X-ray Diffraction Imaging of Nanoscale Materials and Biological Structures

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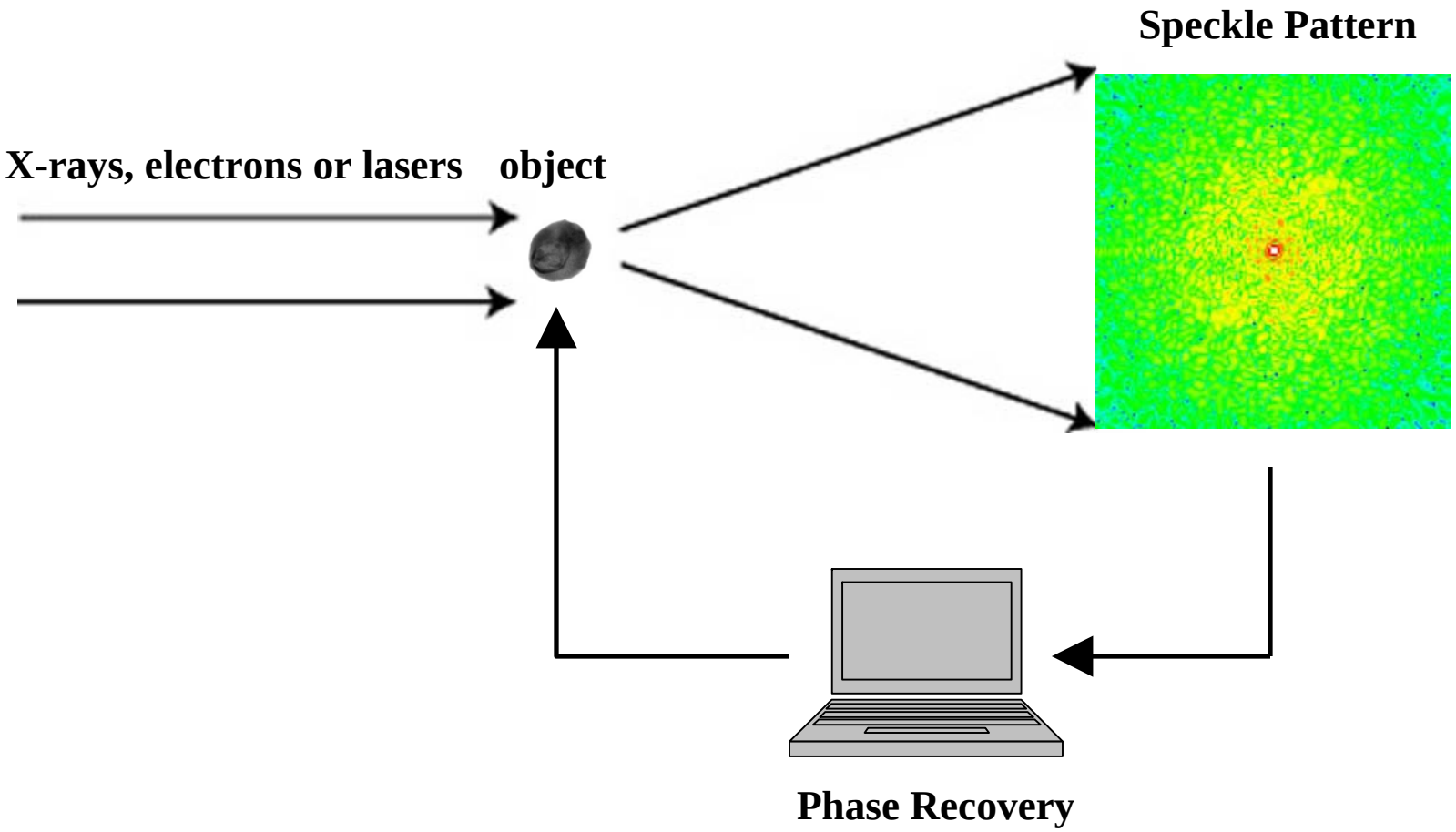
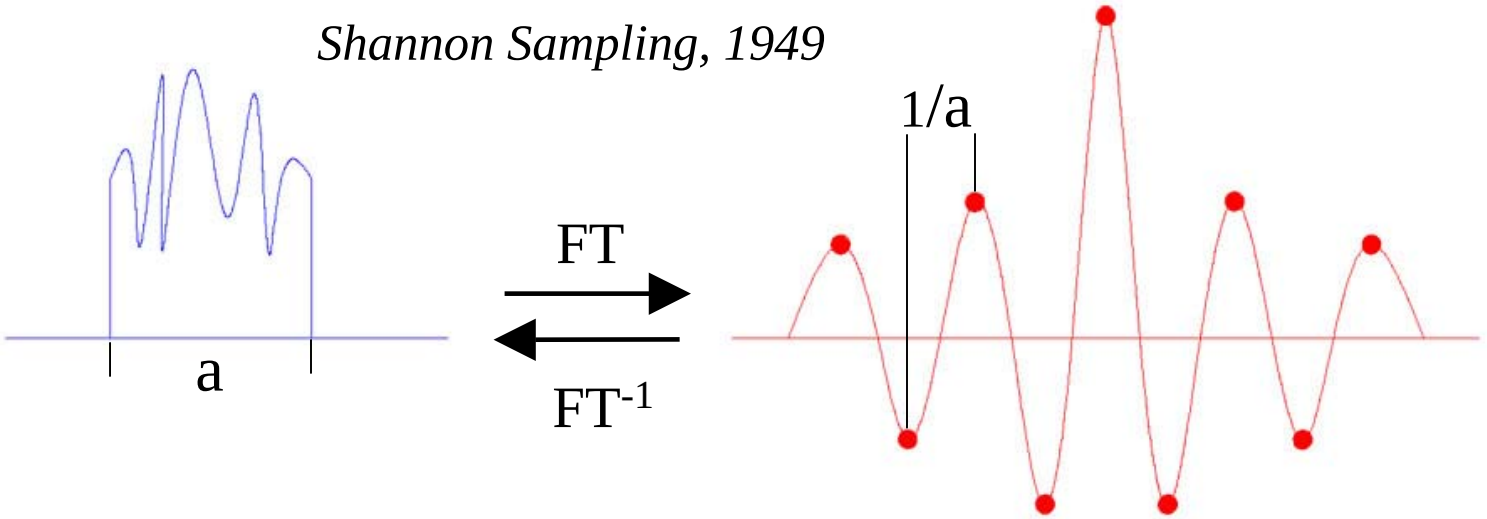
Coherent Diffraction Microscopy (or Lensless Imaging)

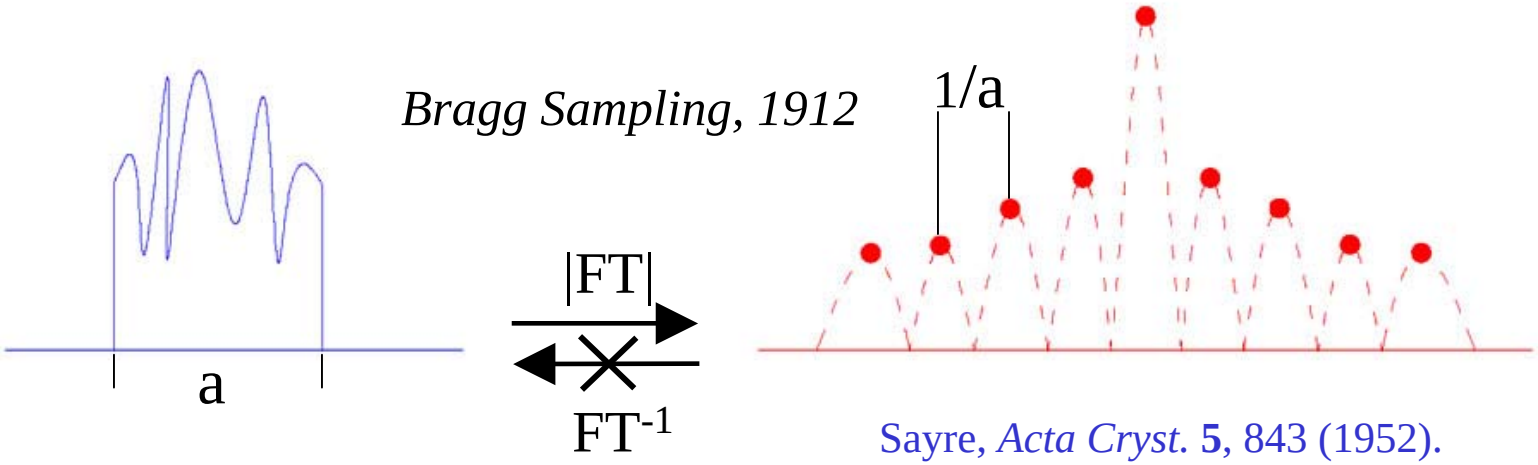


Shannon Sampling vs. Bragg Sampling

Shannon Sampling, 1949

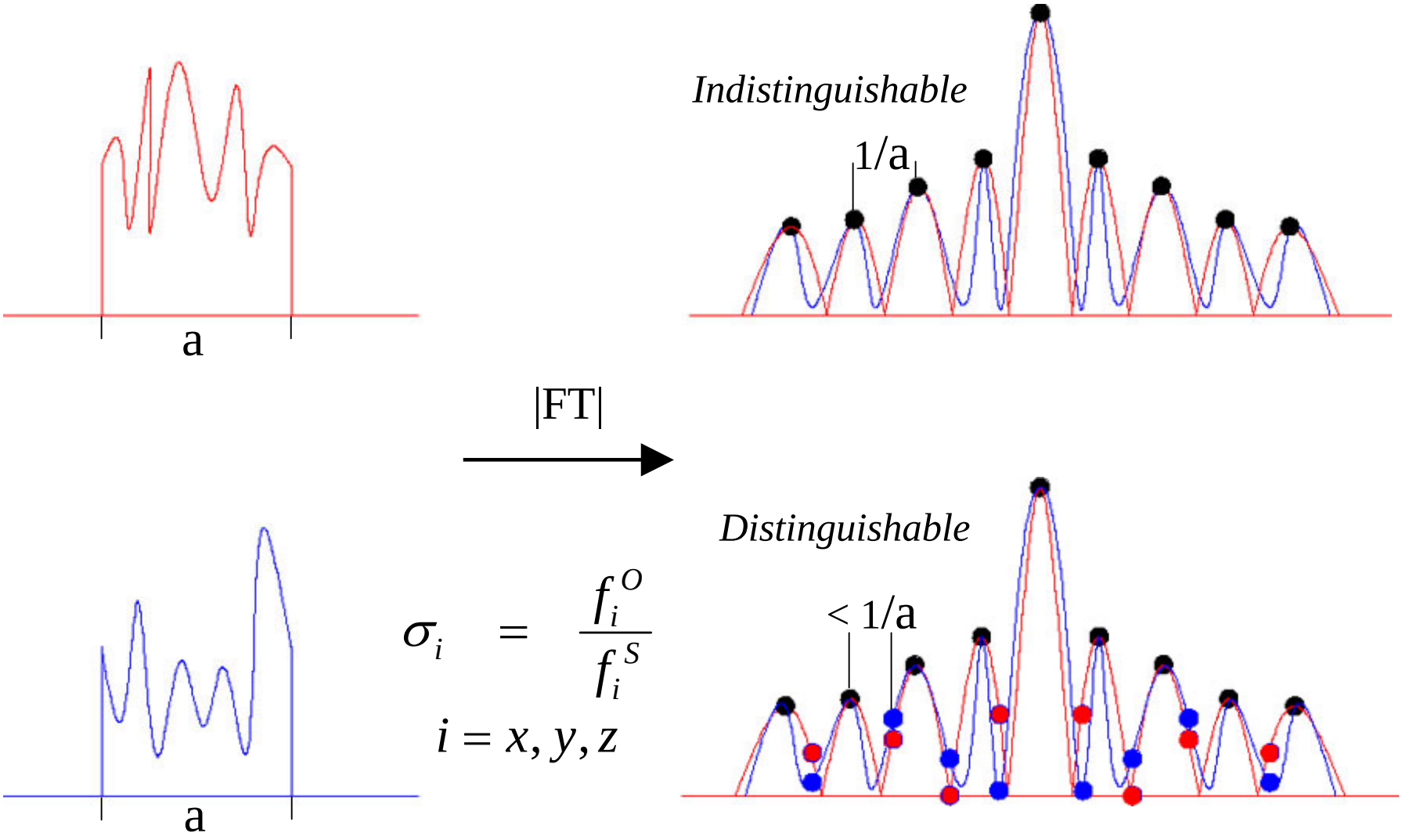


Bragg Sampling, 1912



Sayre, *Acta Cryst.* **5**, 843 (1952).

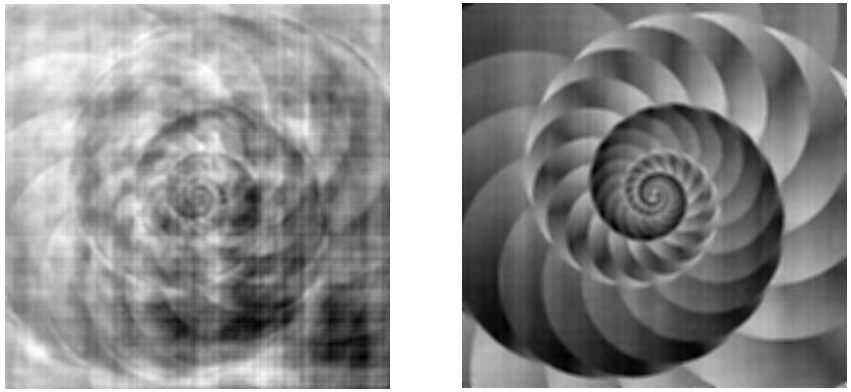
Oversampling



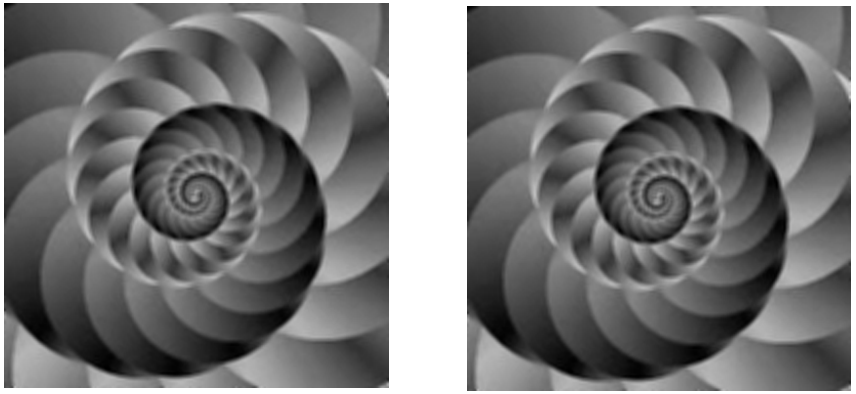
Miao, Sayre & Chapman, *J. Opt. Soc. Am.* A **15**, 1662 (1998).

Intensity Integration vs. Exact Oversampling

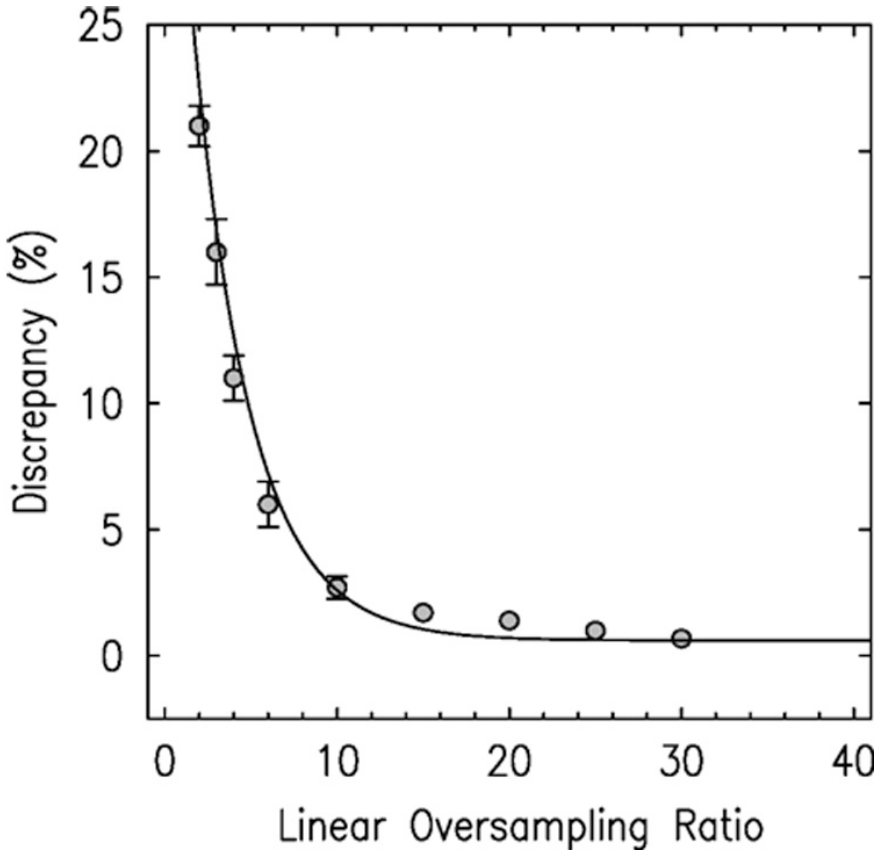
$\sigma_i = 2$ $\sigma_i = 8$



Intensity Integration



Exact Oversampling

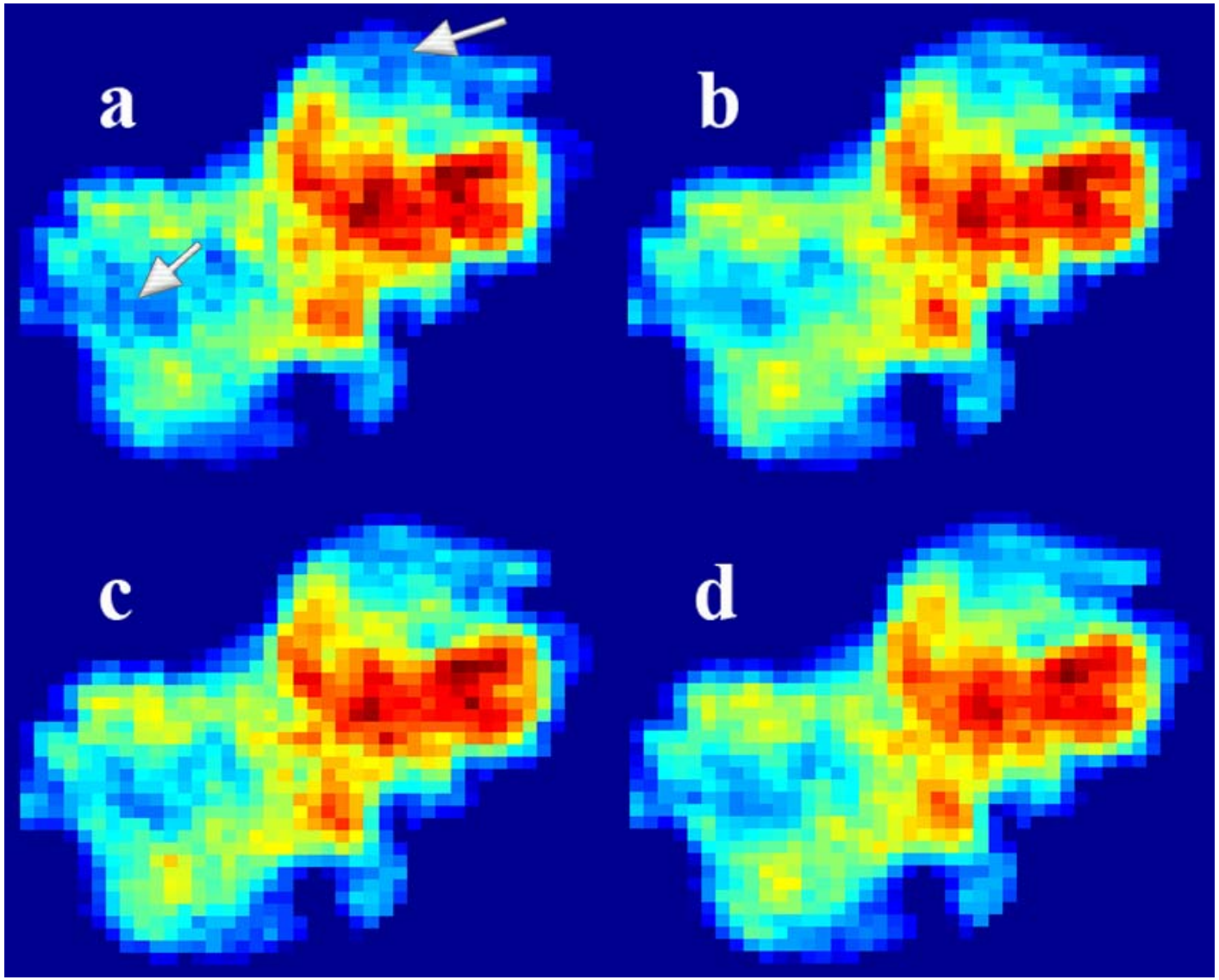


$$I_S(k) = FT\left\{\frac{FT^{-1}\left[I_M(k)\right]}{\mathrm{sinc}(x/M)}\right\}$$

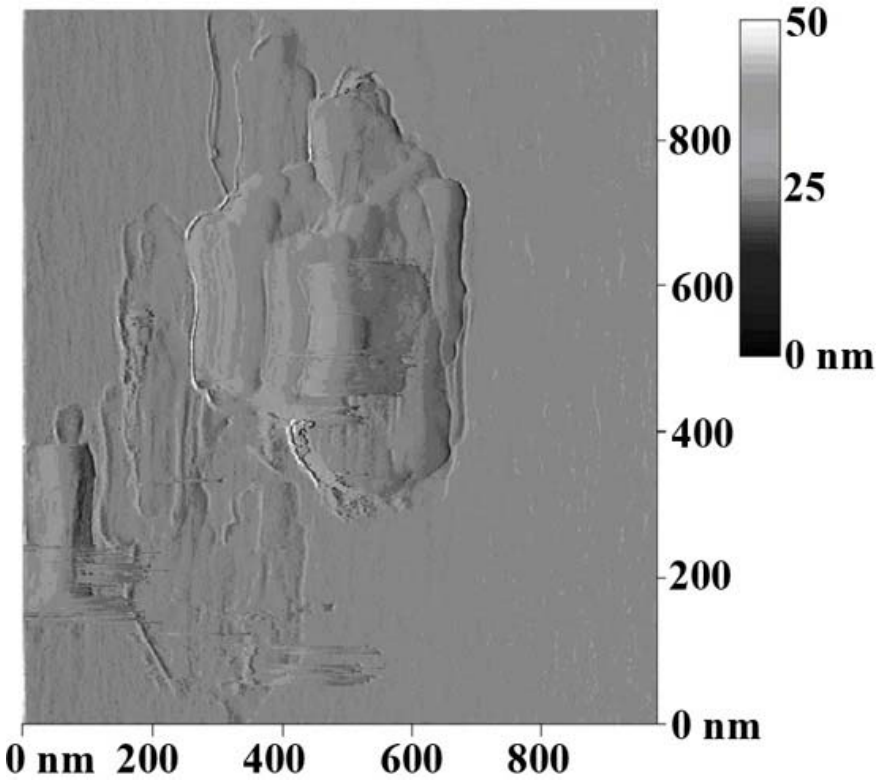
Song *et al*, *PRB* 75, 012102 (2007).

Experimental Verification of Exact Oversampling

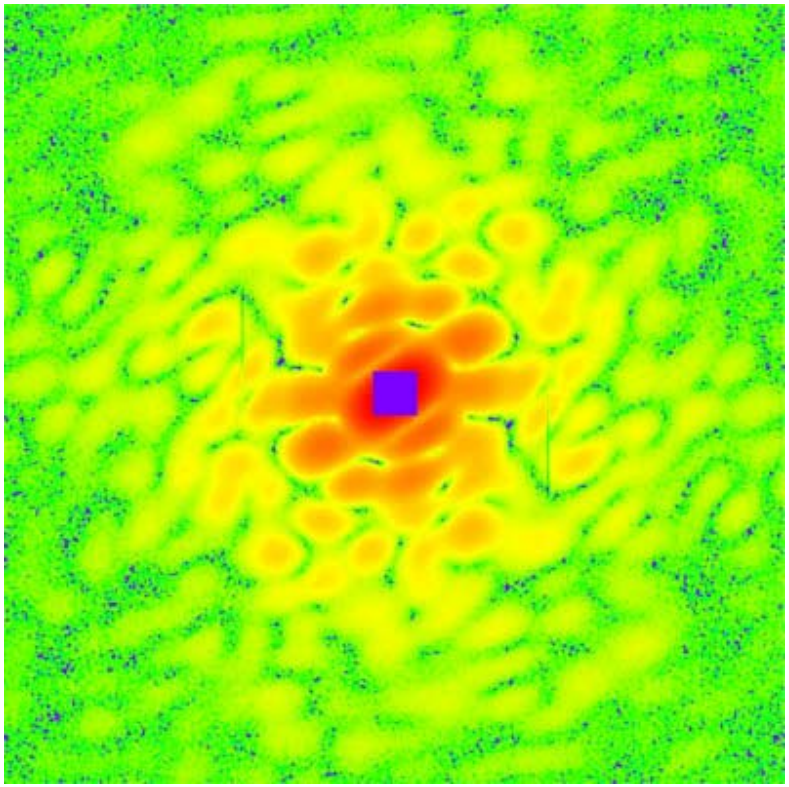
$\sigma_i = 2$ $\sigma_i = 18$



The Missing Center Problem



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



Oversampled diffraction pattern from a GaN quantum dot nanoparticle

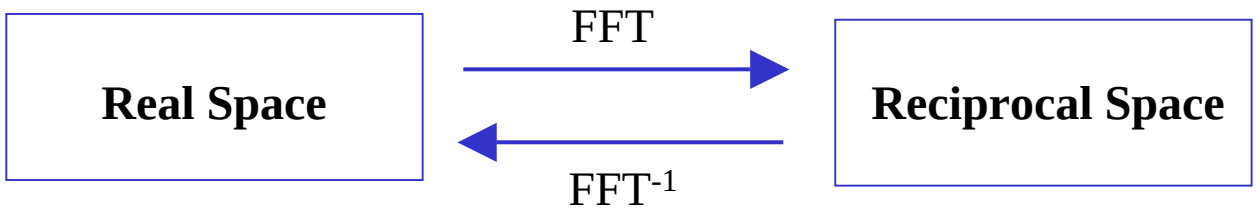
$$\eta_i = \frac{D_i - 1}{2\sigma_i} \quad i = x, y, z$$

Miao *et al.*, *PRL* **95**, 085503 (2005).

The Guided Hybrid Input-Output (GHIO) Algorithm

i) Start with 16 independent reconstructions.

ii) For each reconstruciton:



iii) Calculate the *R*-value,

$$R = \sum \left\| F_{\exp} \right| - \alpha \left| F_{cal} \right\| \Big/ \sum \left| F_{\exp} \right|$$

iv) Select a seed out of 16 images (ρ_{seed}) with the smallest *R*-value.

v)

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

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

Chen *et al.*, *PRB* 76, 064113 (2007).

Image Reconstruction Using the GHIO Algorithm at 0th Generation

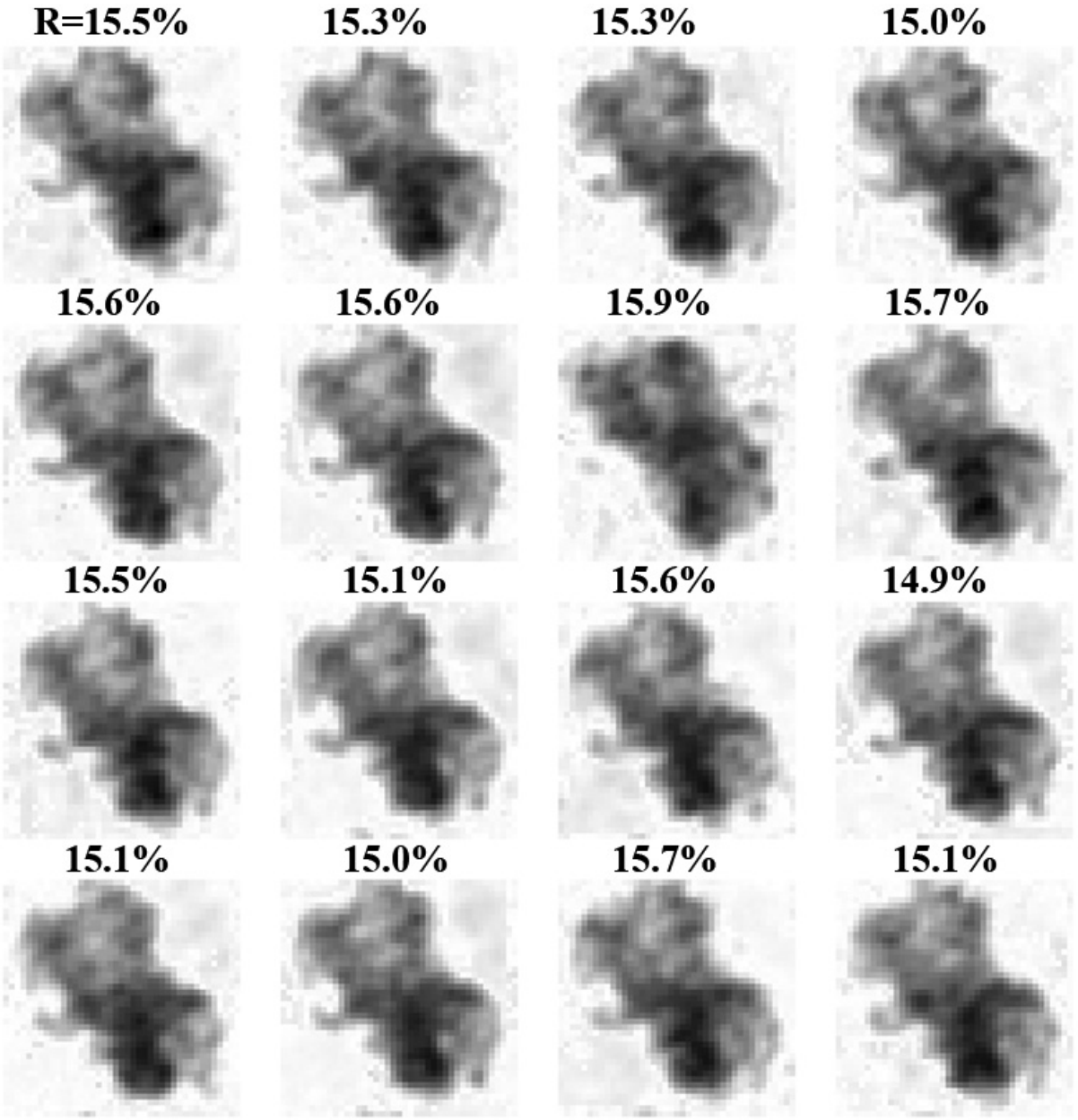
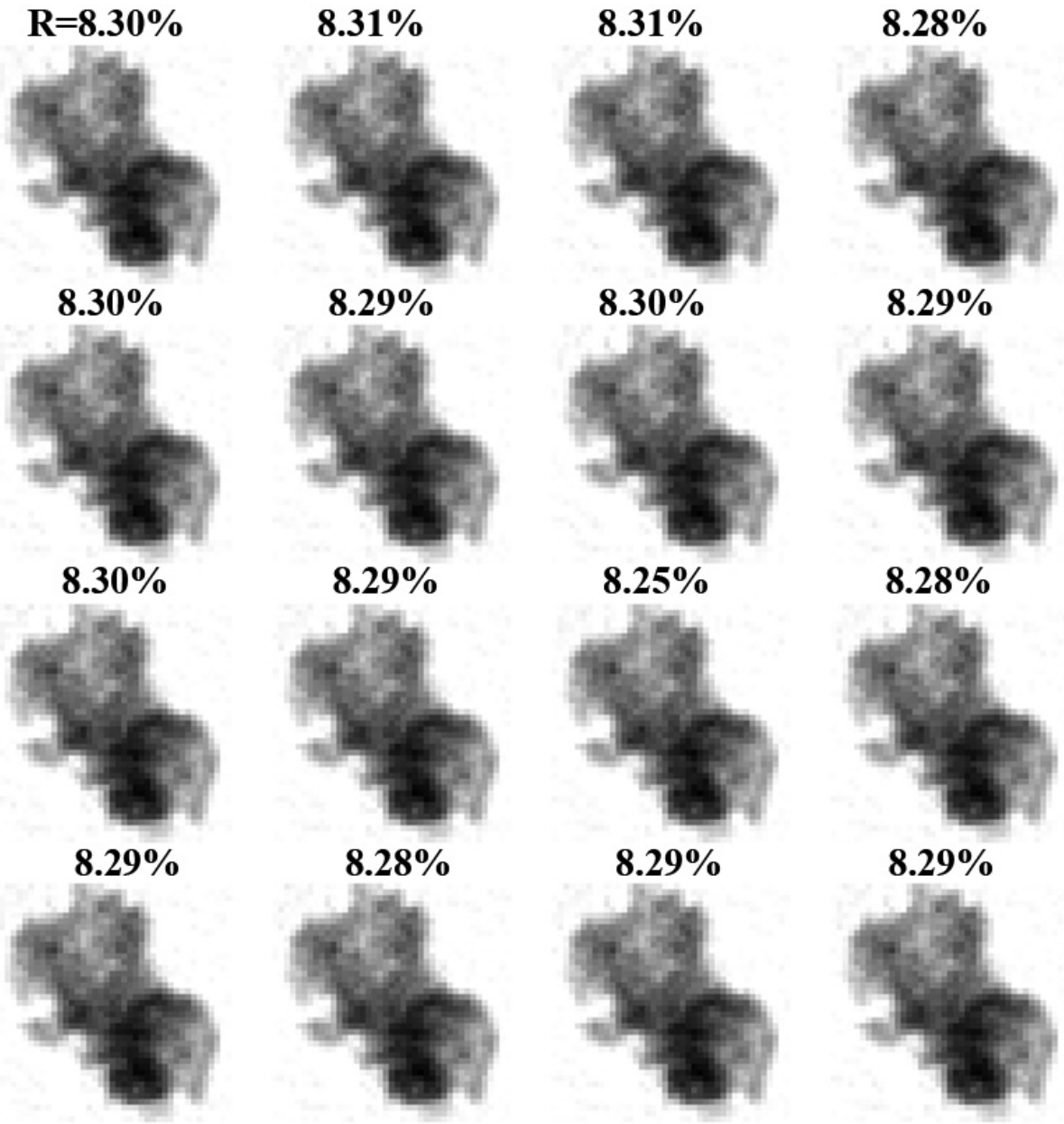
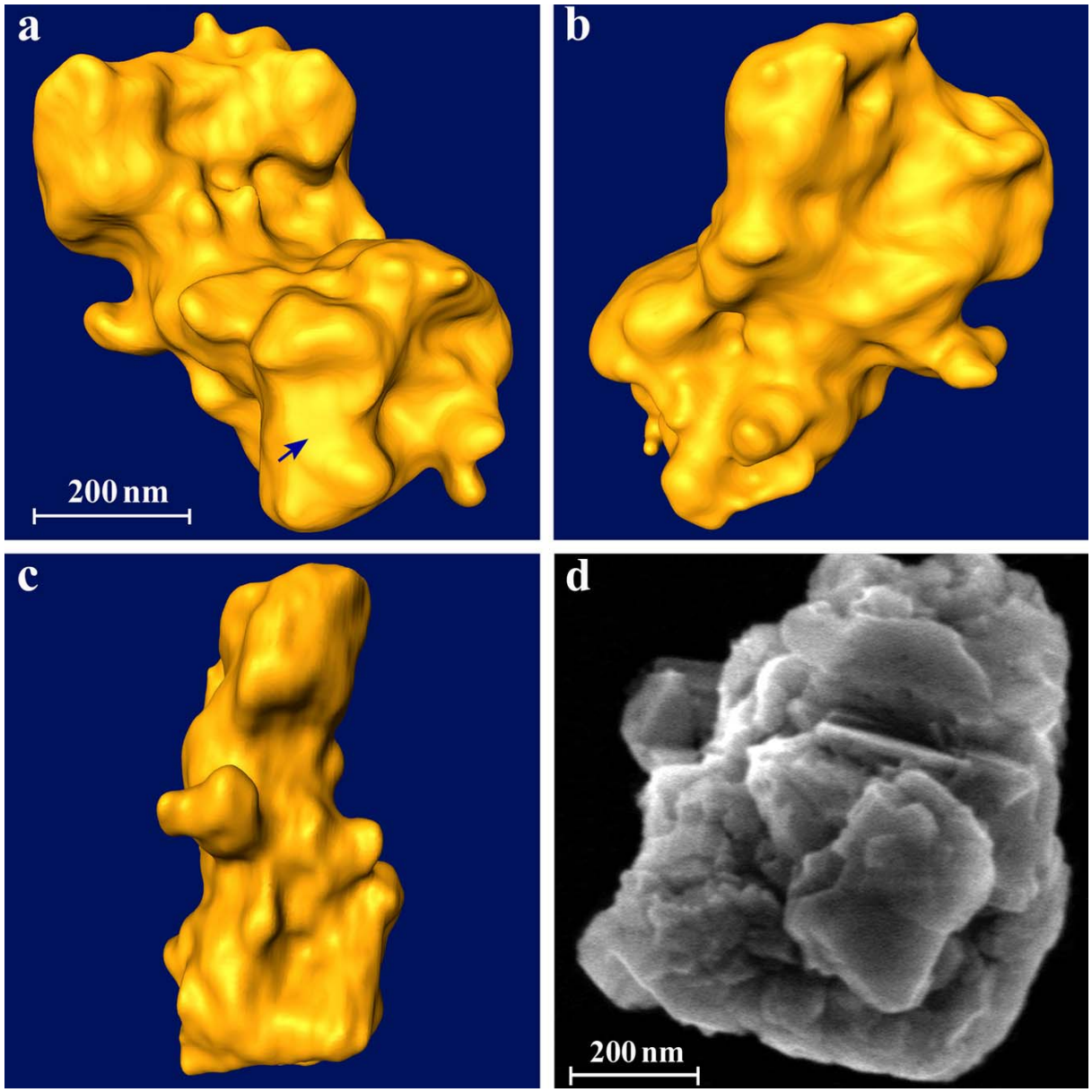


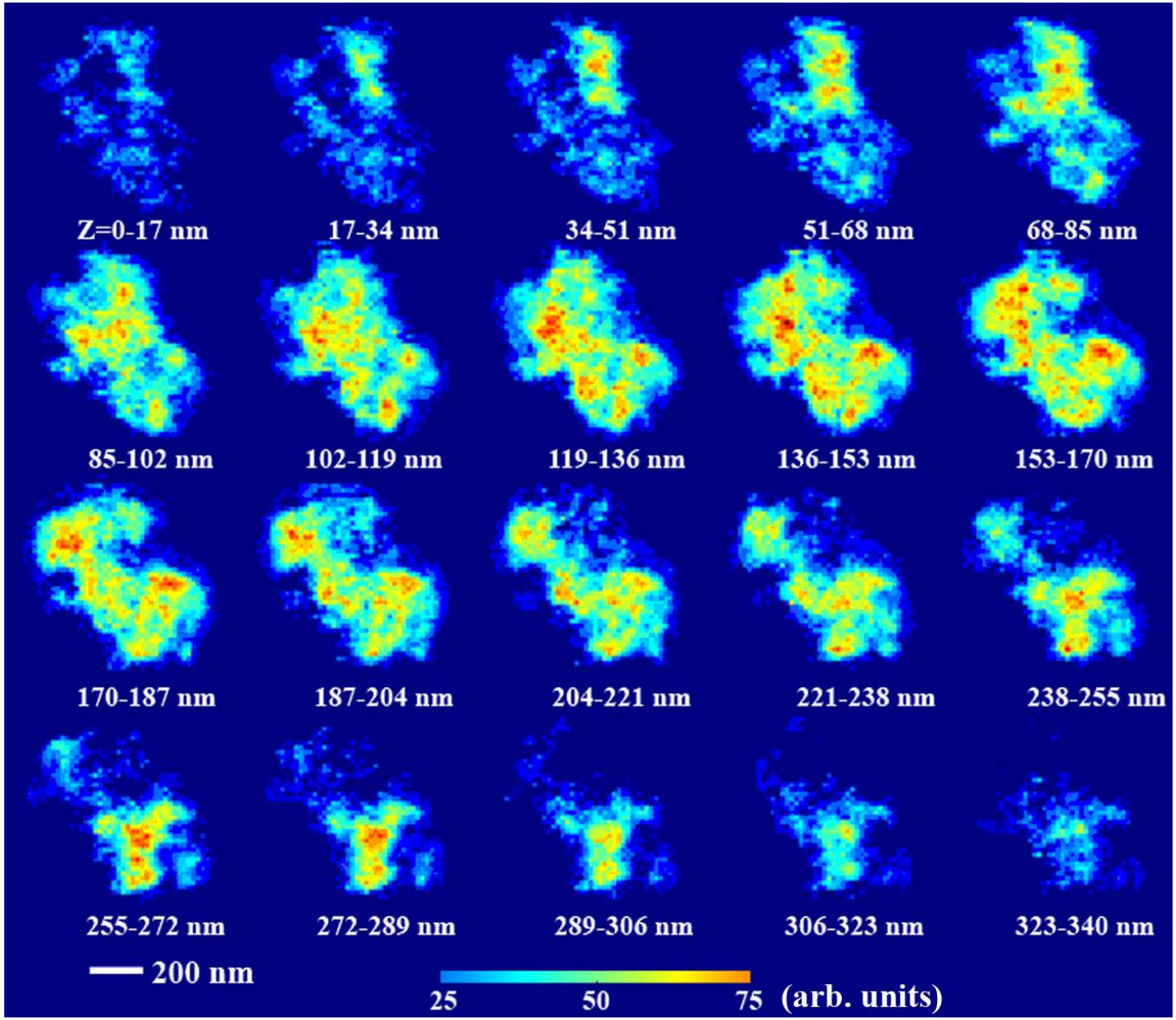
Image Reconstruction Using the GHIO Algorithm at 8th Generation



3D Surface Morphology of Nanoparticles

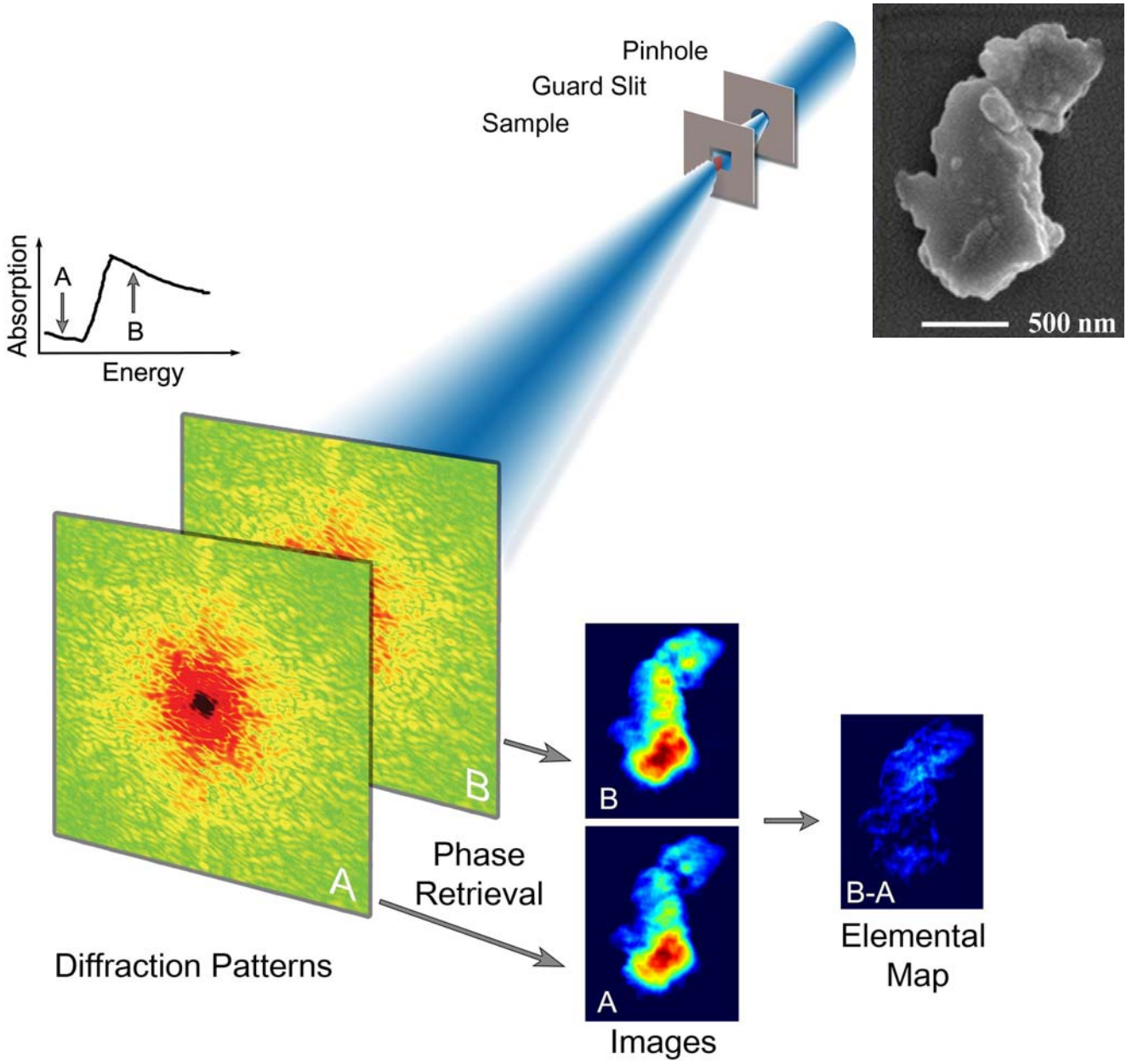


Revealing 3D GaN-Ga_2O_3 Core Shell Structure

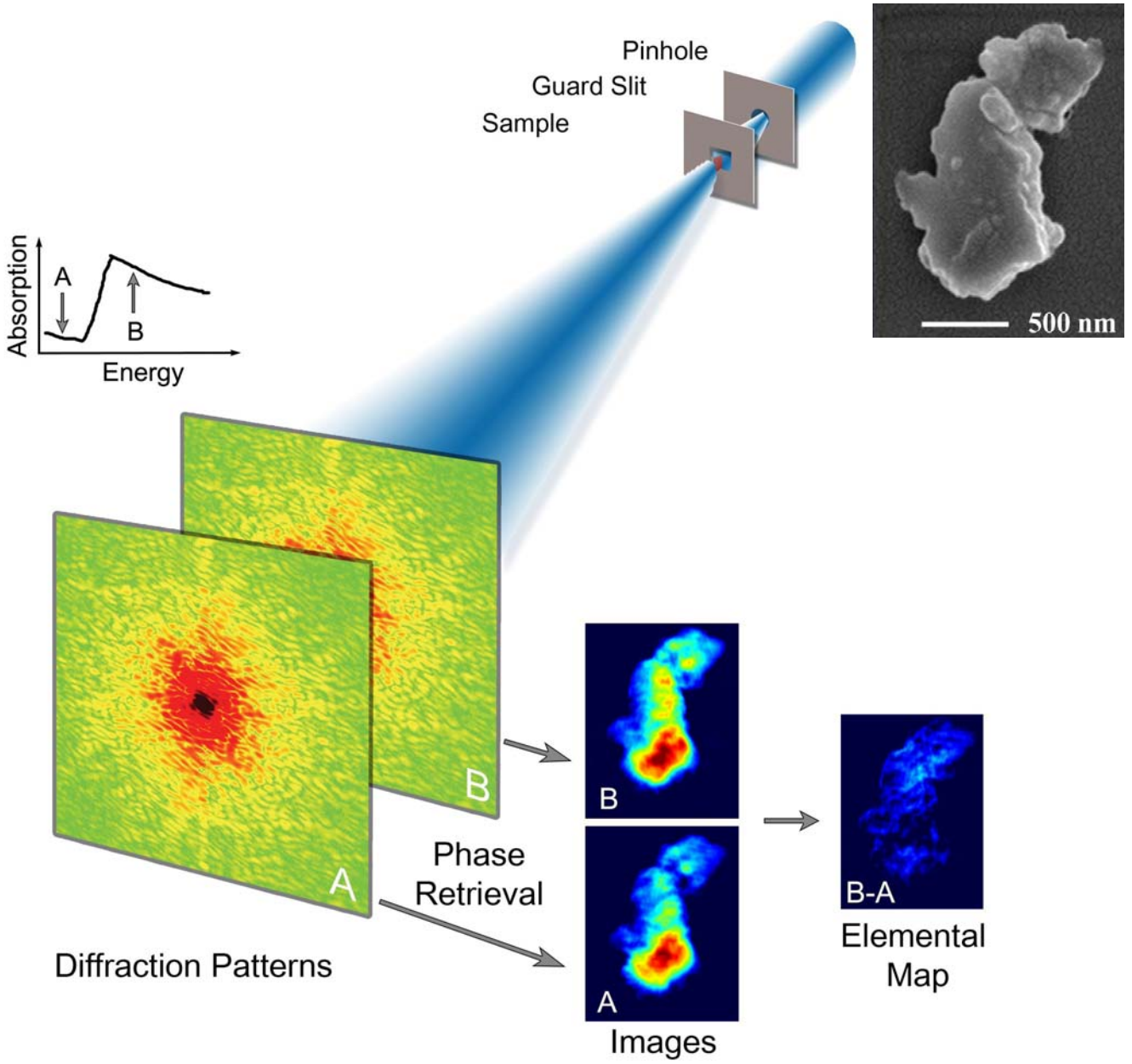


Miao *et al.*, *PRL* **97**, 215503 (2006).

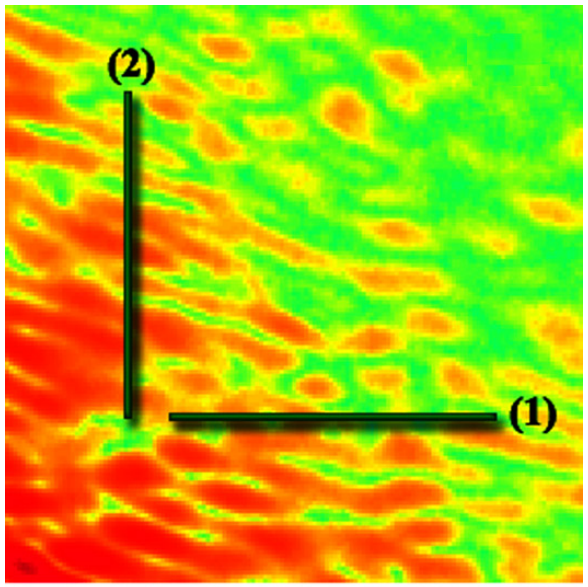
Schematic Layout of Resonant X-ray Diffraction Microscopy

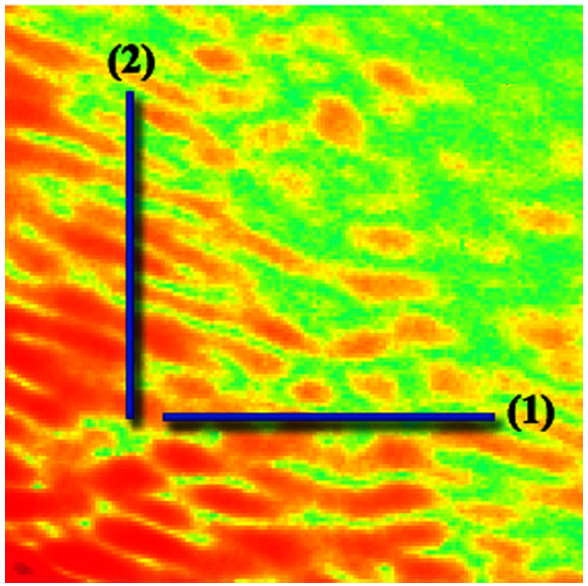


Schematic Layout of Resonant X-ray Diffraction Microscopy



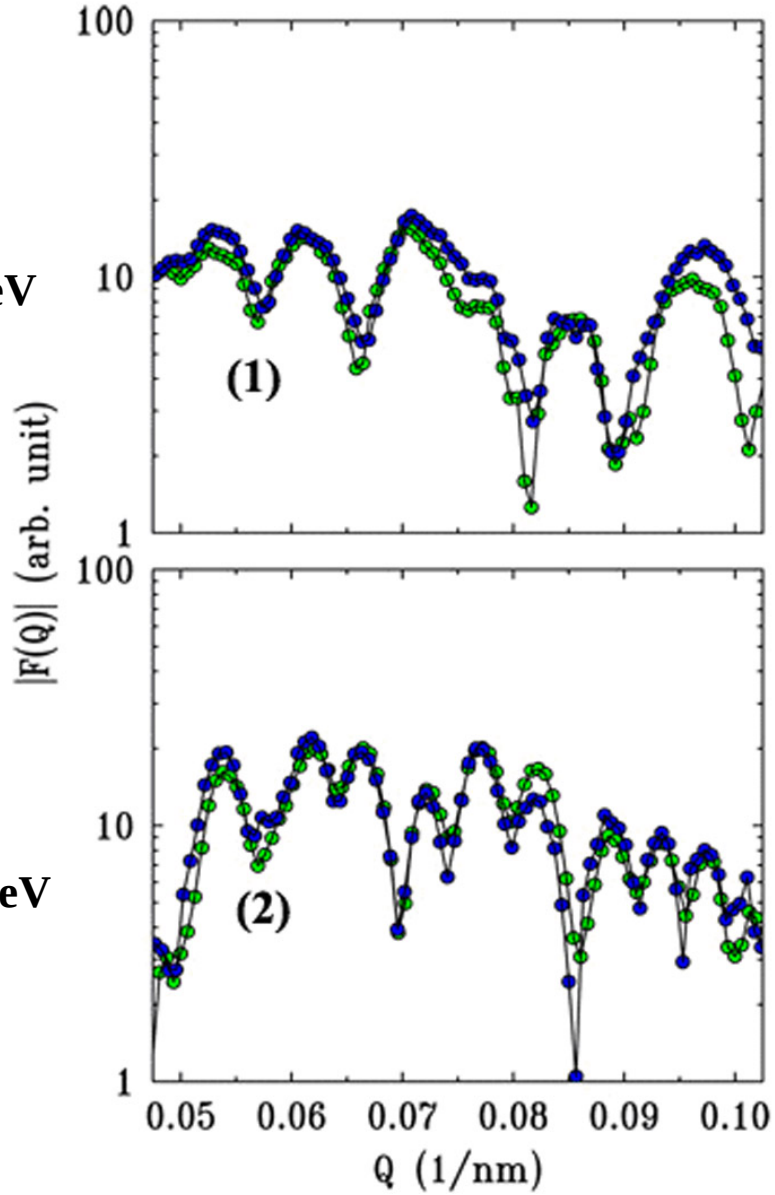
X-ray Diffraction Patterns of a Bi Doped Si Crystal at E=2.550 and 2.595 keV



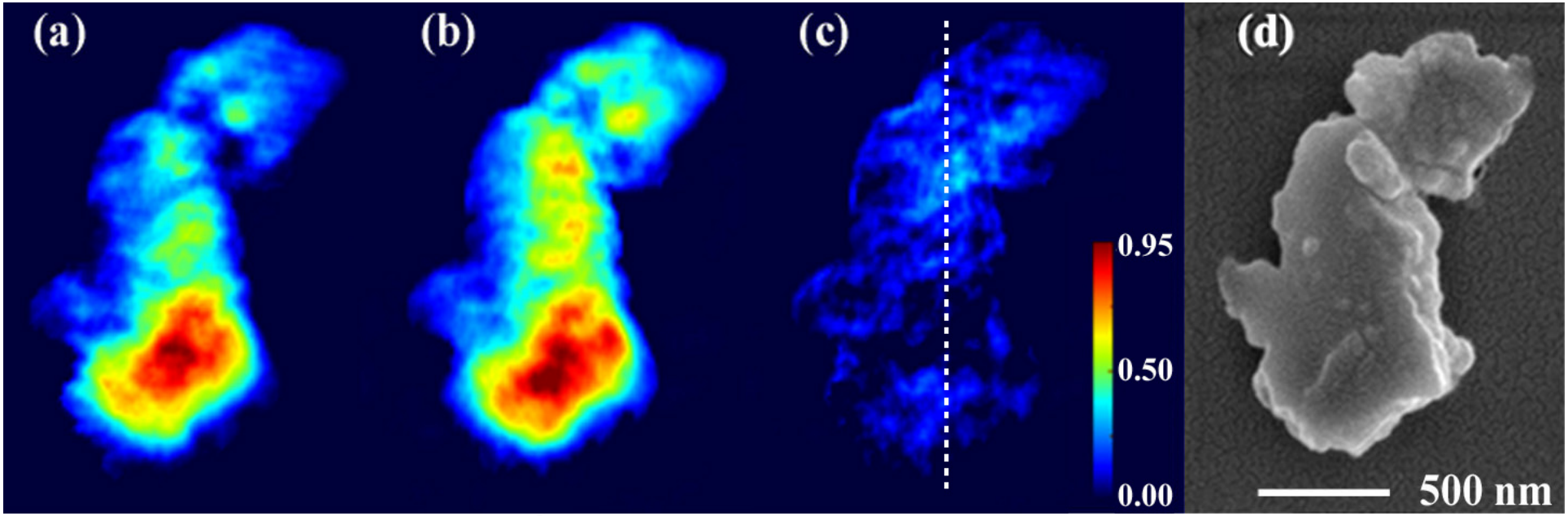


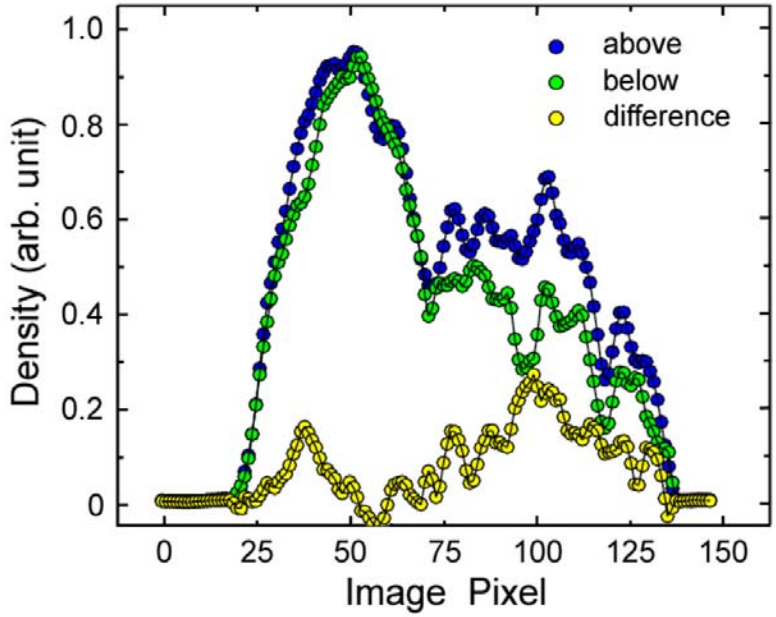
E=2.550 keV

E=2.595 keV



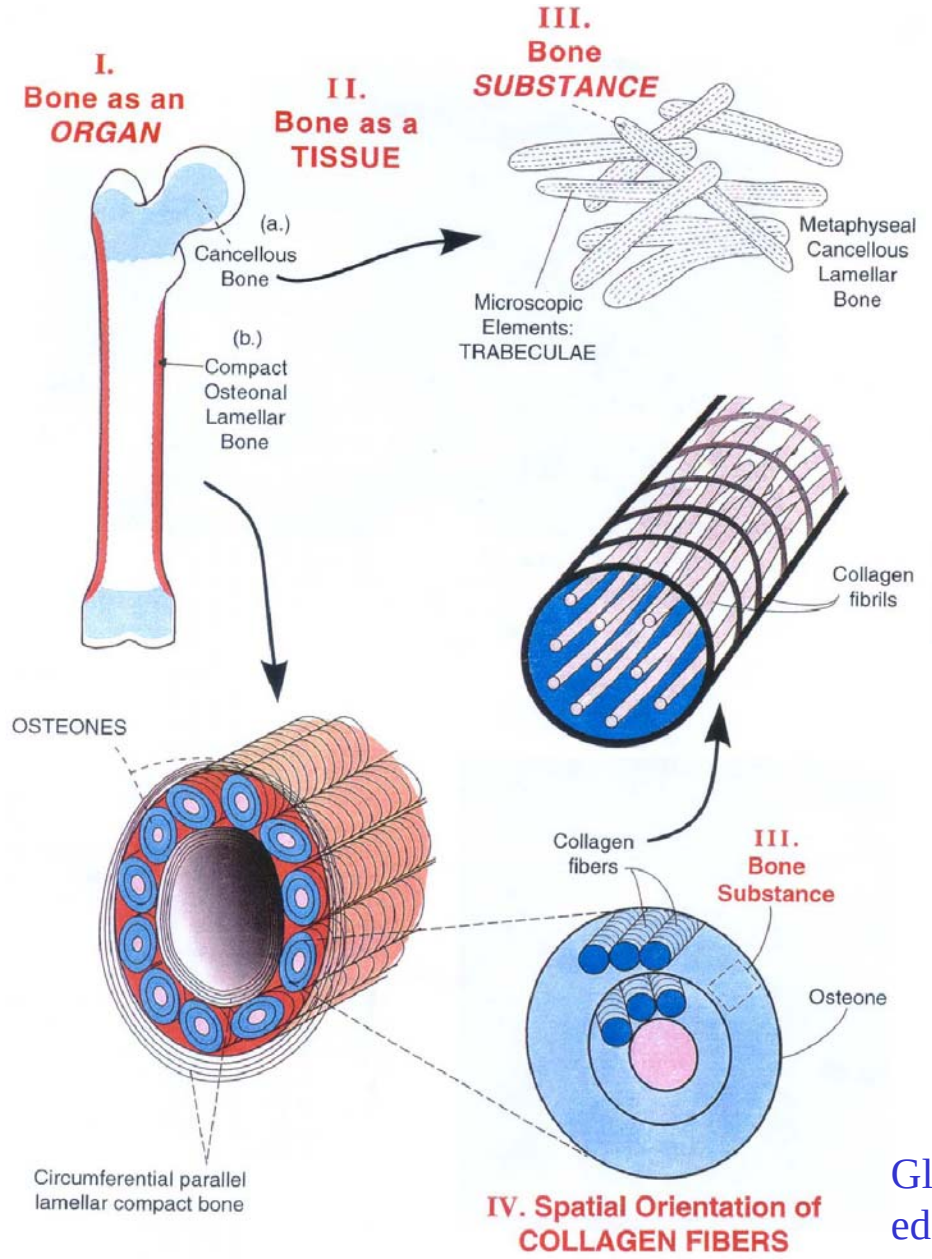
Elemental Mapping of Buried Bi Structure

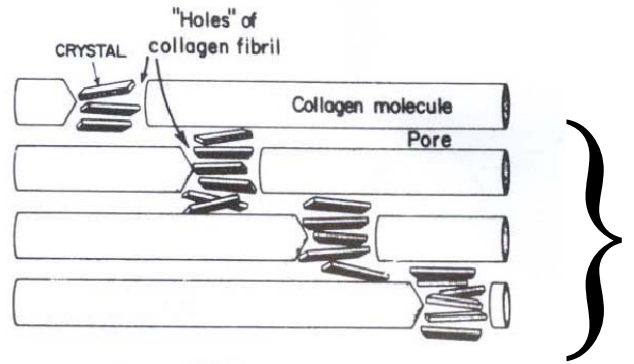




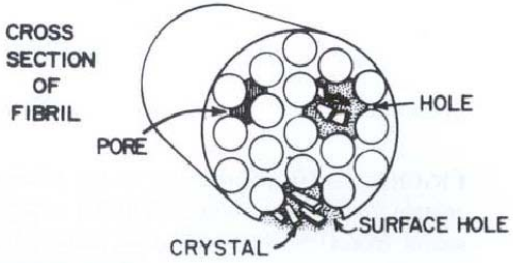
Song *et al.*, *PRL* **100**, 025504 (2008).

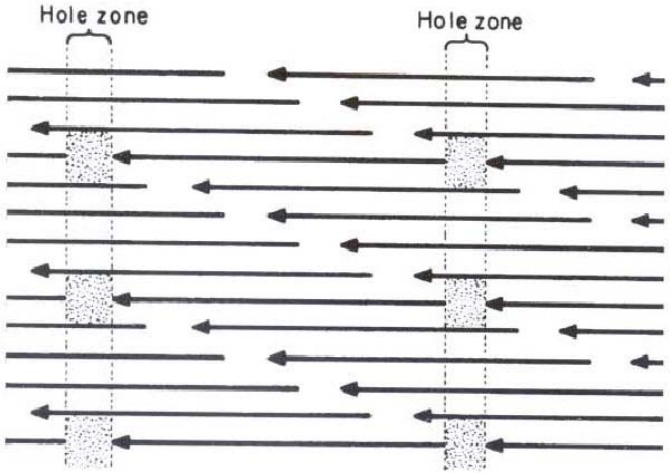
Hierarchical Structures in Bone





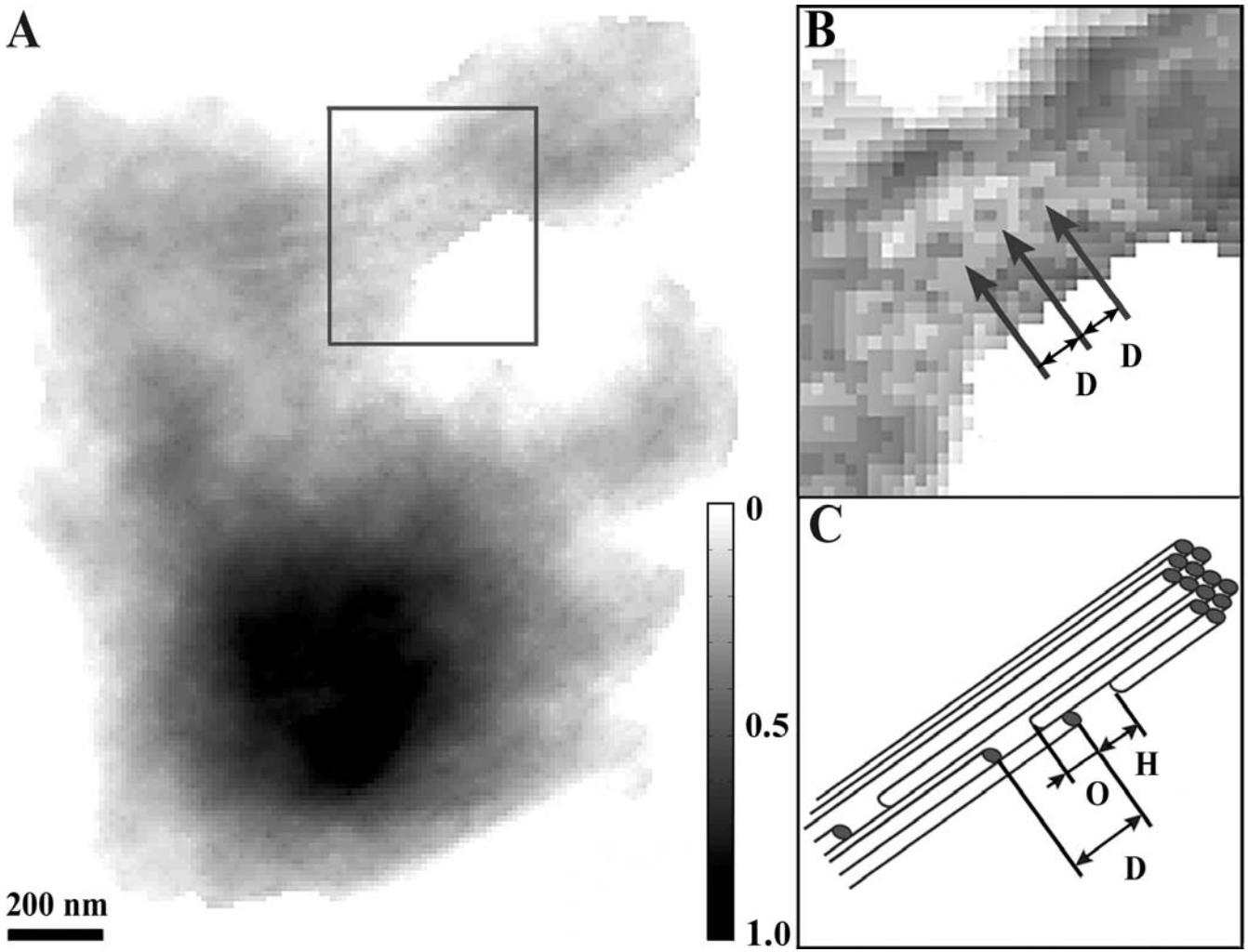
Collagen fibril



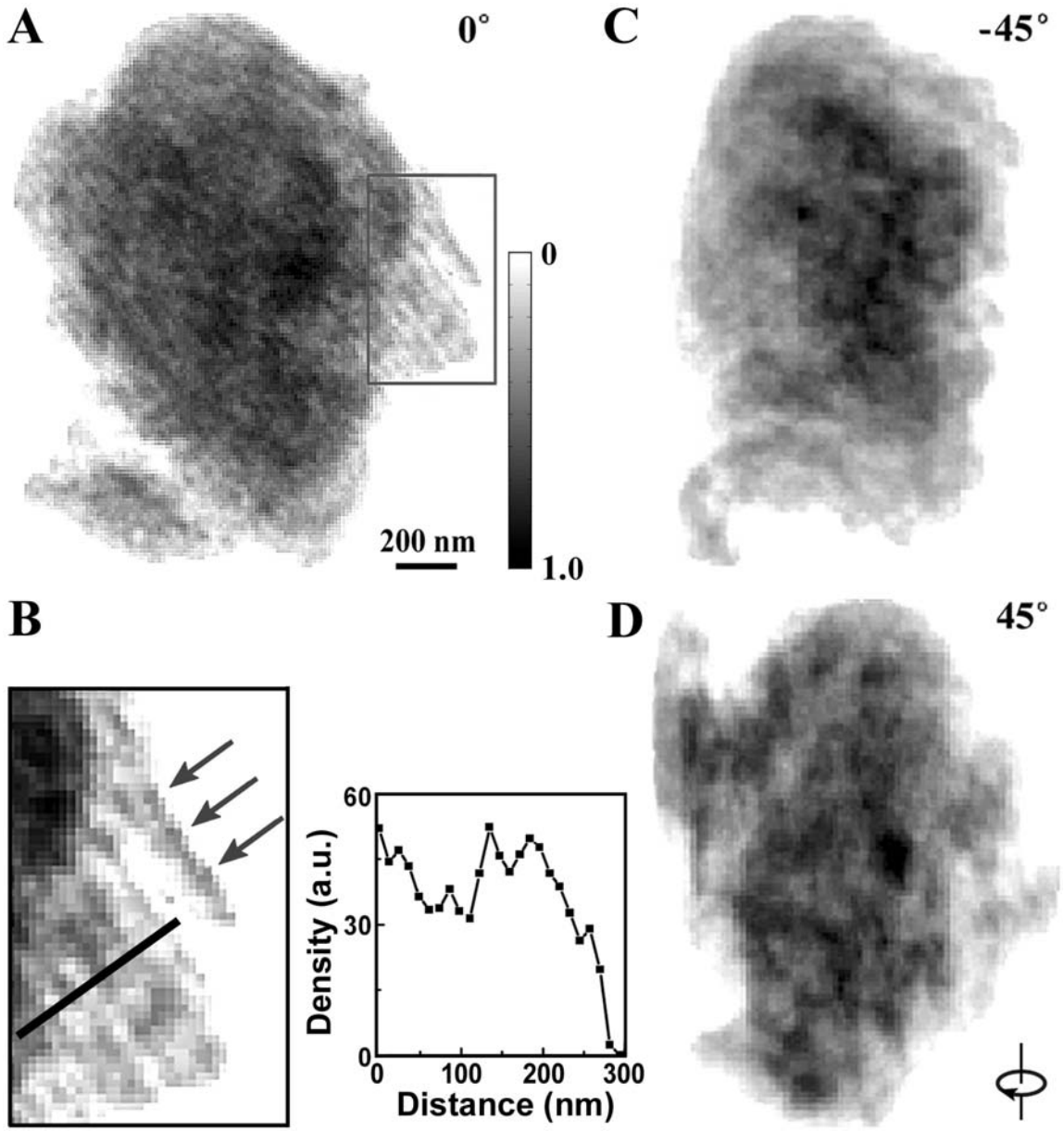


Glimcher (1998) in *Metabolic Bone Disease*, eds Avioli, Krane (Academic Press, San Diego)

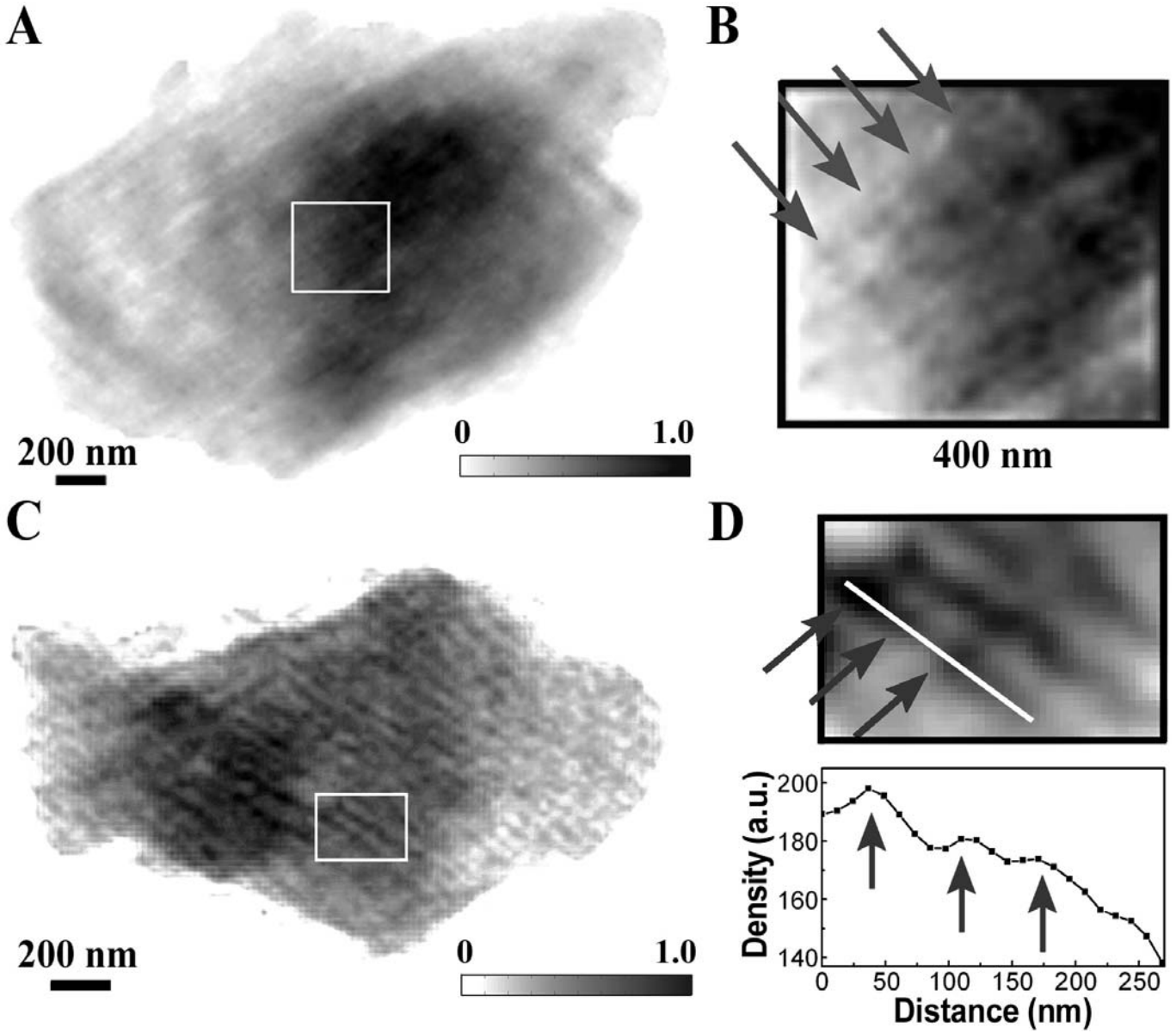
X-ray Diffraction Imaging of Unmineralized Bone Particles



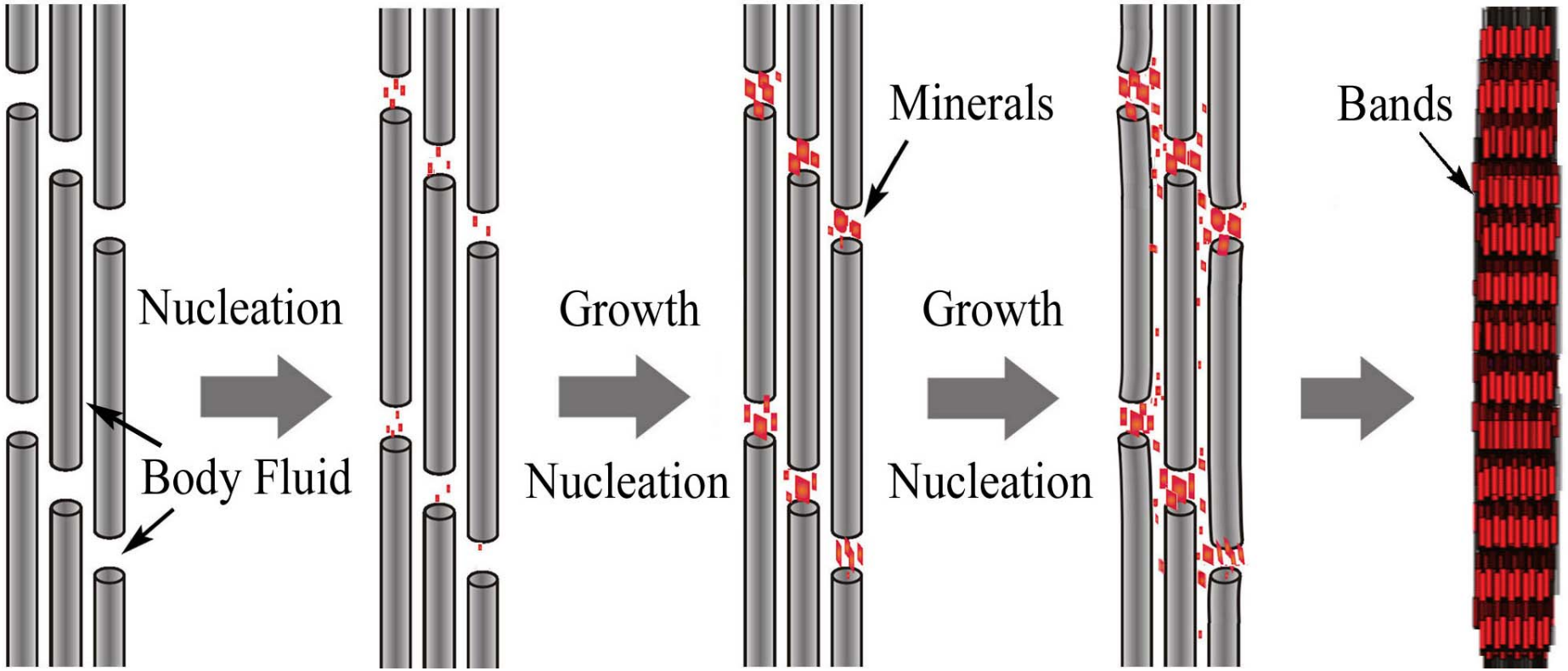
X-ray Diffraction Imaging of Low Mineralized Bone Particles



X-ray Diffraction Imaging of Highly Mineralized Bone Particles



Dynamic 3D Structure Model of the Mineral Phase in Bone



Jiang *et al.*, *PRL* **100**, 038103 (2008).

Summary

- Oversampling the diffraction intensities $\Rightarrow$ the phase information.
- Imaged nanoscale materials and biological structures in 2- and 3-dimensions.
- Resonant X-ray diffraction microscopy for element specific imaging of buried structures.
- Towards 3D structural determination of noncrystalline materials at the near atomic resolution using future brighter X-ray sources such as NSLS-II.

Collaborators

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Harvard Medical School	*M.J. Glimcher, L. Graham*