Quantitative 3D Imaging of Nanomaterials by Using Coherent X-rays

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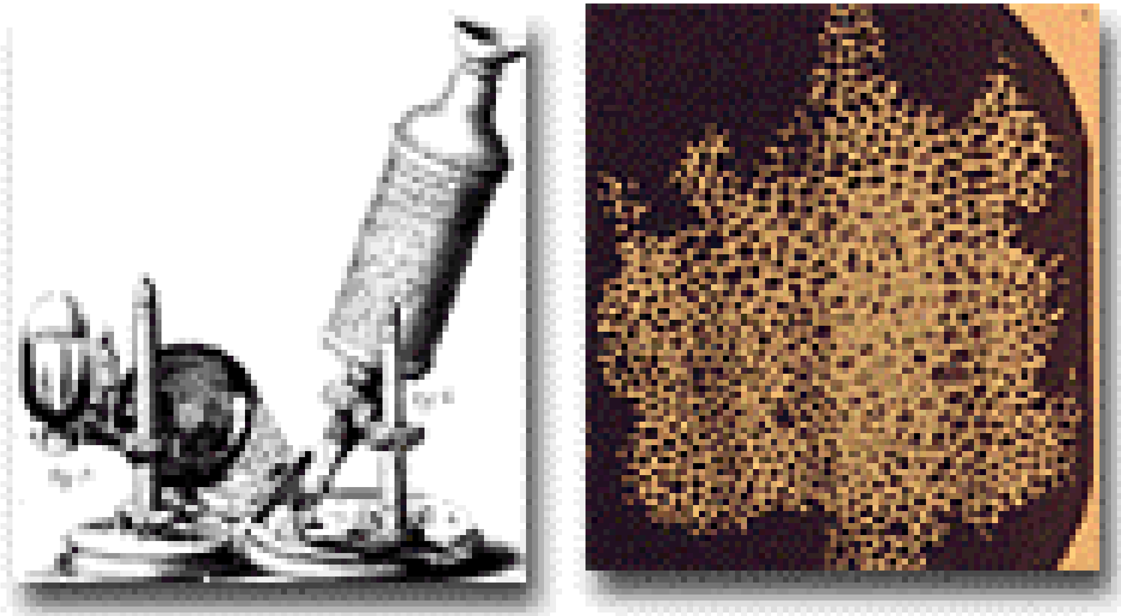
Workshop on Almost Impossible Materials Science:
Pushing the Frontier with ERL X-ray Beams, June 16 & 17, 2006

The First Compound Light Microscope Based on a Three Lenses Conformation

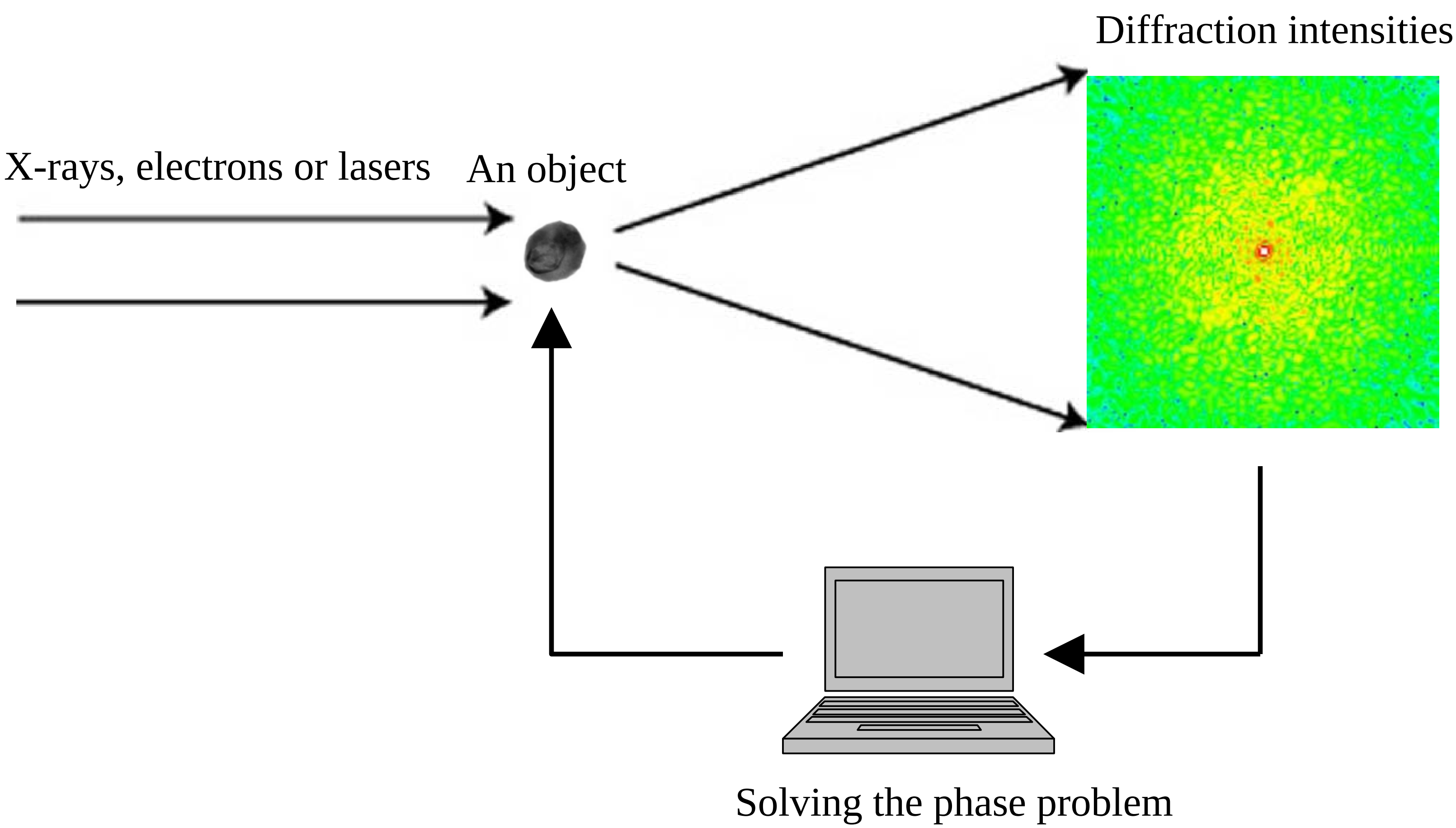


Hooke’s compound light microscope and a drawing of cork made by Hooke.

1611 **Kepler** suggested that a compound light microscope could be constructed based on a three lenses conformation.

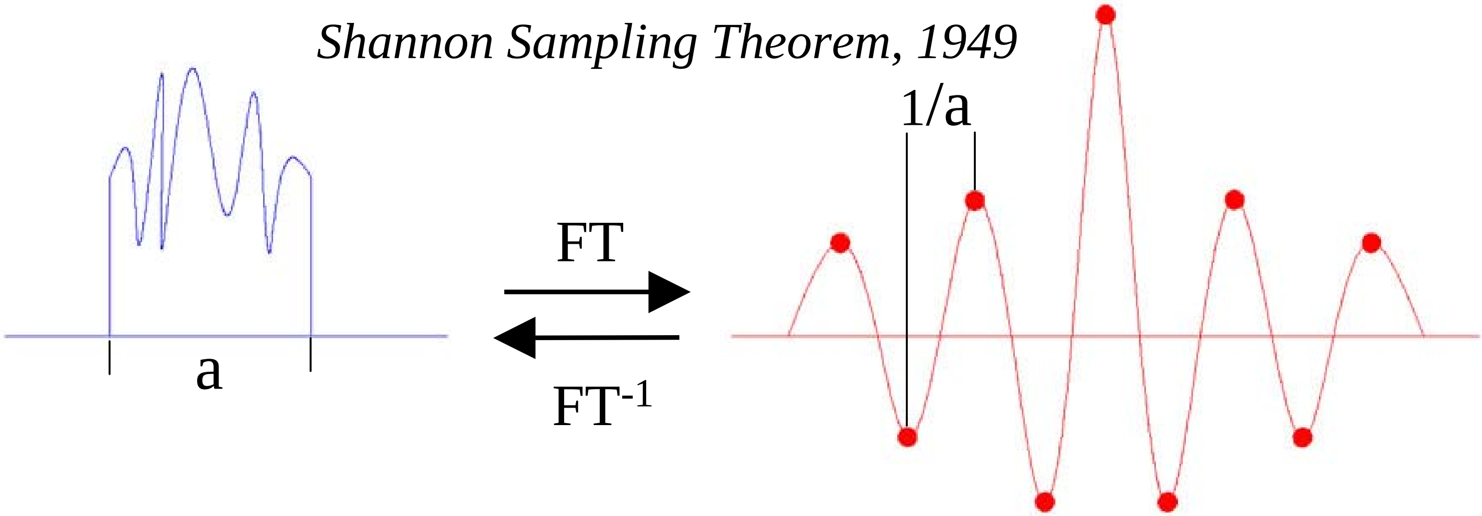
1665 **Hooke** built the 1st compound light microscope and imaged small pores in sections of cork he called “cells”

A New Type of Microscopy – Coherent (*i.e.* Lensless) Imaging

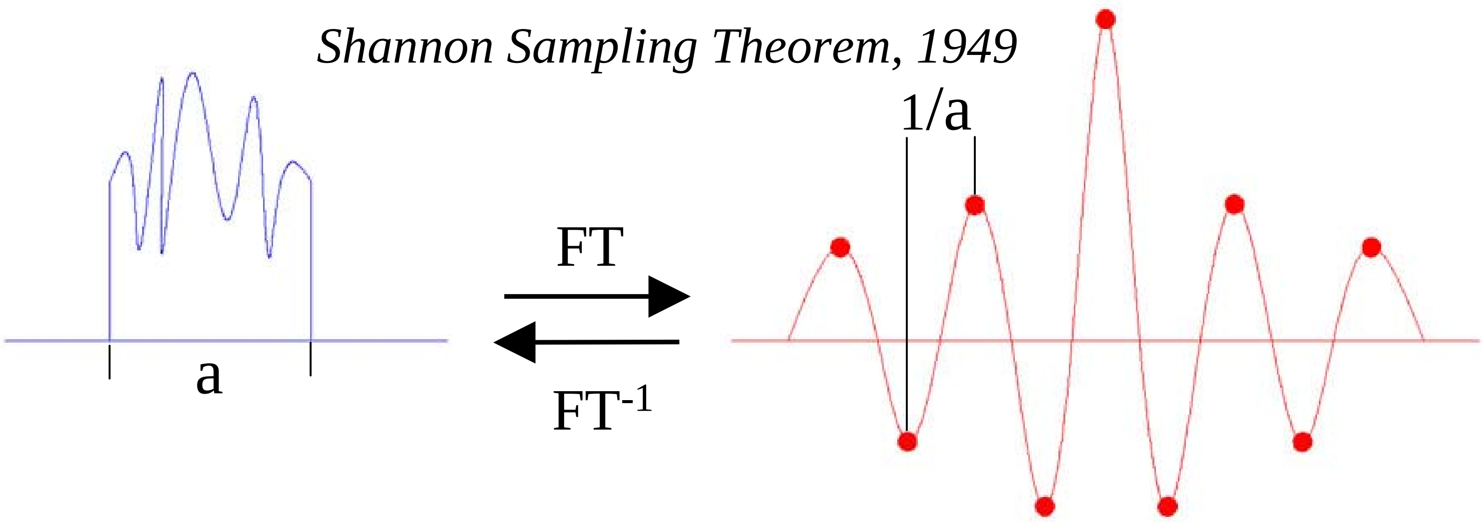


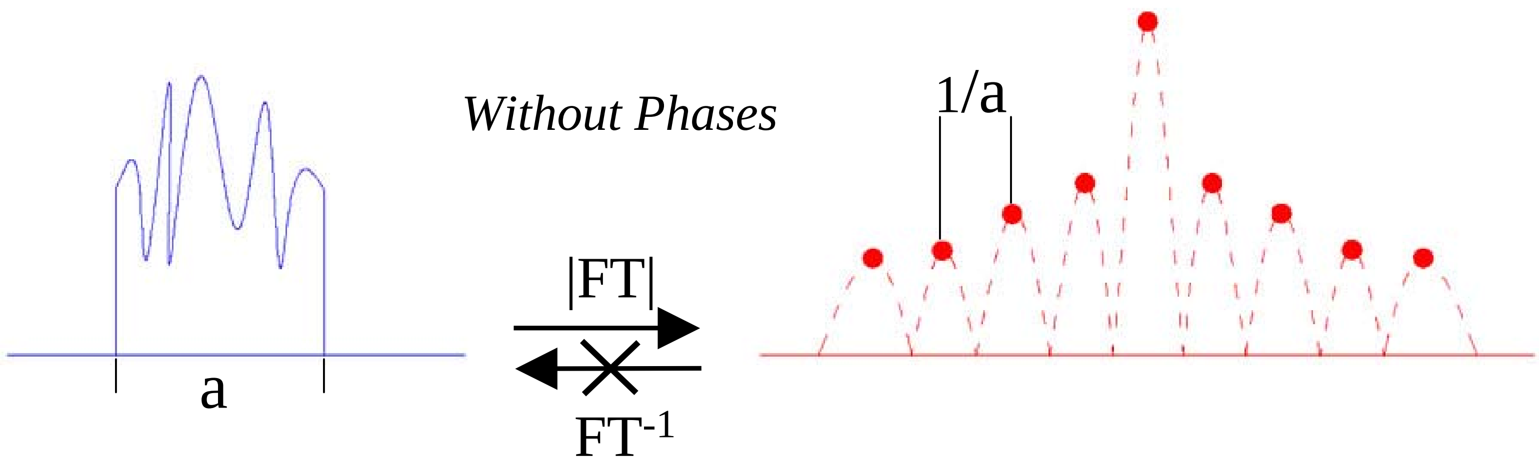
The Shannon Sampling Theorem

Shannon Sampling Theorem, 1949

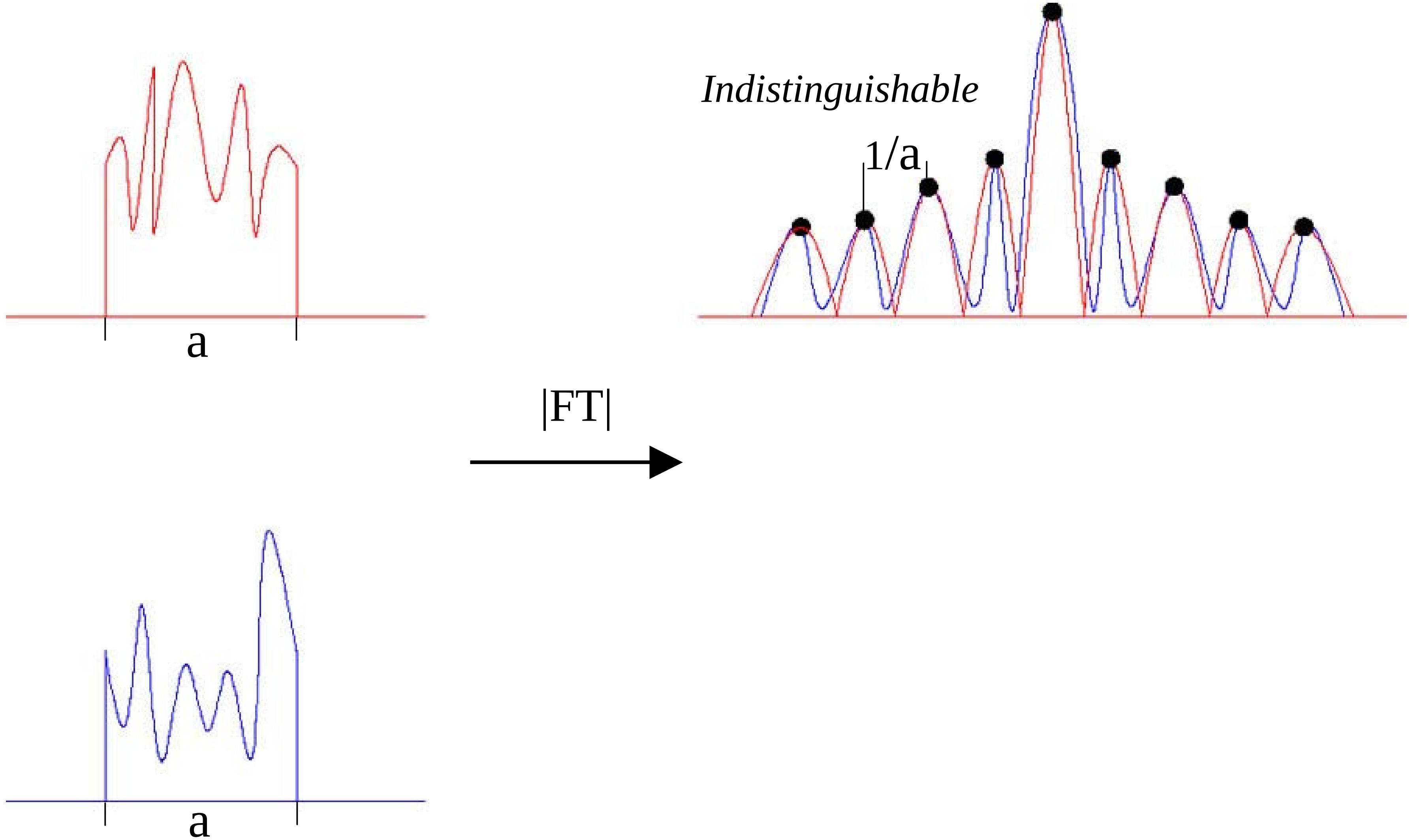


The Shannon Sampling Theorem

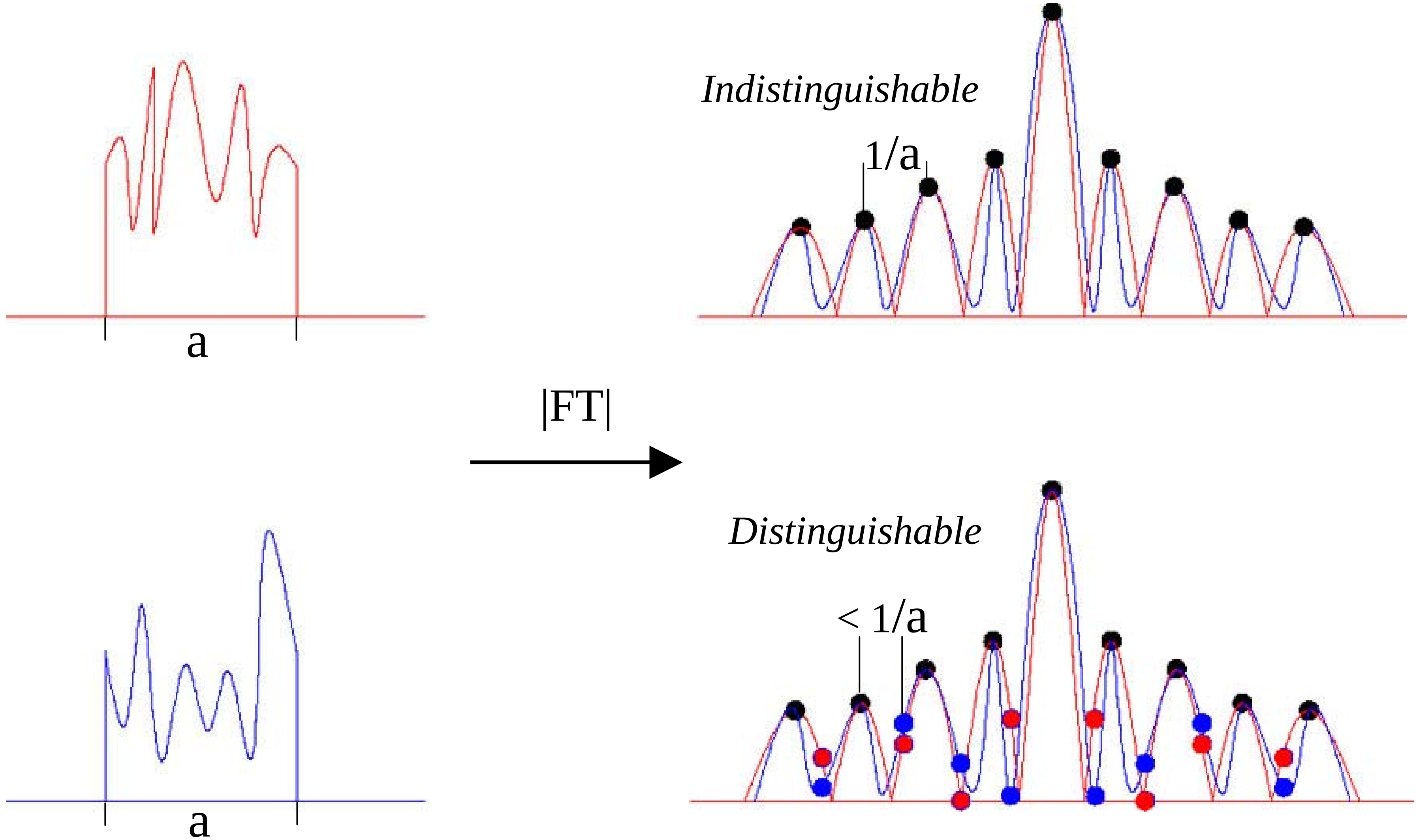




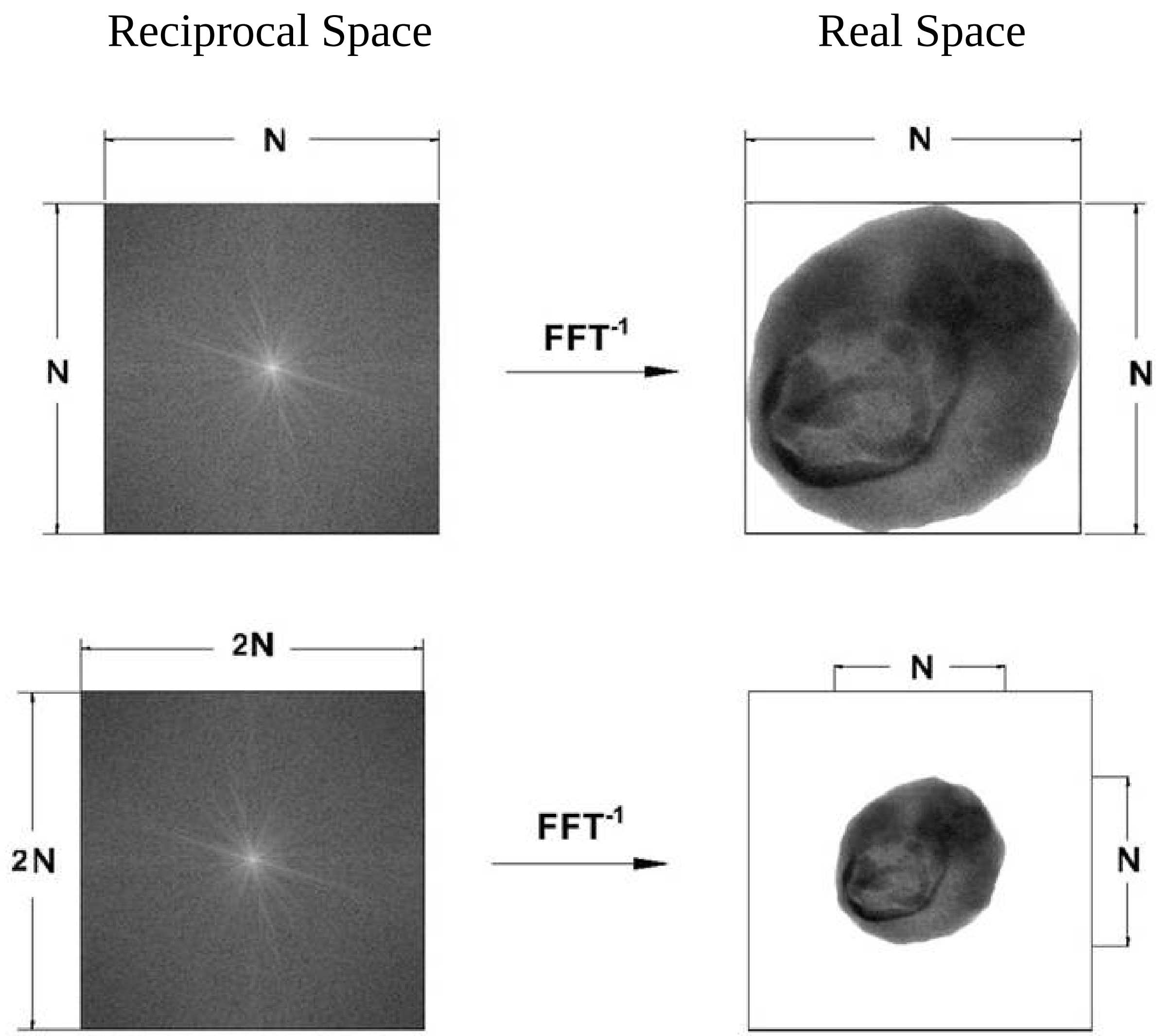
The Oversampling Method



The Oversampling Method

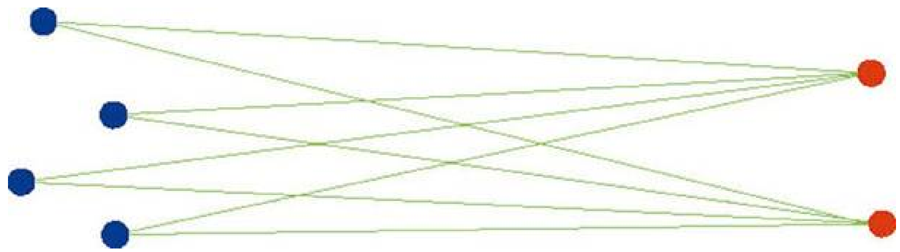


Experimental Implementation of the Oversampling Method

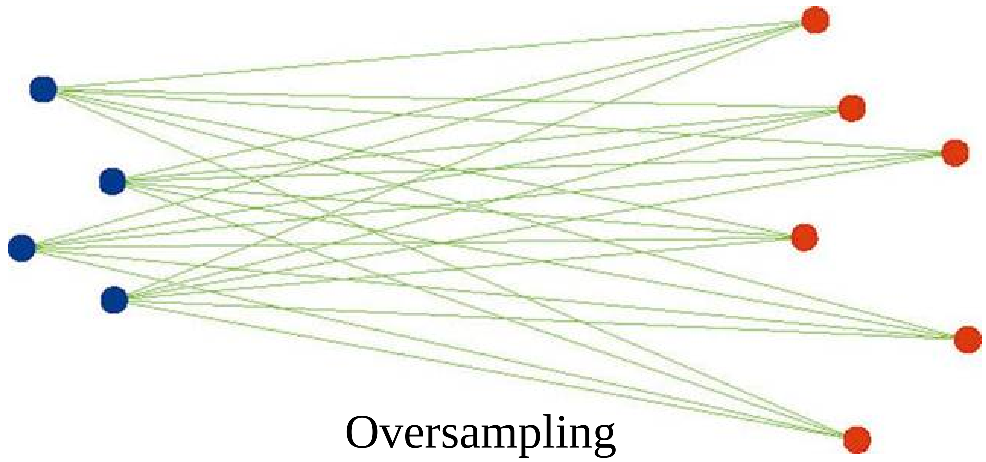


The Physical Explanation to the Oversampling Method

Real Space | Reciprocal Space



Nyquist sampling frequency



Oversampling

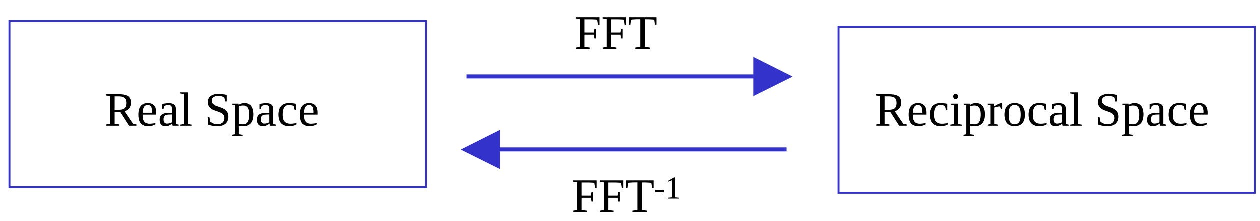
Better coherence ⇒ More correlated intensity points ⇒ Phase information

Miao, Sayre & Chapman, *J. Opt. Soc. Am.* A **15**, 1662 (1998).

The Guided Hybrid Input-Output Algorithm

(i) Started with 16 independent reconstructions.

(ii) For each reconstruciton:



(iii) Select a seed out of 16 images, ρ_{seed}, corresponding to the smallest R-value.

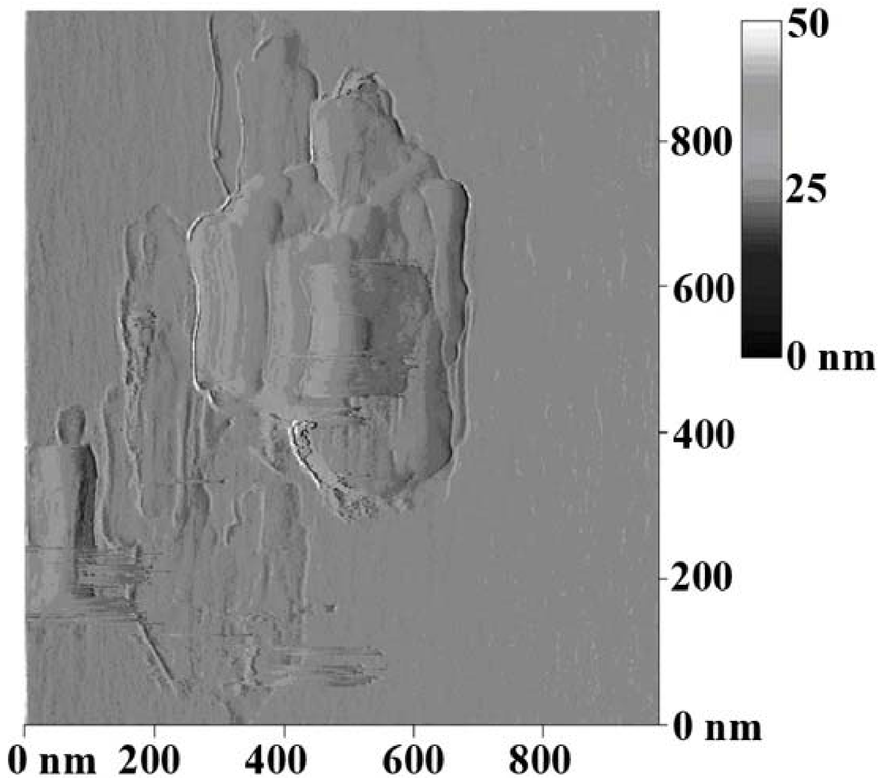
$$R = \sum \left| F_{\exp} - \alpha F_{cal} \right| \Big/ \sum F_{\exp}(k_x, k_y)$$

(iv)

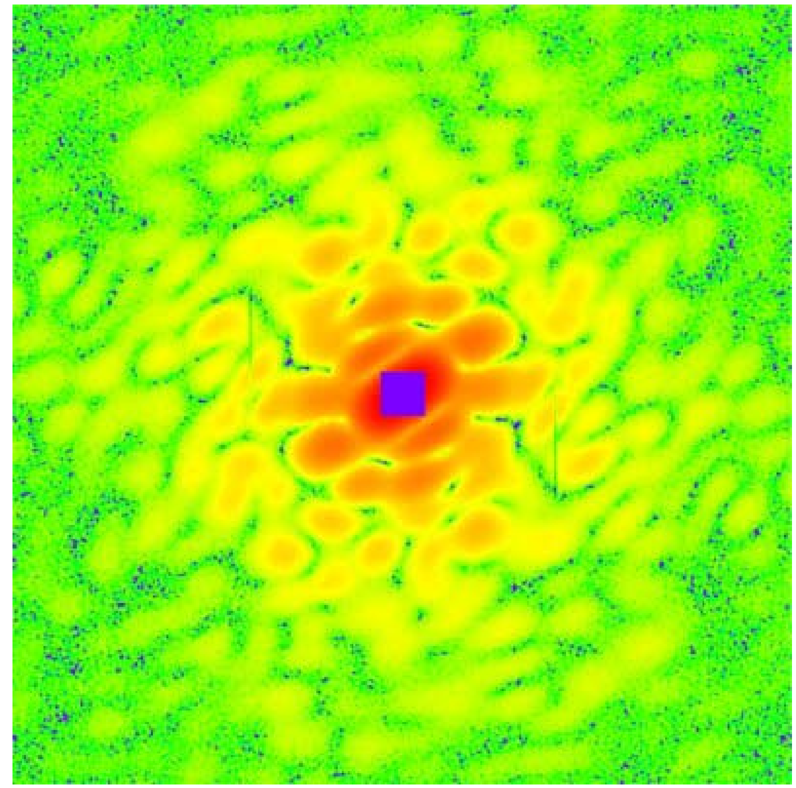
$$\rho^i_{new} = \sqrt{\rho_{seed} \times \rho^i_{old}}$$

$$i = 1, 2, \cdots, 16$$

Coherent X-ray Diffraction Pattern from a Single GaN Quantum Dot Nanoparticle

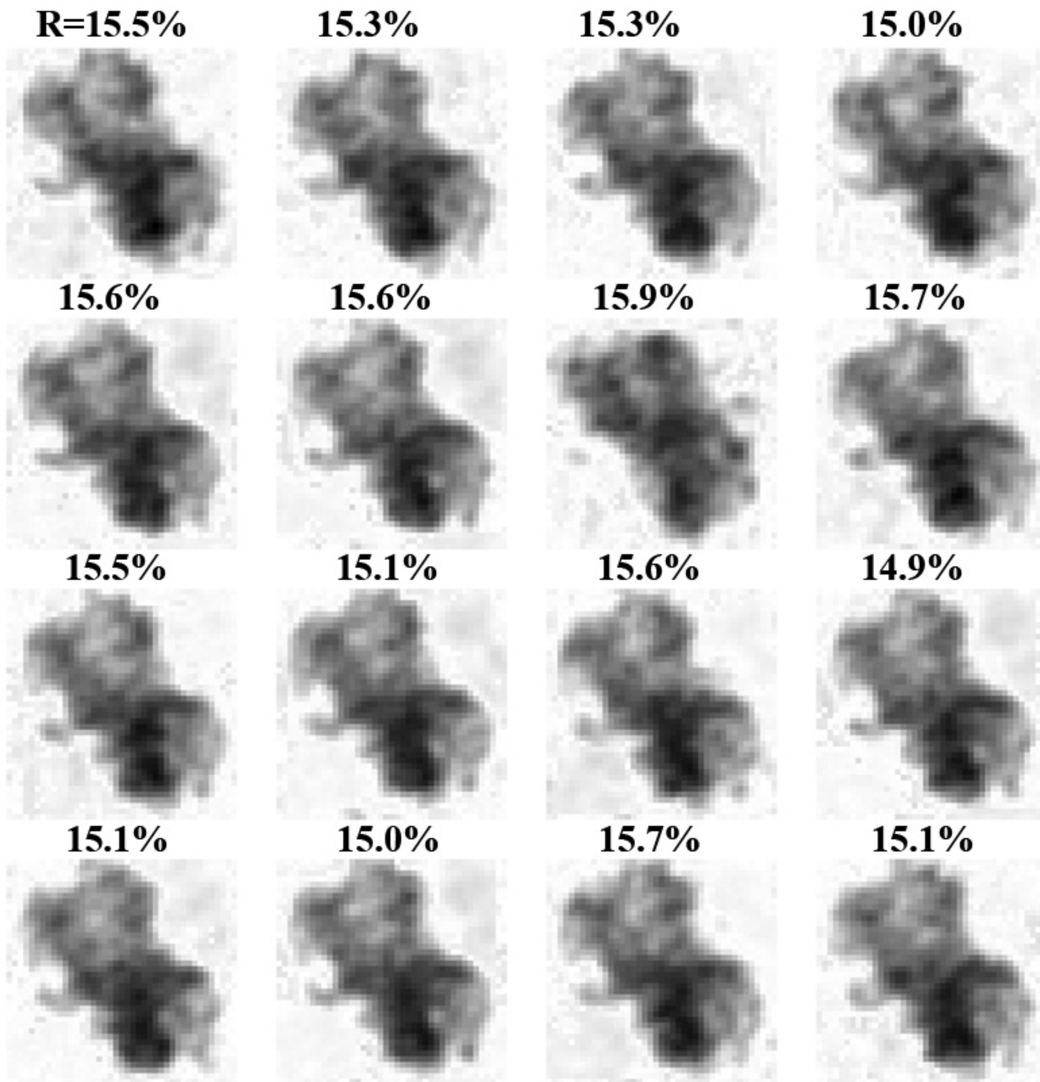


An AFM Image of GaN quantum dots, showing the platelet structures.



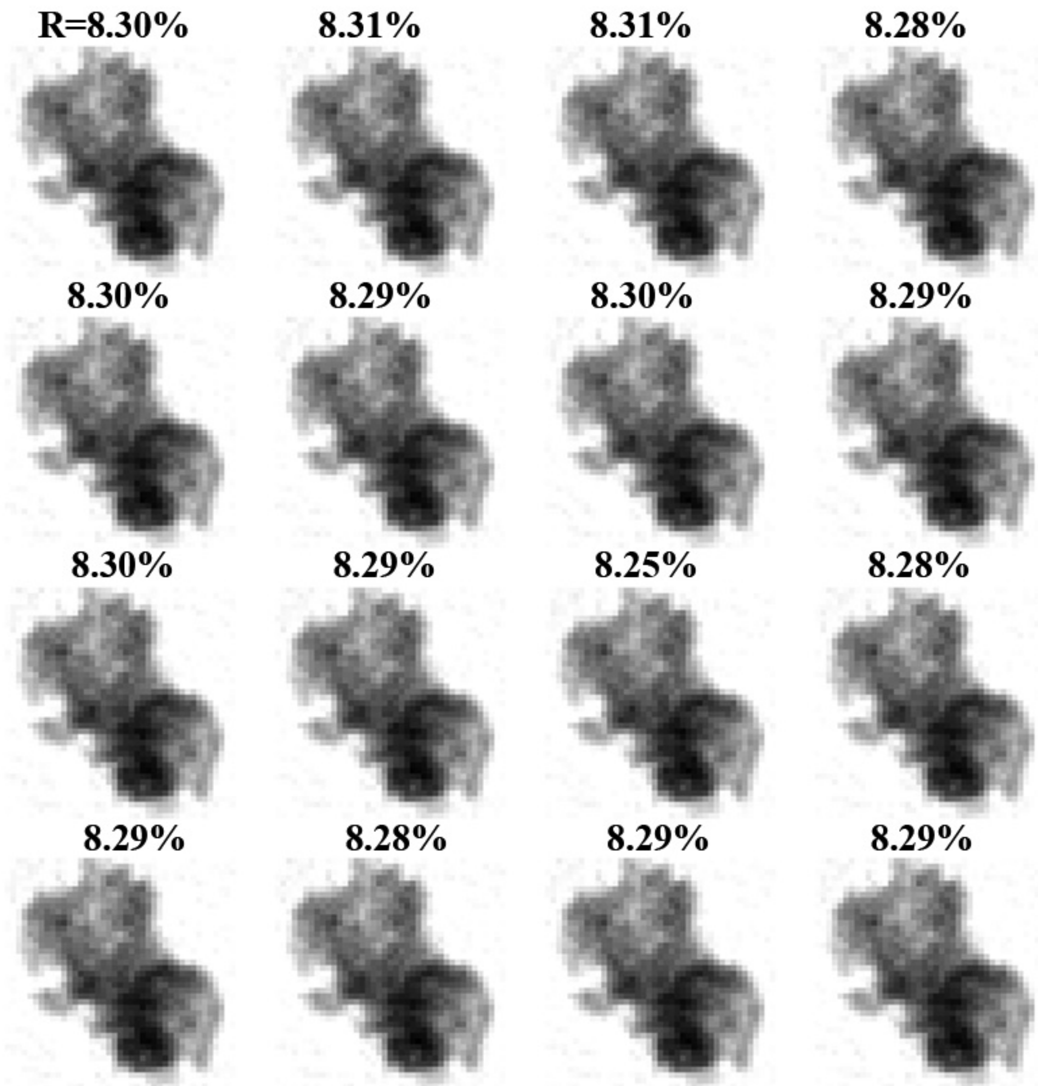
An oversampled diffraction pattern from a single GaN quantum dot at 0°

Image Reconstruction Using the gHIO Algorithm



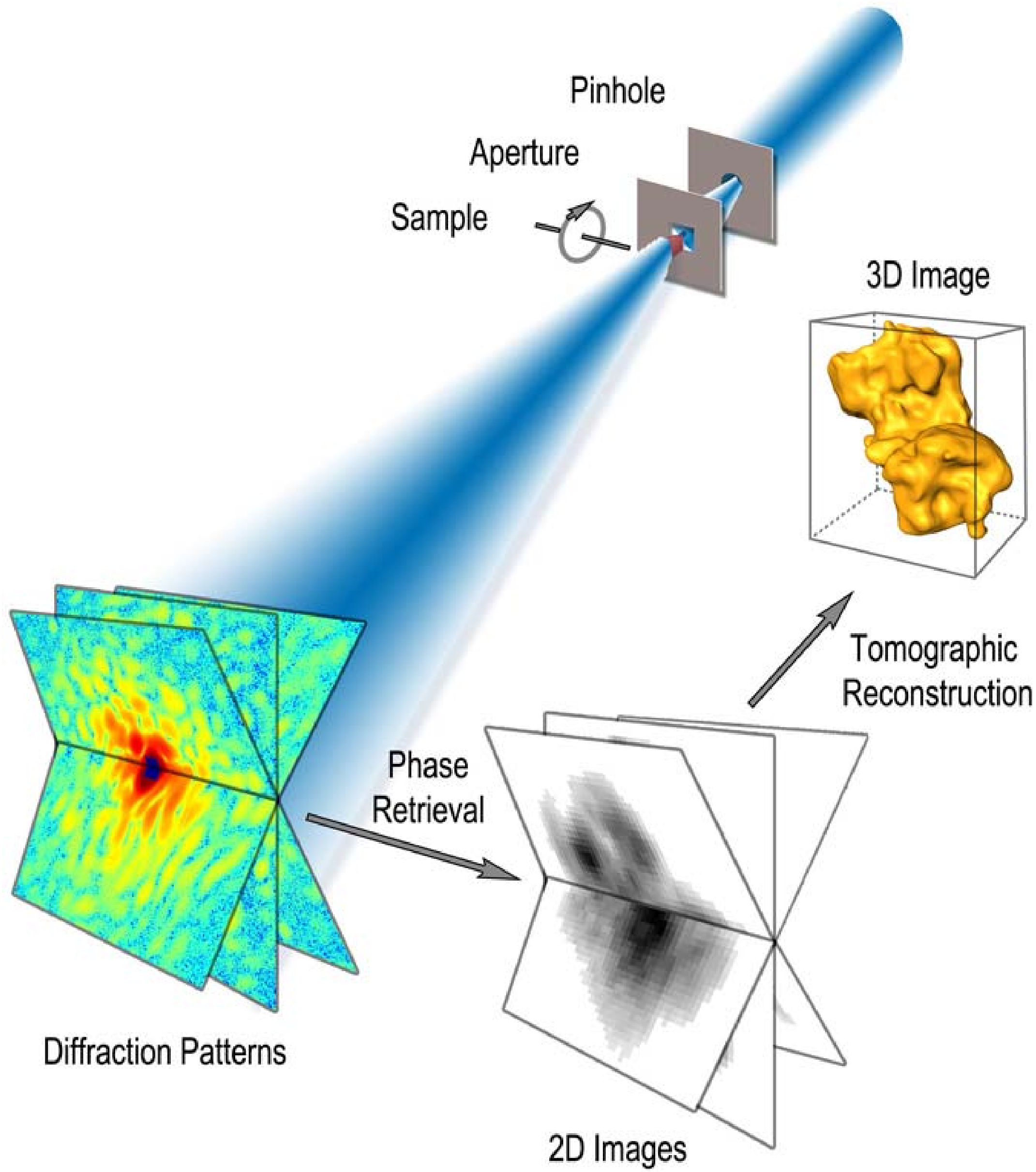
The 0th generation

Image Reconstruction Using the gHIO Algorithm

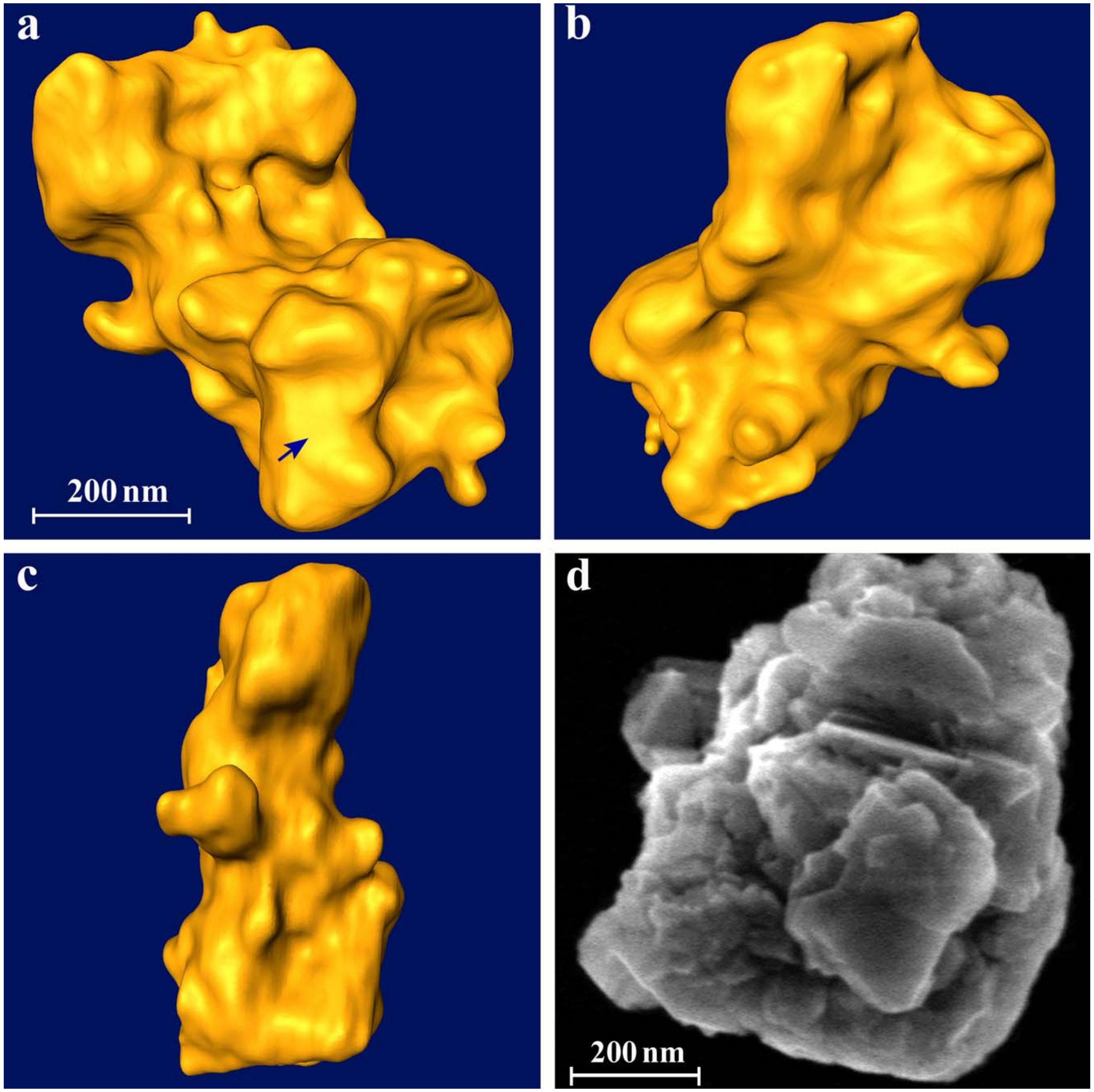


The 8th generation

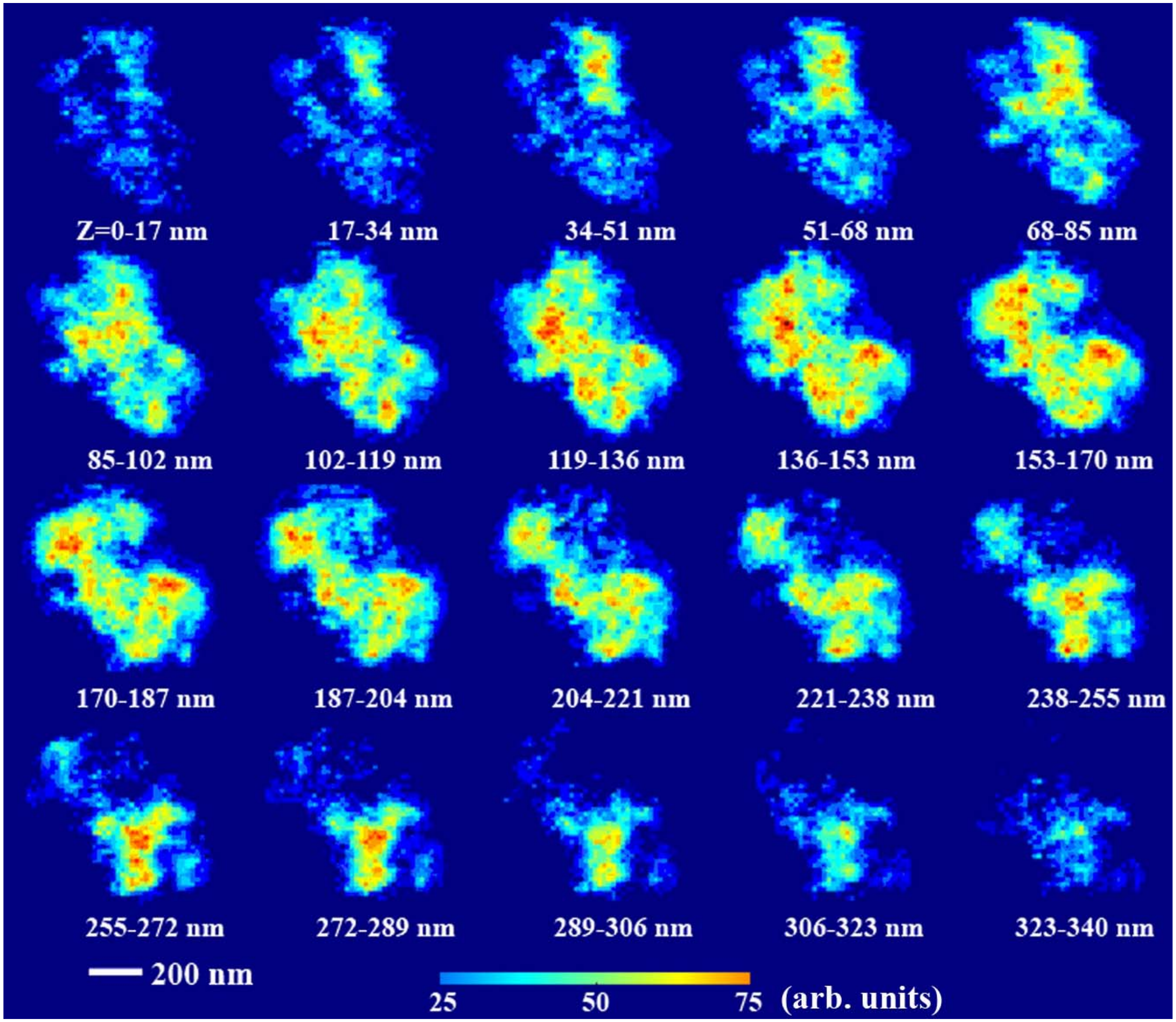
A New Strategy for 3D Lensless Imaging



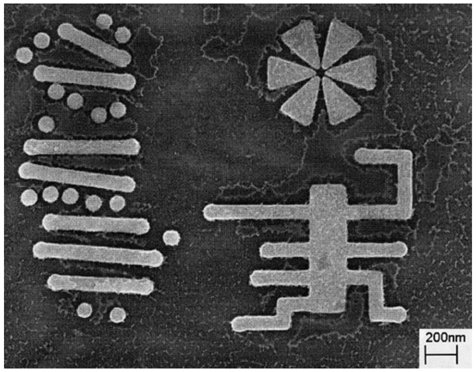
3D Surface Morphology of the GaN Quantum Dot Nanoparticle



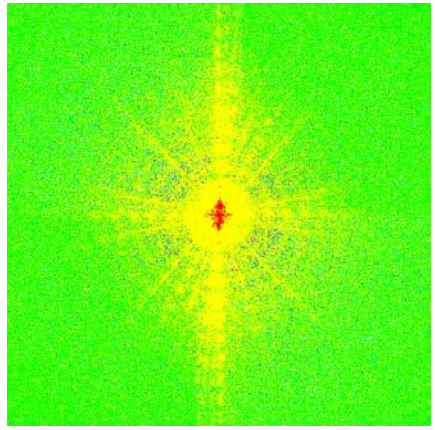
Quantitative 3D Internal View of the GaN Quantum Dot Nanoparticle



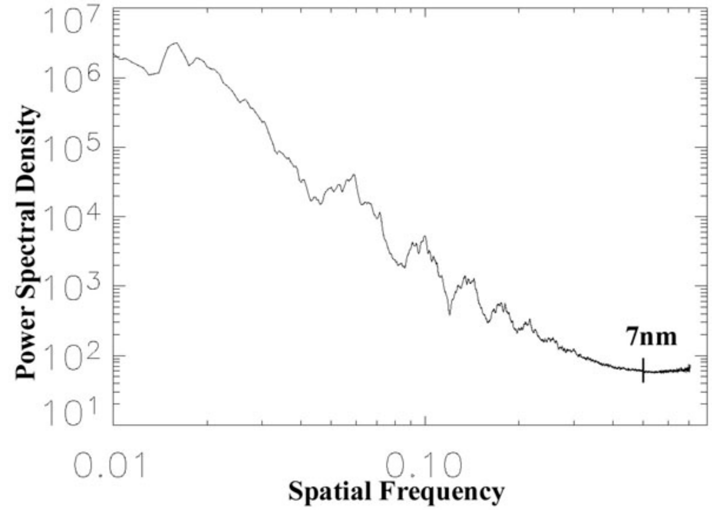
Imaging Nanostructures at 7 nm Resolution



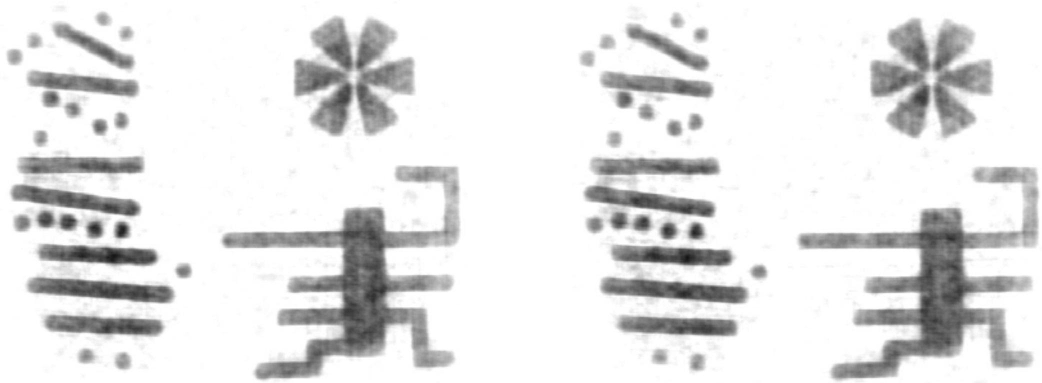
(a) A SEM image of a patterned sample made of Au



(b) A coherent diffraction pattern from (a)

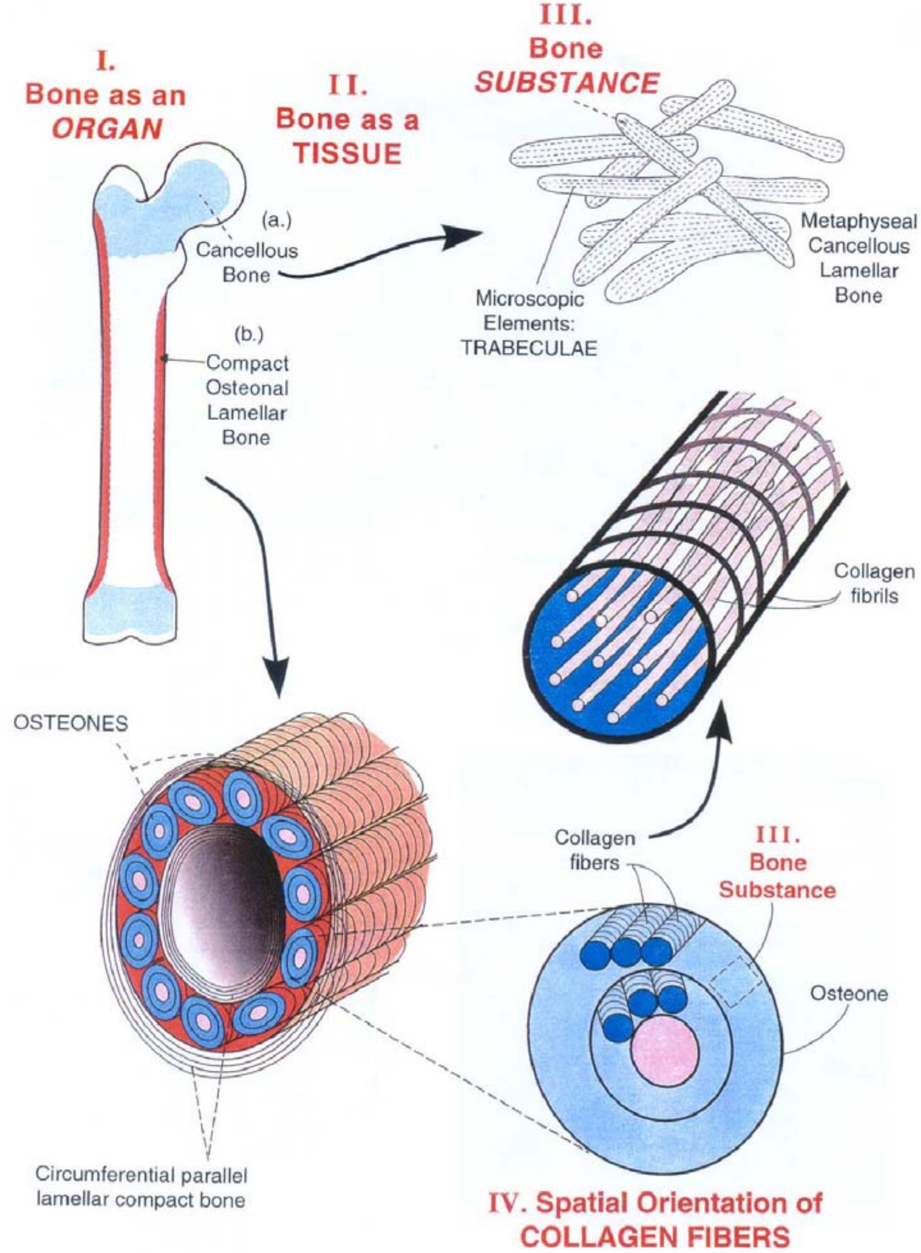


(c) Power spectral density of the diffraction pattern

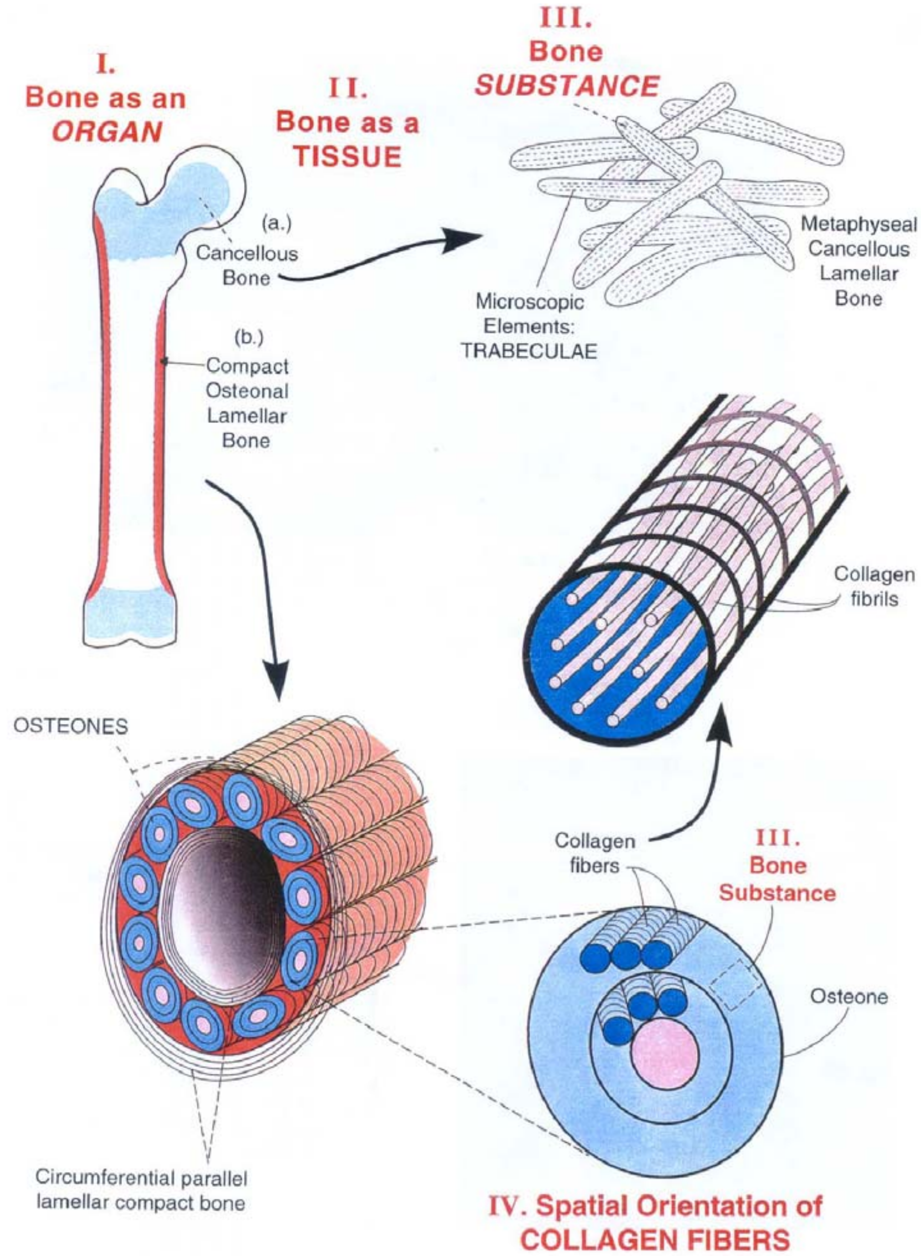


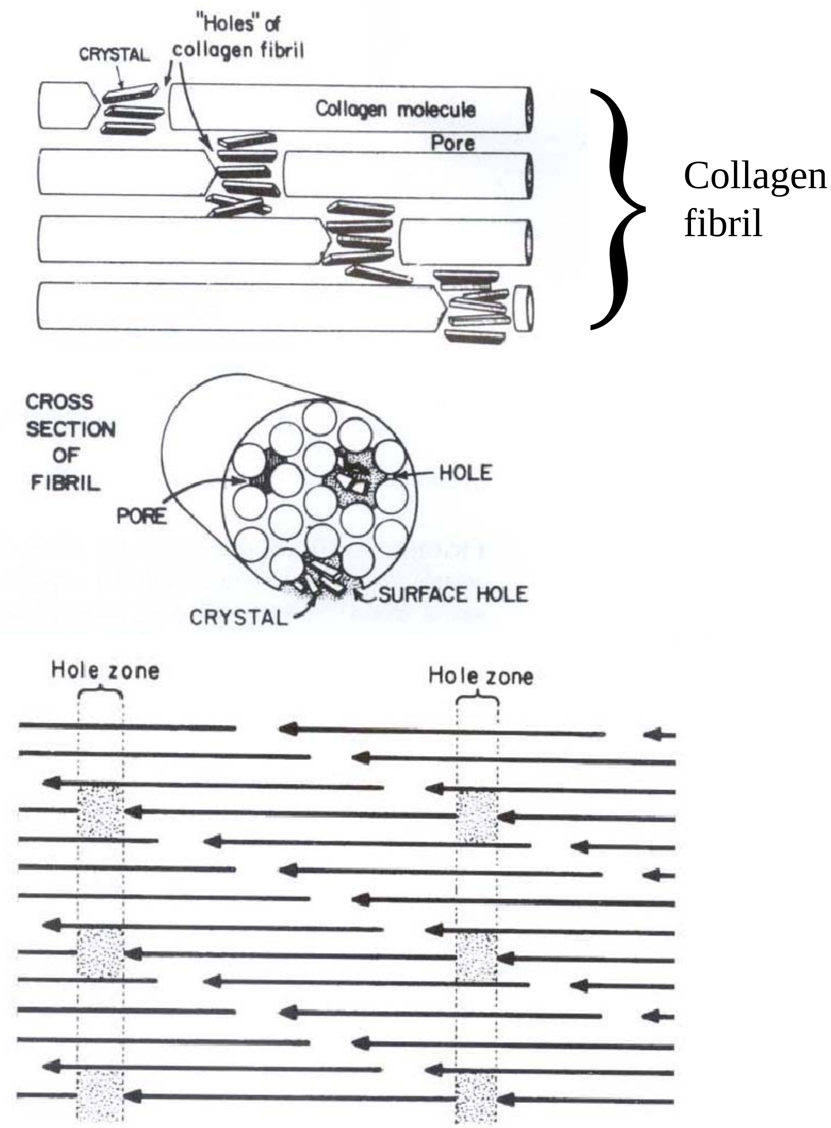
(d) Images reconstructed from (b) with two different initial seeds.

Hierarchic Structure of Bone and the Hodge Model (1963)

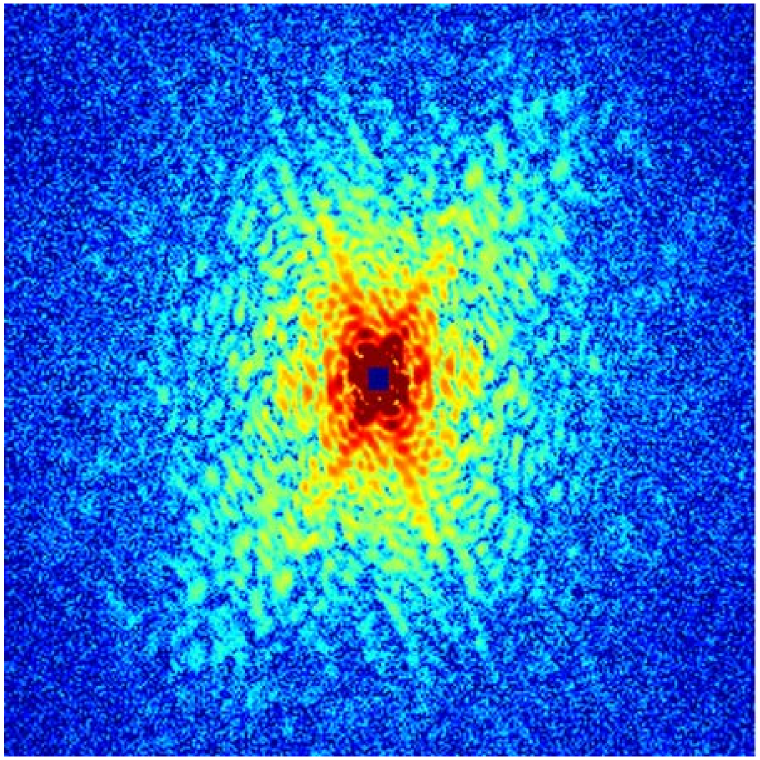


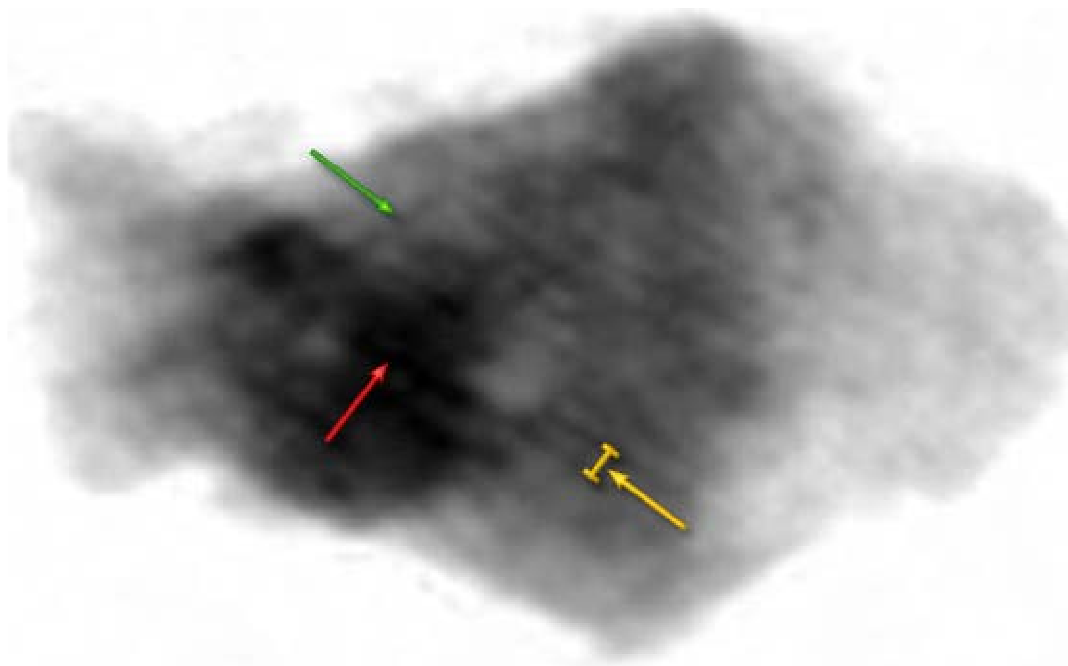
Hierarchic Structure of Bone and the Hodge Model (1963)



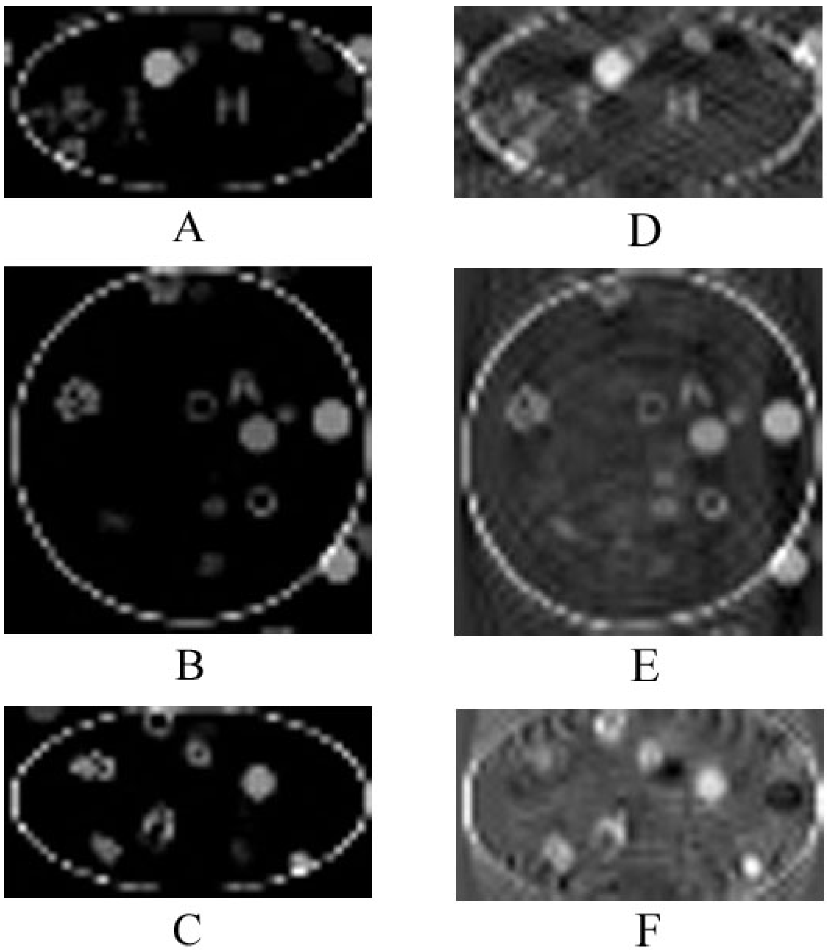


Imaging of a Herring Fish Bone Particle with a High Content of Mineral Crystals

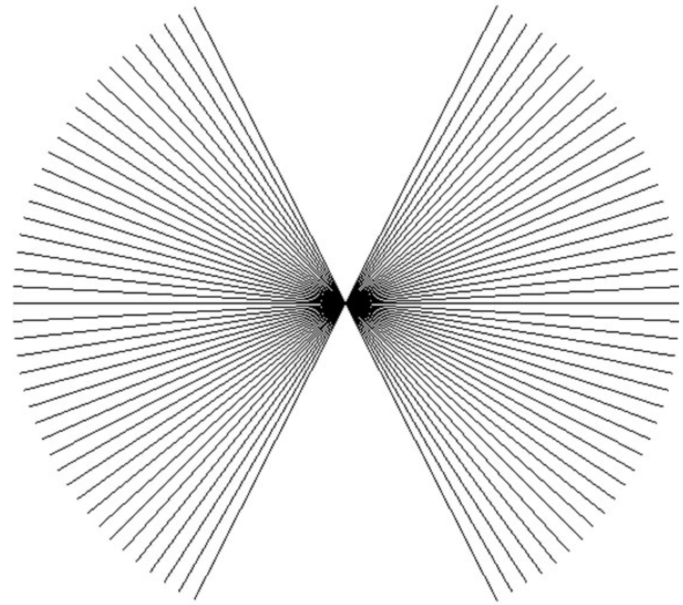




Artifacts in 3D Image Reconstruction with Conventional Tomography



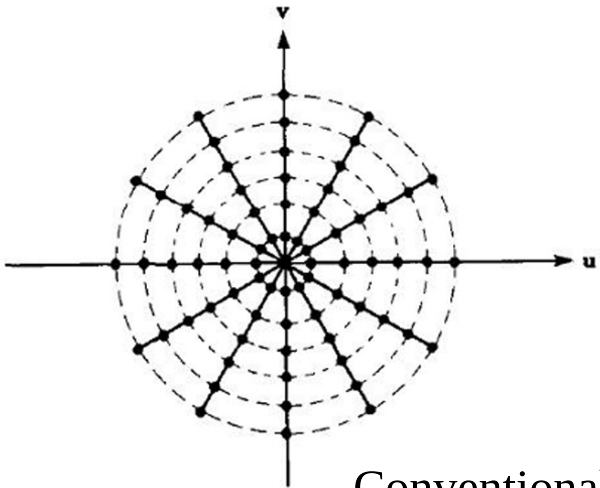
Reconstruction of a simulated vesicle
by using conventional tomography
(27 projections ranging from -69 ° to +69 °)



"Despite advanced image-acquisition procedures and the application of denoising techniques, cryoelectron tomograms still suffer from substantial residual noise and distortions because of missing data."

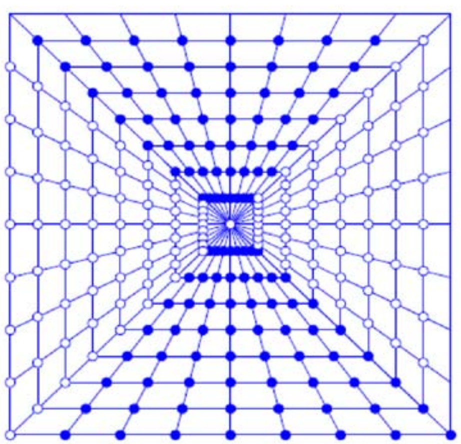
Medalia *et al*., *Science* 298, 1209 (2002).

Pseudo-Polar Fast Fourier Transform (PPFFT)



$P_\theta(\mathrm{r, z}) \xrightarrow{\text{Interpolation}} \rho(\mathrm{x, y, z})$

Conventional tomographic reconstruction



$F_\theta(\mathrm{R, Z}) \underset{\text{PPFFT}}{\overset{\text{PPFFT}^{-1}}{\rightleftarrows}} \rho(\mathrm{x, y, z})$

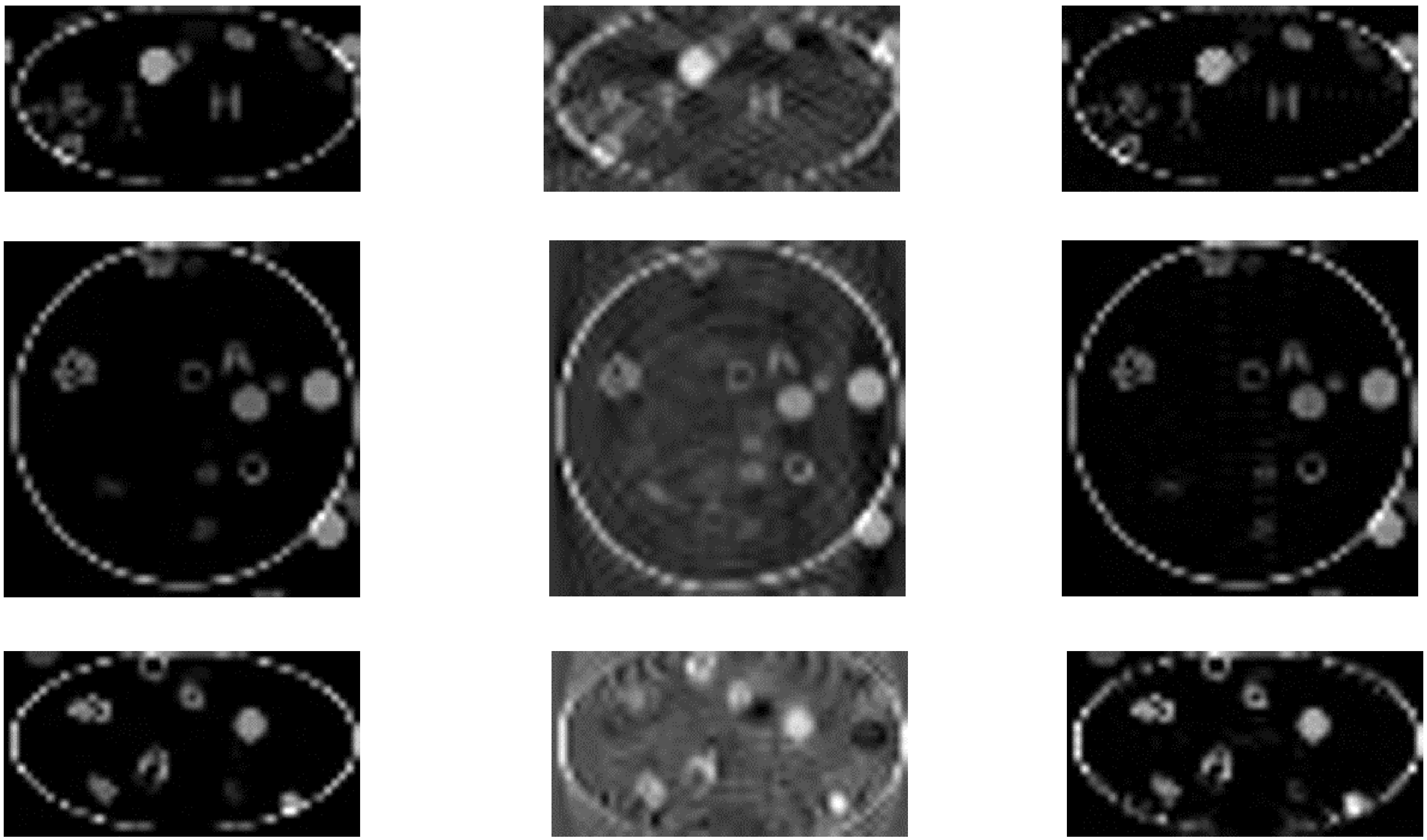
PPFFT: Equal $\Delta(\tan\theta)$ instead of equal $\Delta\theta$

Equally Sloped Tomography: A Combination of PPFFT with the Oversampling Method

(a) An original 3D object

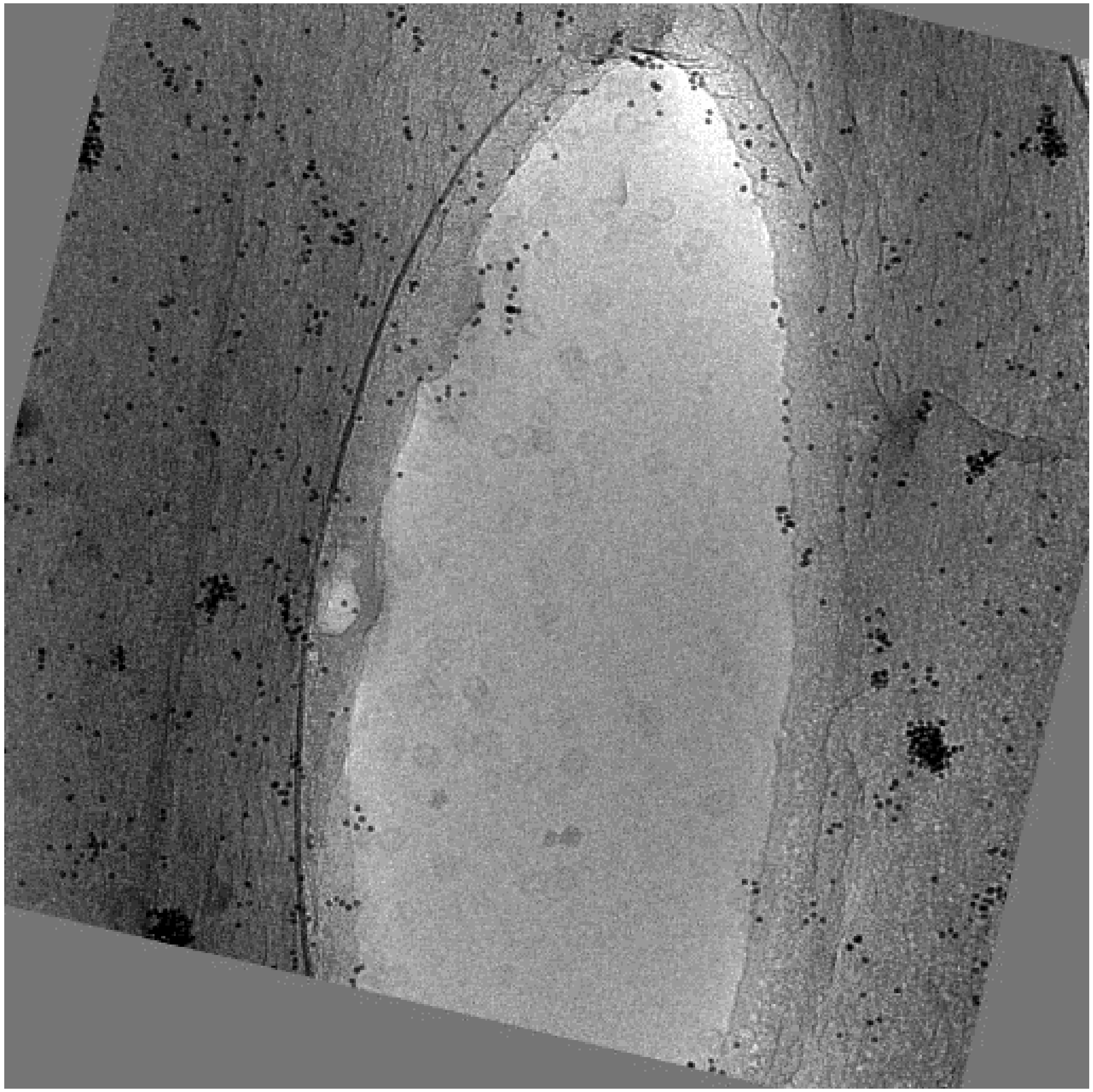
(b) Reconstruction using conventional tomography

(b) Reconstruction using equally sloped tomography



Miao, F. Förster & O. Levi, *Phys. Rev.* B. **72**, 052103 (2005).

3D Imaging of Hemocyanin Molecules Using Equally Sloped Tomography



Summary

- Oversampling the diffraction intensities $\Rightarrow$ the phase information.
- Coherent (*i.e.* lensless) imaging $\Rightarrow$ structure determination of nanomaterials and biological samples in two- and three-dimensions.
- Application of coherent imaging: materials science, nanoscience and biology.
- Equally sloped tomography $\Rightarrow$ 3D image reconstruction at higher quality
- A bright future with the emerging of more coherent and brilliant X-ray sources such as ERLs and X-FELs.

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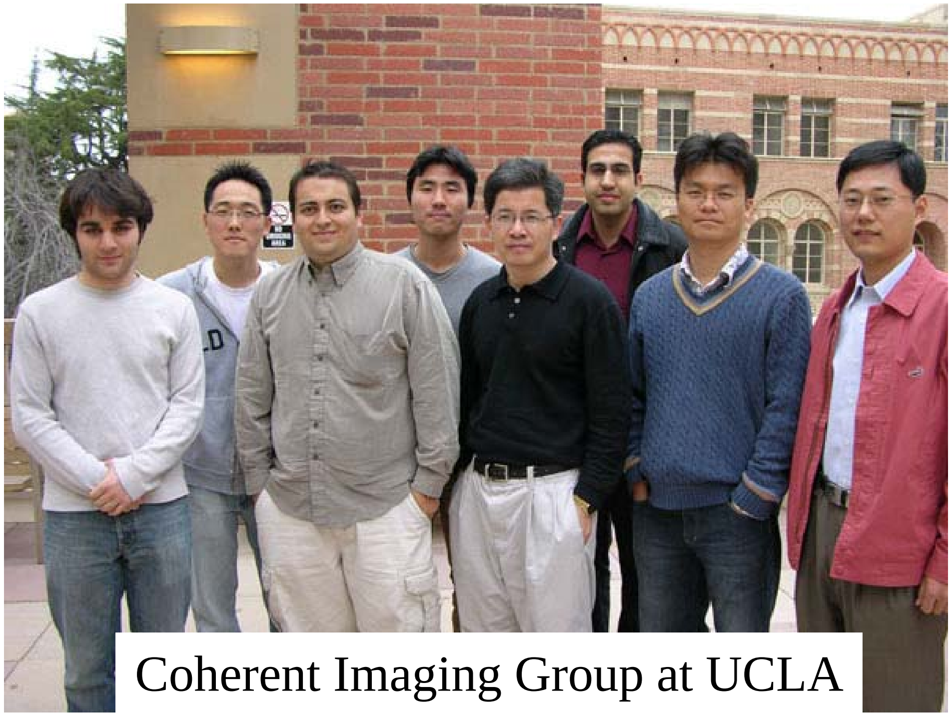

Coherent Imaging Group at UCLA