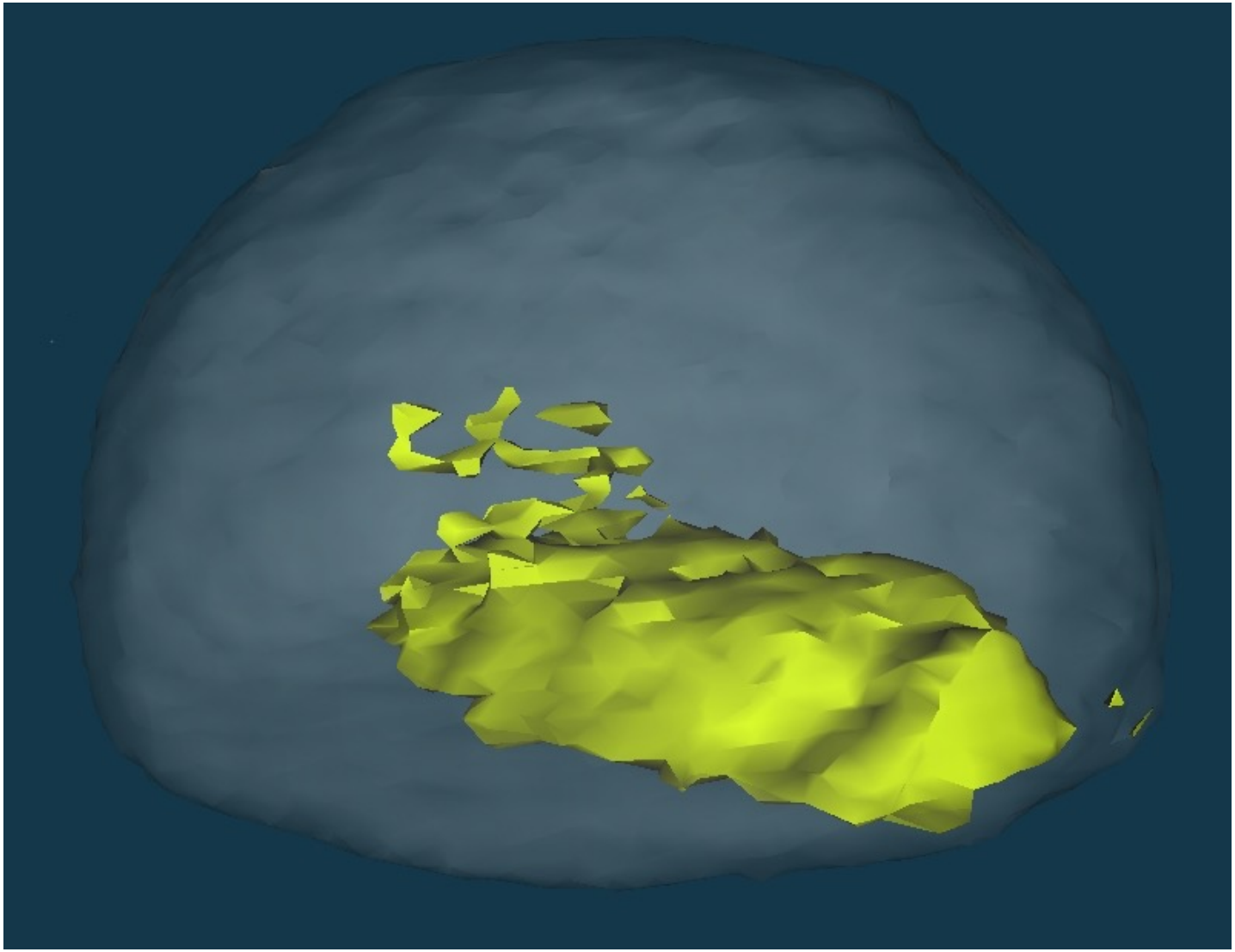
$$A \sim \sum e^{i\mathbf{Q}\cdot(\mathbf{R}_j+\mathbf{u}_j)}$$
$$\approx \sum e^{i\mathbf{Q}\cdot\mathbf{R}_j}(1+i\mathbf{Q}\cdot\mathbf{u}_j)$$

Imaginary density

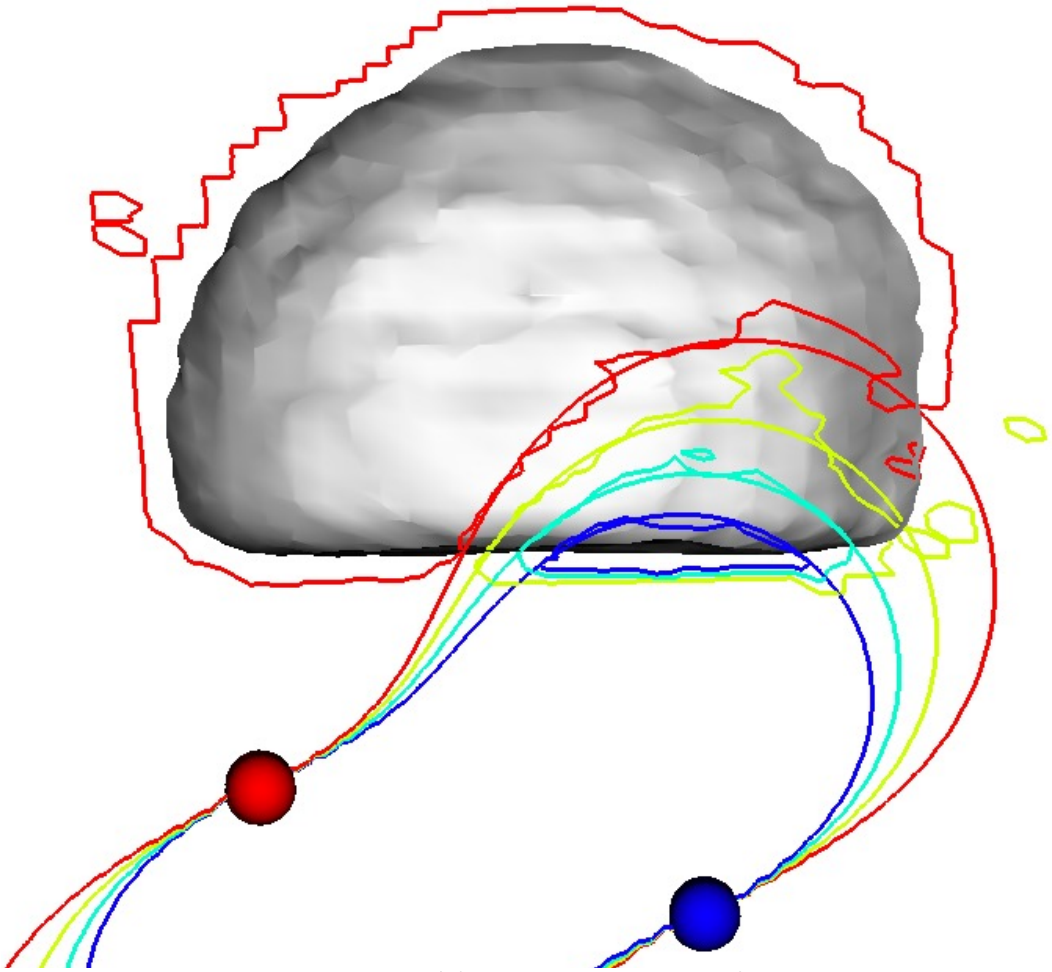




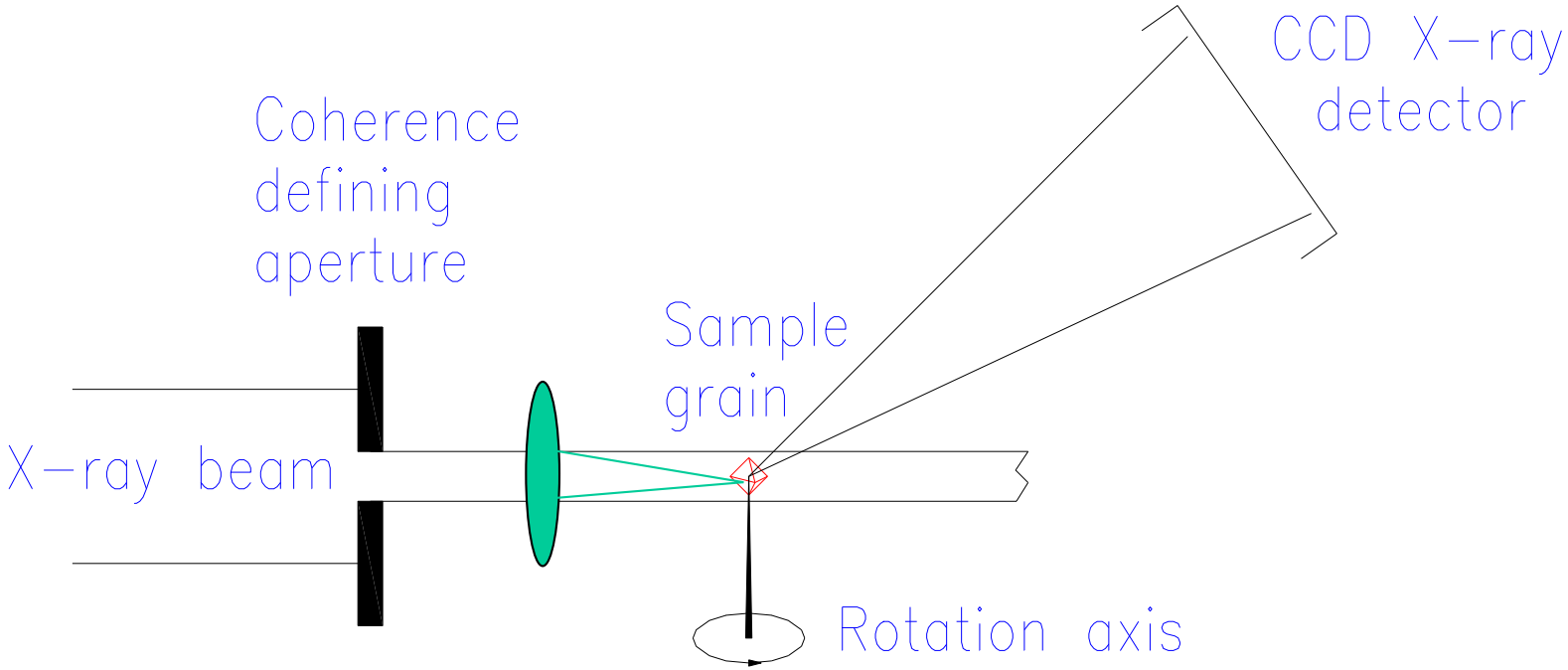
Modeling of 3D Phase Bump



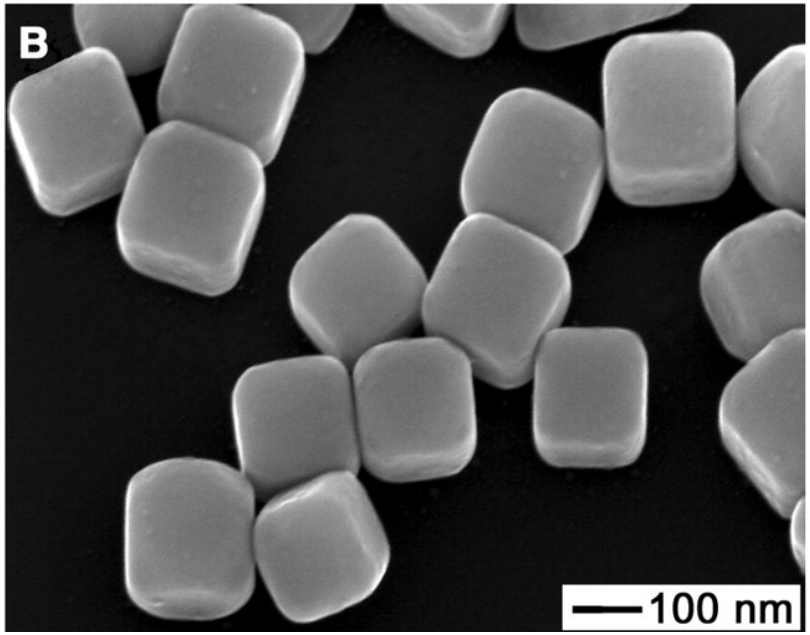
Field lines of Point Charges

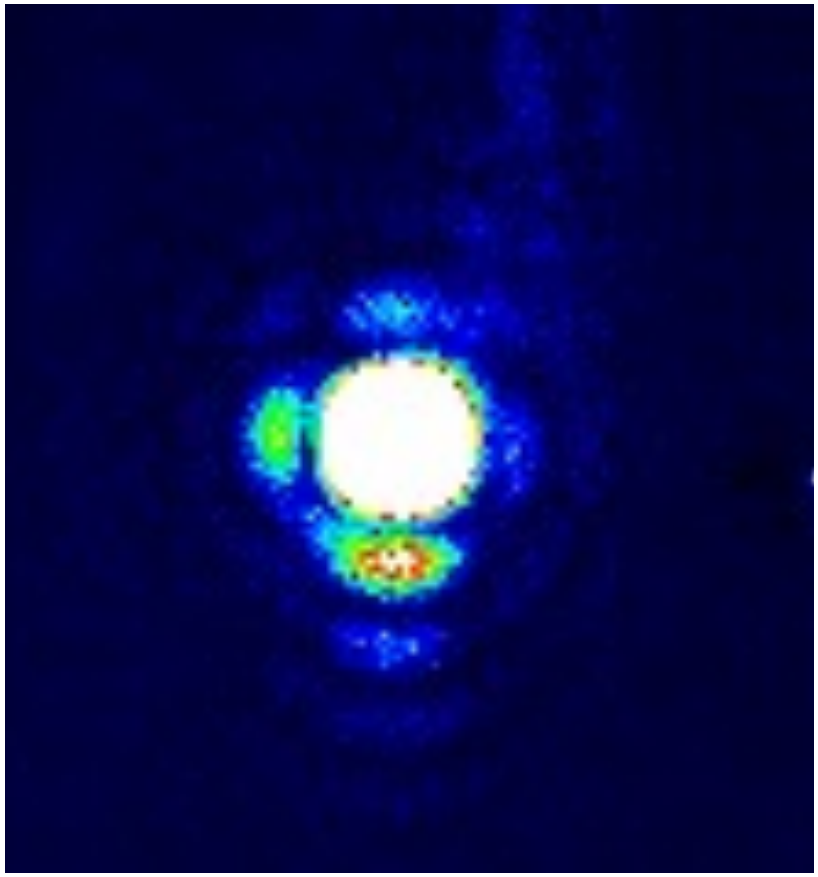


Lensless X-ray Microscope



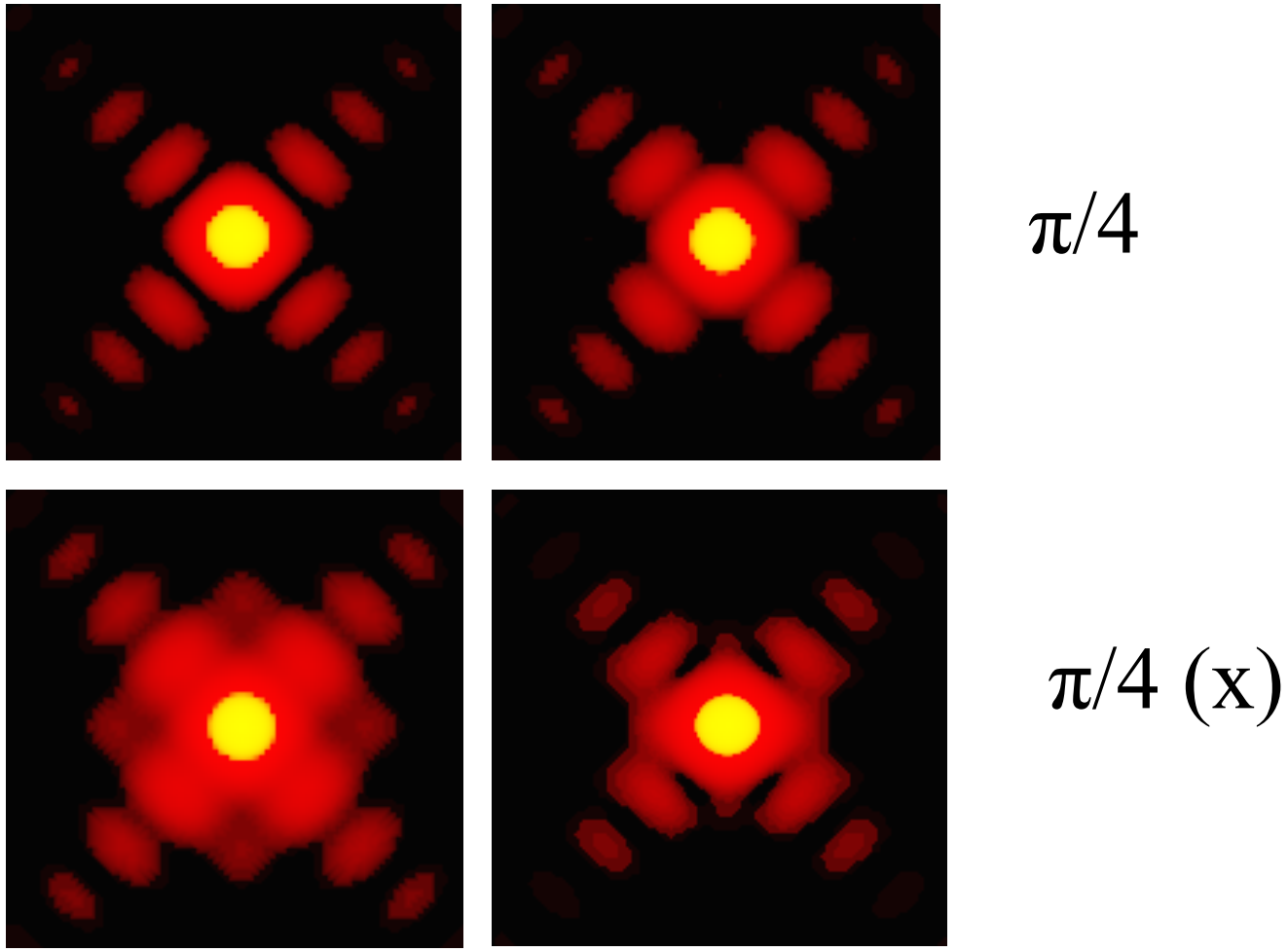
CXD from Silver Nanocubes





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

Spherical and cylindrical waves

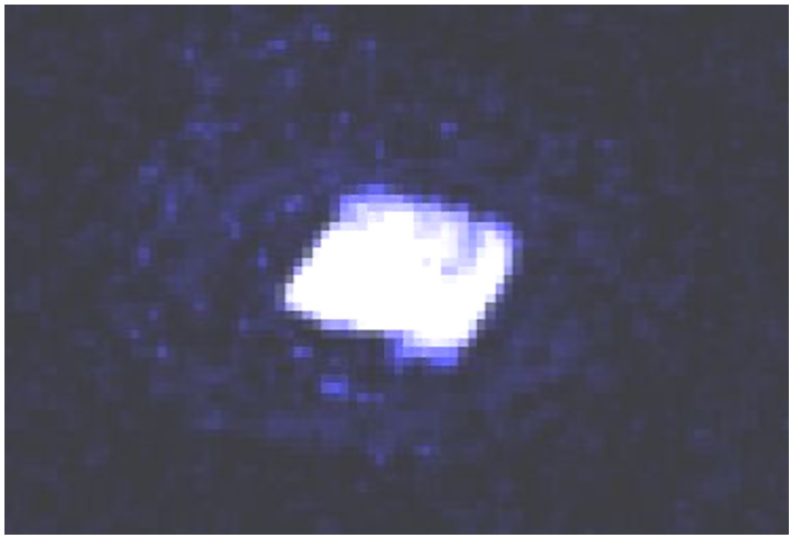


π/4

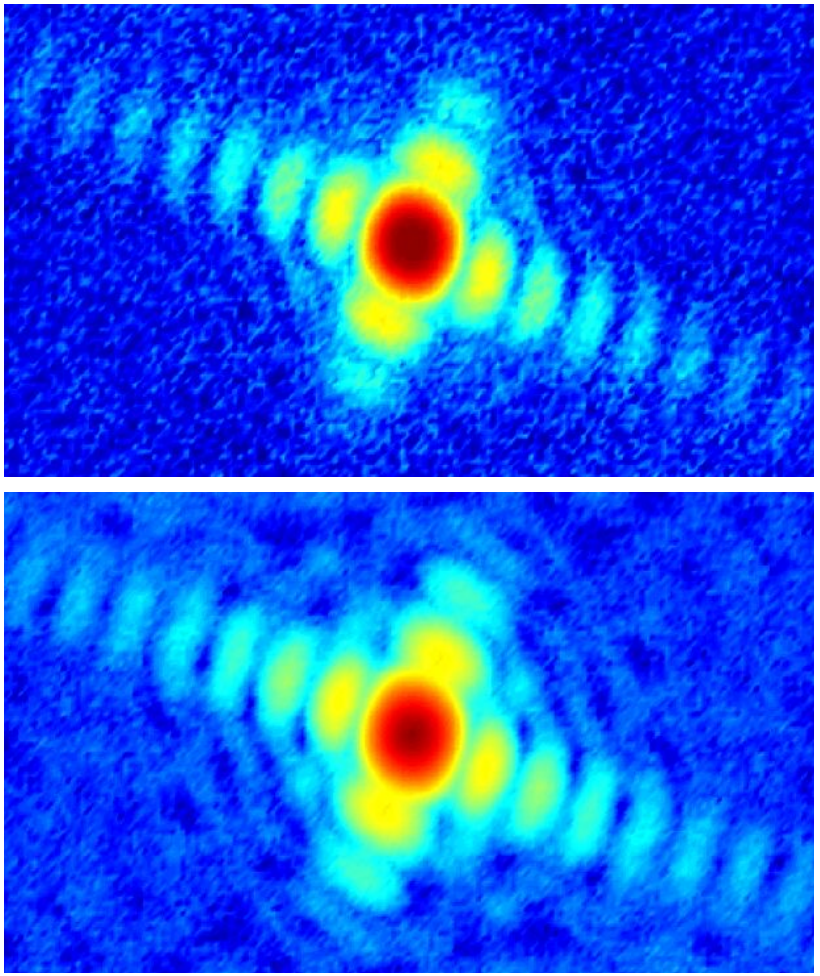
π/2

π/4 (x)

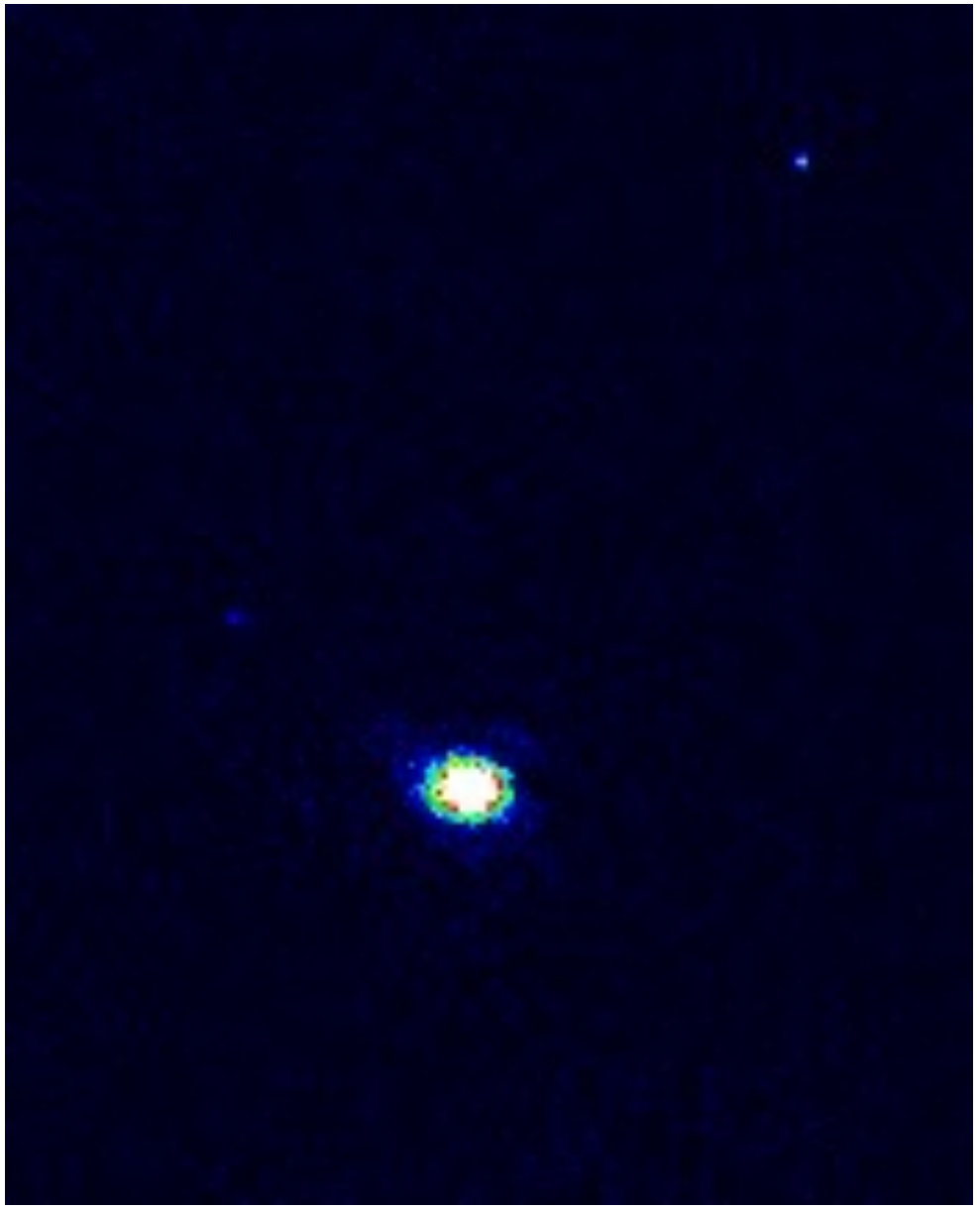
Reconstruction of Ag Nanocrystal

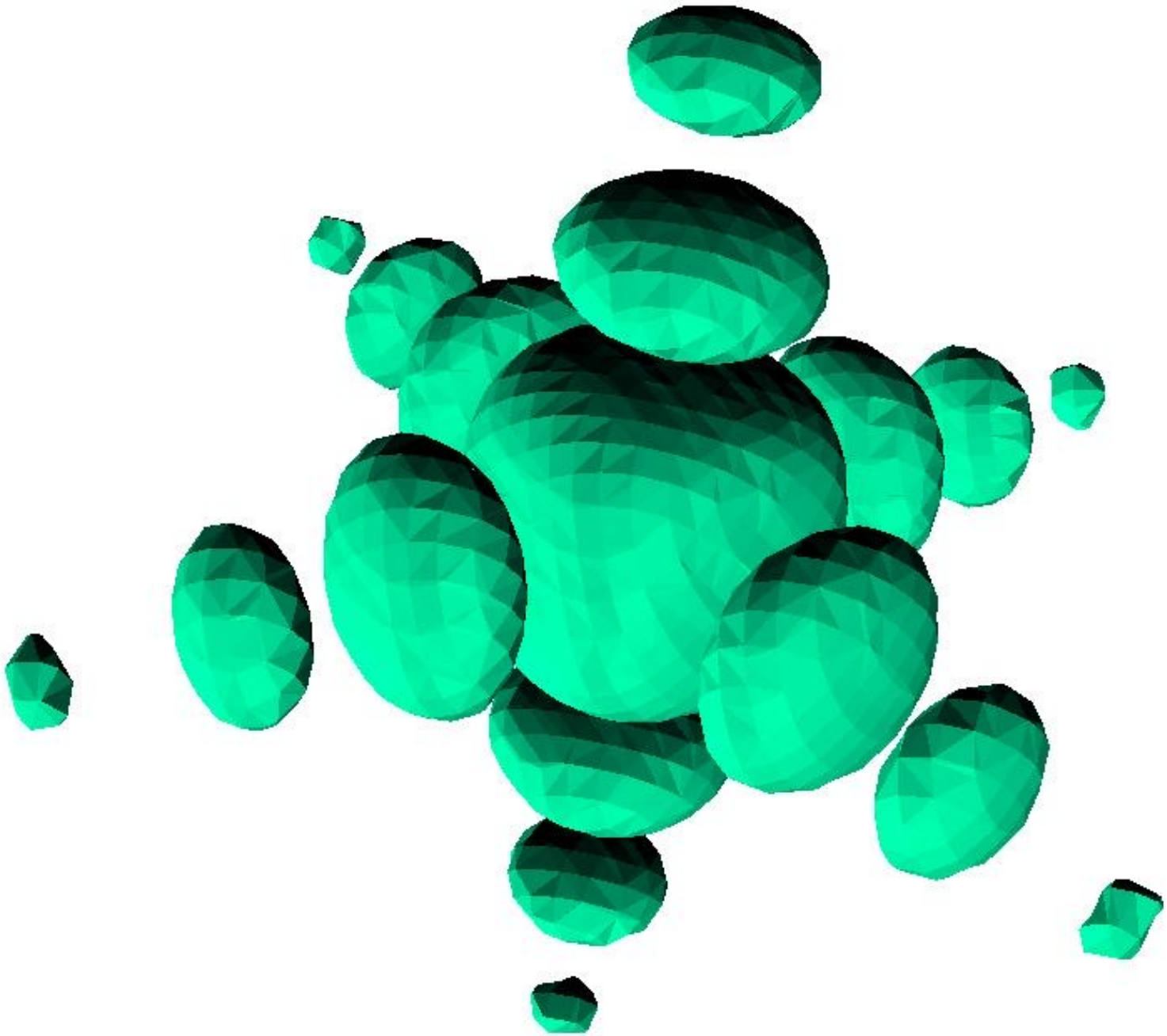


200nm



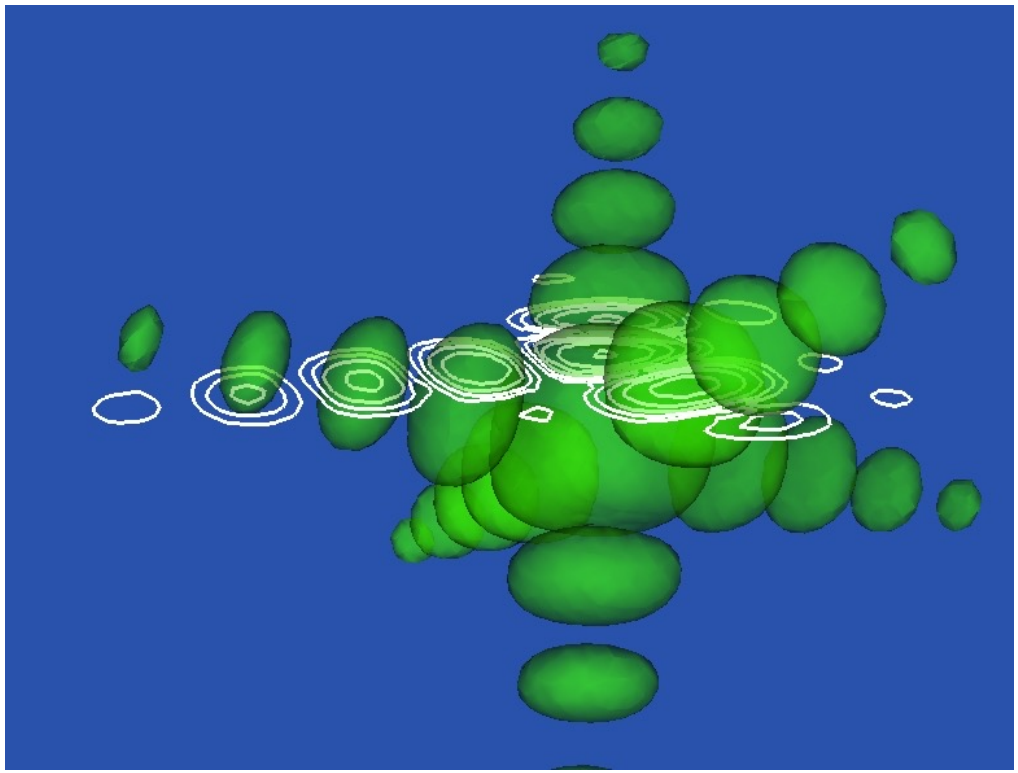
Rocking scan of Ag cubes with 0.01° steps





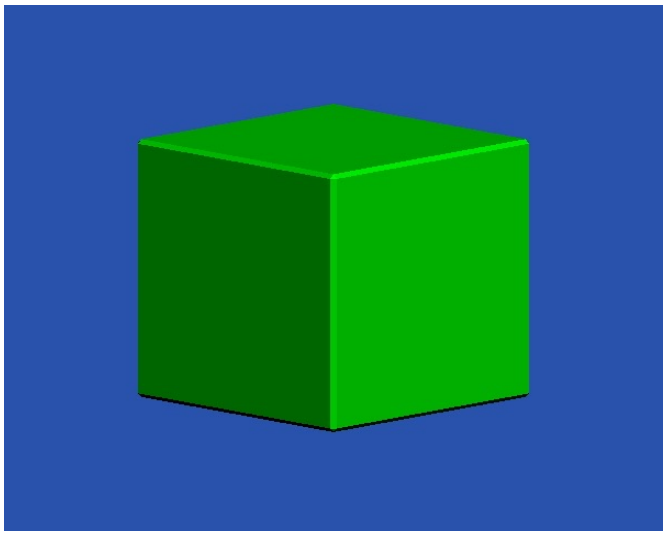
Miscentered Non-Centrosymmetric Reciprocal Space Slice

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

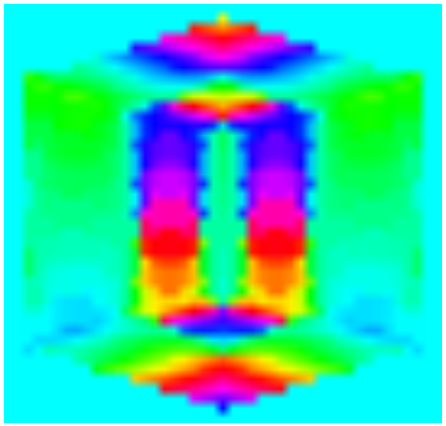


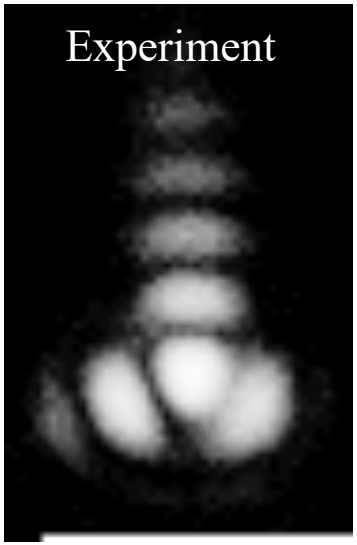
Real-space phase.

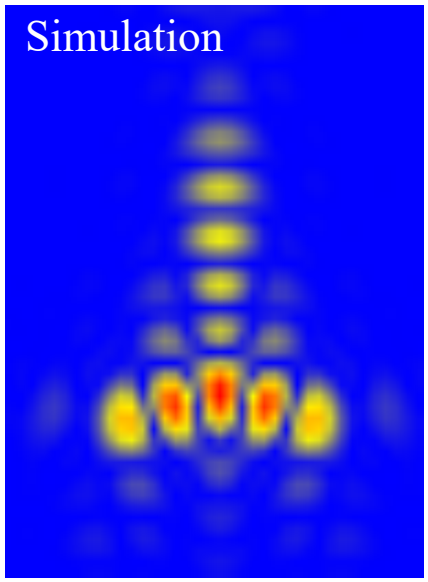
What can we expect to see?



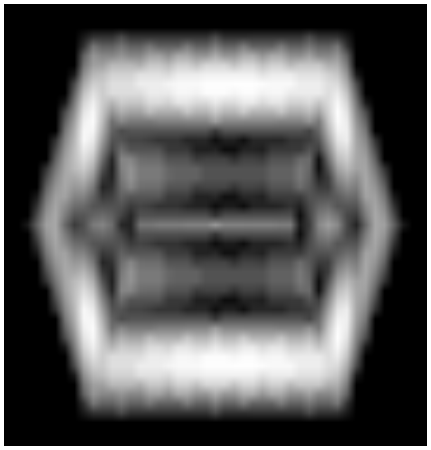
$$A(\bar{q}_o+\bar{q}_z)=\sum_i \sum_z \underbrace{\rho(x,y,z)}_{u_i\{x,y\}} e^{2\pi i \bar{q}_z\cdot\bar{z}_i} e^{2\pi i\{\bar{q}_o\}\cdot\bar{r}_i}$$

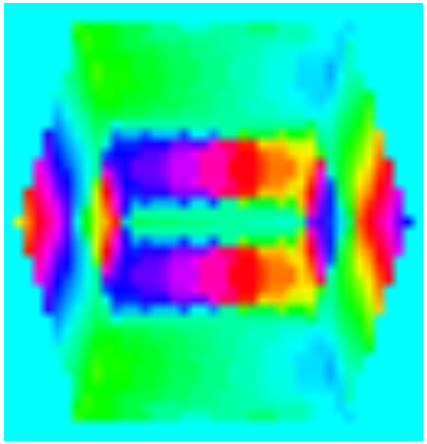


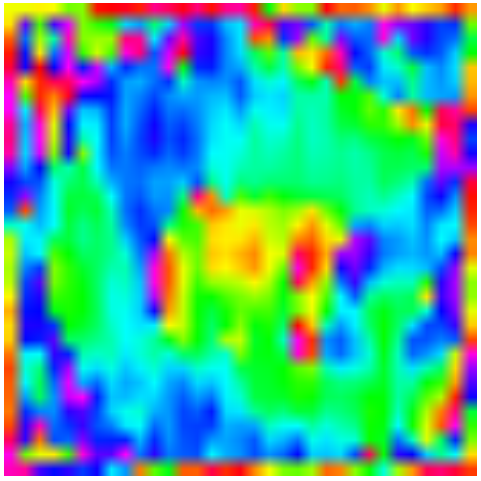


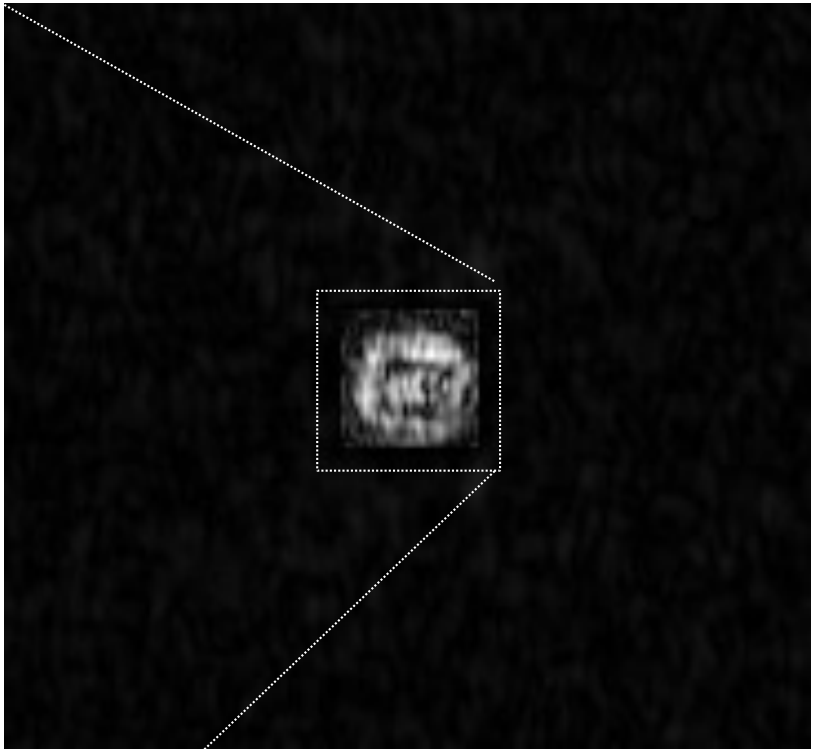


Direct Space Result (1000 Iterations)



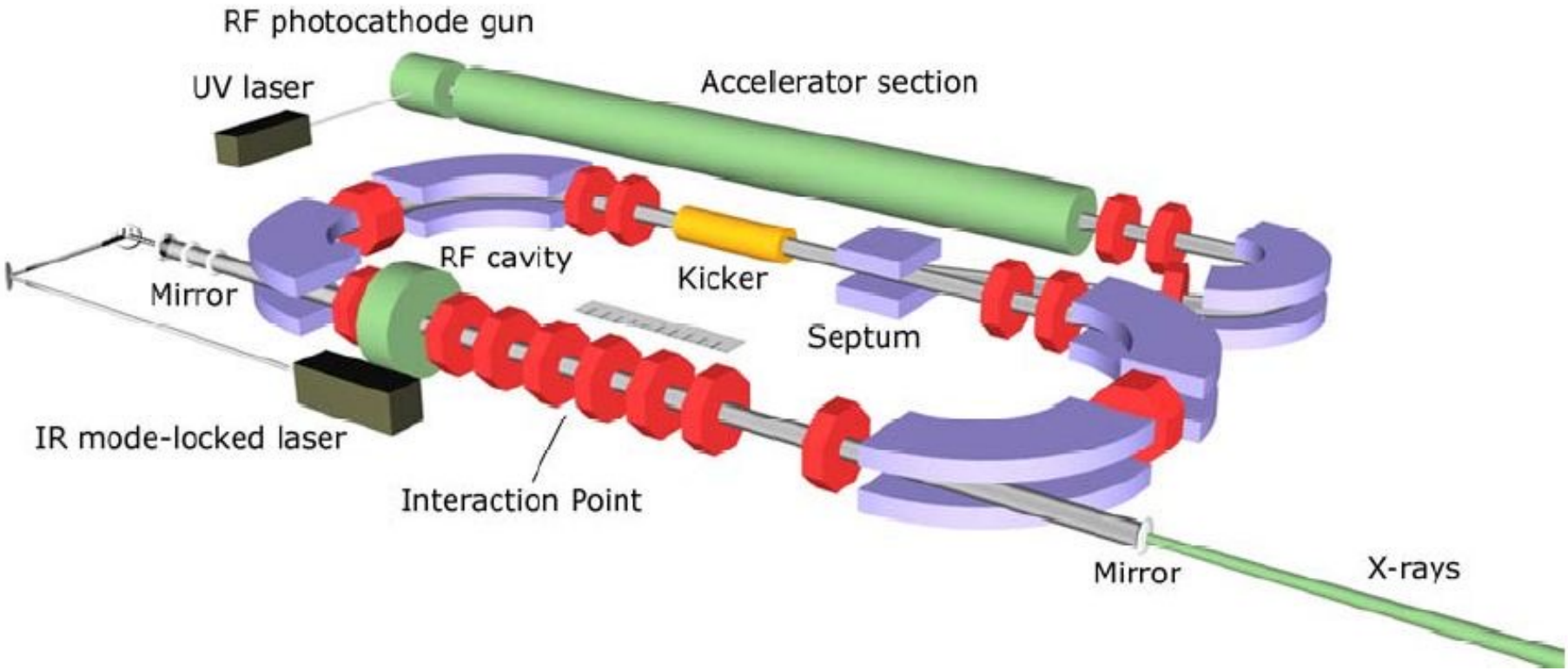


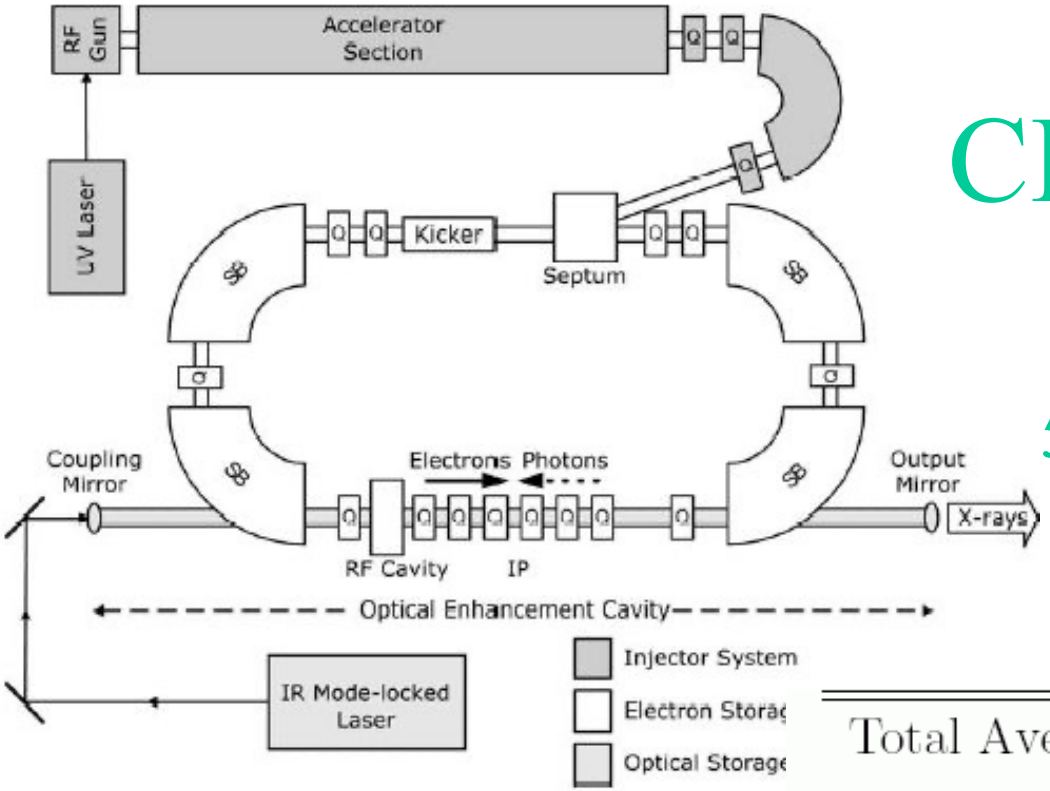




Compact Light Source

Ron Ruth, Lyncean Technologies





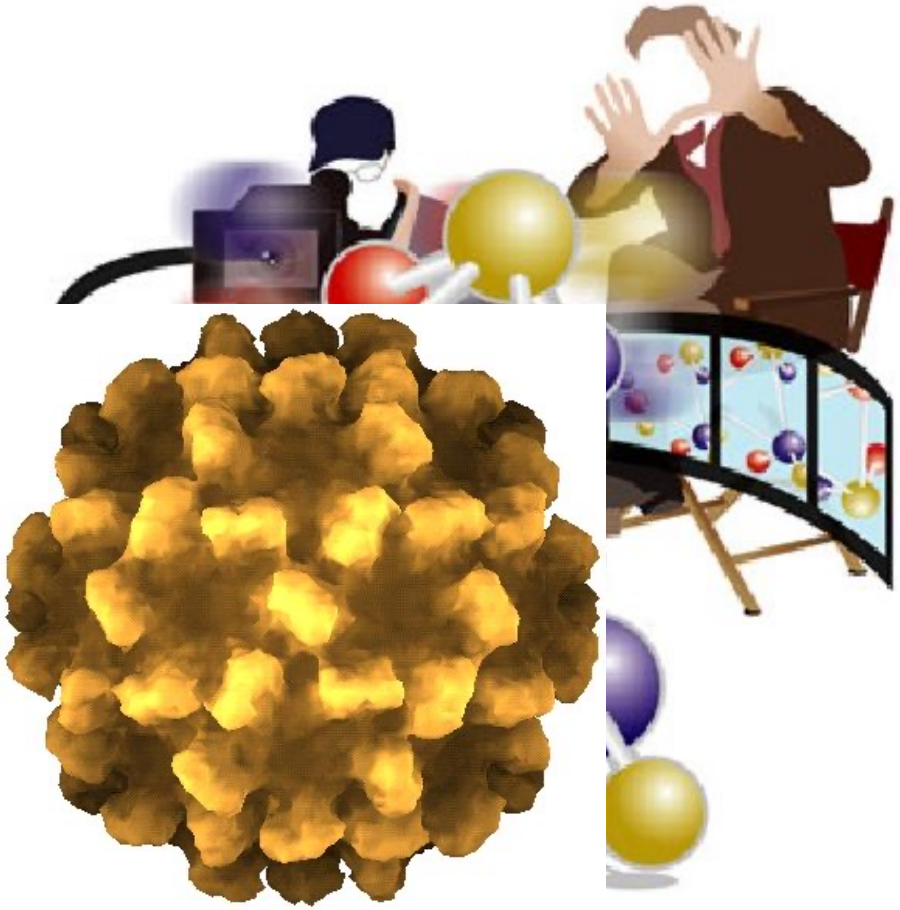
CLS Specifications

R. J. Loewen, Ph.D. Thesis
SLAC (2003)
50MeV (γ=100) + 1μm laser

$$\omega = \frac{4\gamma^2}{(1+\gamma^2\theta^2)}\,\omega_0$$

Total Average Flux	$\gtrsim 10^{13}$ ph/s
Avg. "Monochromatic" Flux*	$\approx 10^{10}$ ph/s
Source Spot Size†	30 μm radius
Source Divergence†	$\approx$ 3 mrad
Source Brightness	$\gtrsim 10^{11}$
X-ray Energy Range‡	12 keV $\pm$ 6 keV

Molecular Movies using XFEL



I. K. Robinson ICTP, Trieste

Conclusions

- Imaging of nanocrystals by phase retrieval
- 3D imaging to see inside structure
- Phase contrast to access strains
- Off-center diffraction implies phase also
- Extension to CLS and XFEL