3D Coherent X-ray Diffraction Microscopy: The Present and the Future

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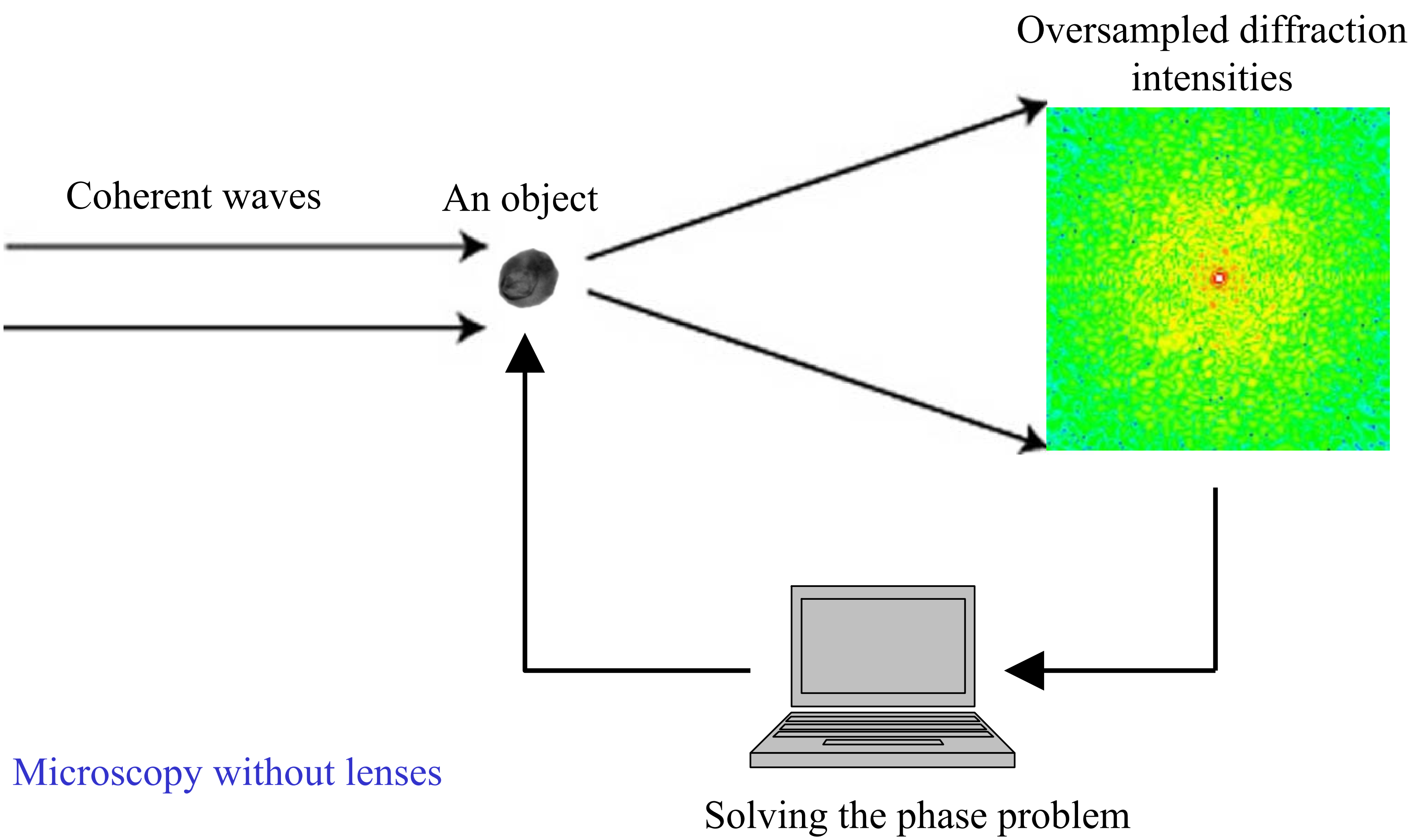
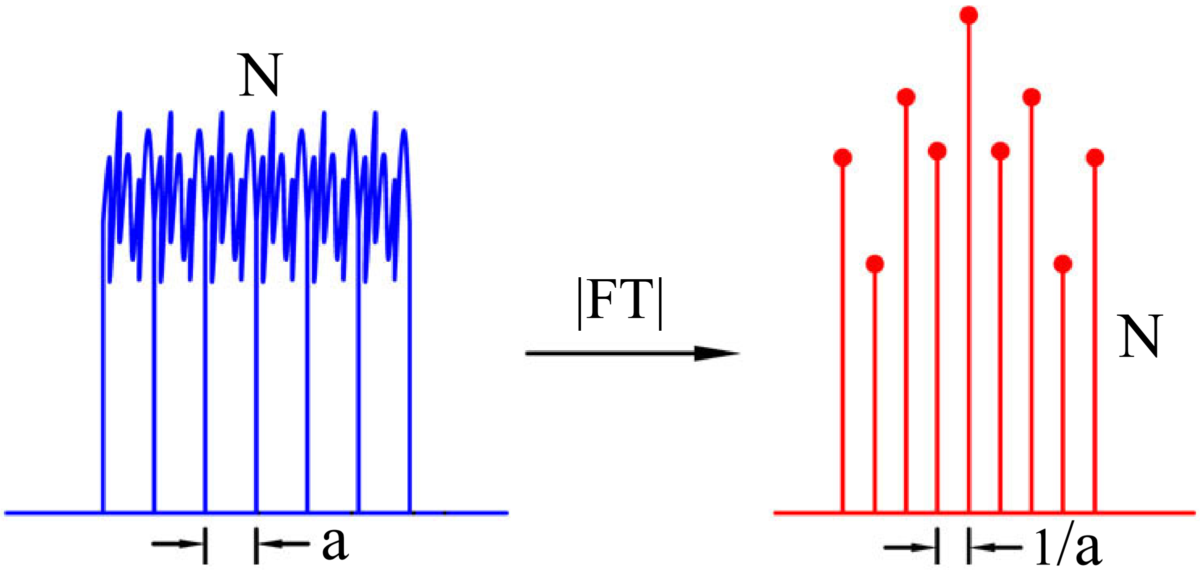
The Principle of Diffraction Microscopy



Microscopy without lenses

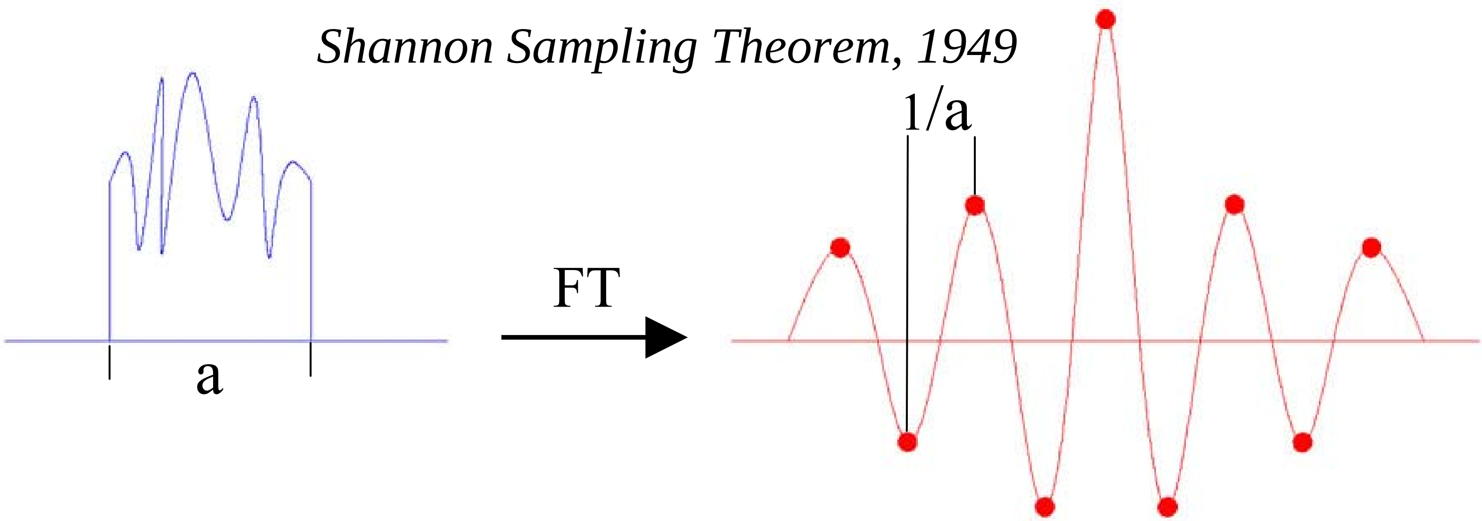
X-ray Diffraction by Crystals

Laue, W. Bragg and L. Bragg, 1912

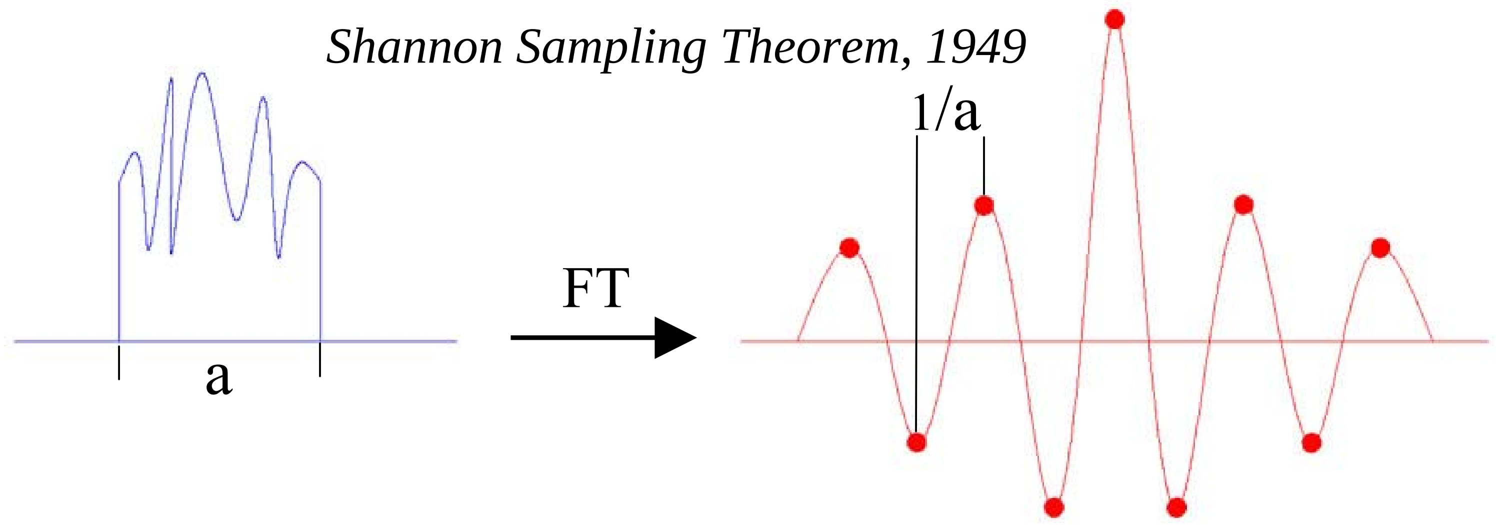


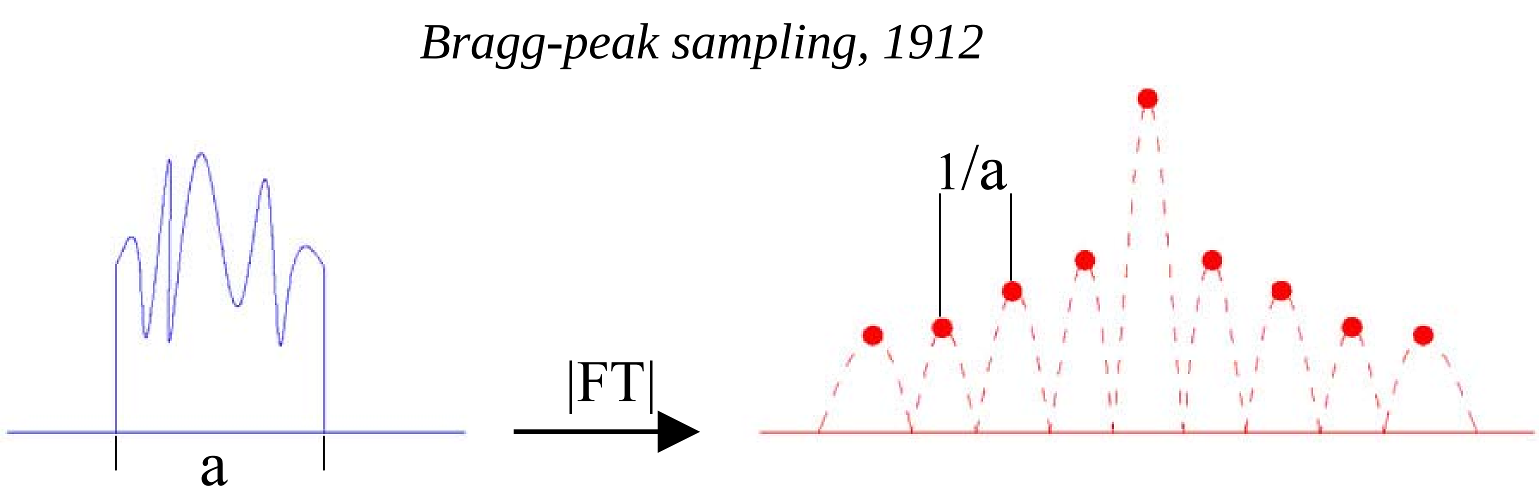
Shannon Sampling vs. Bragg-peak Sampling

Shannon Sampling Theorem, 1949

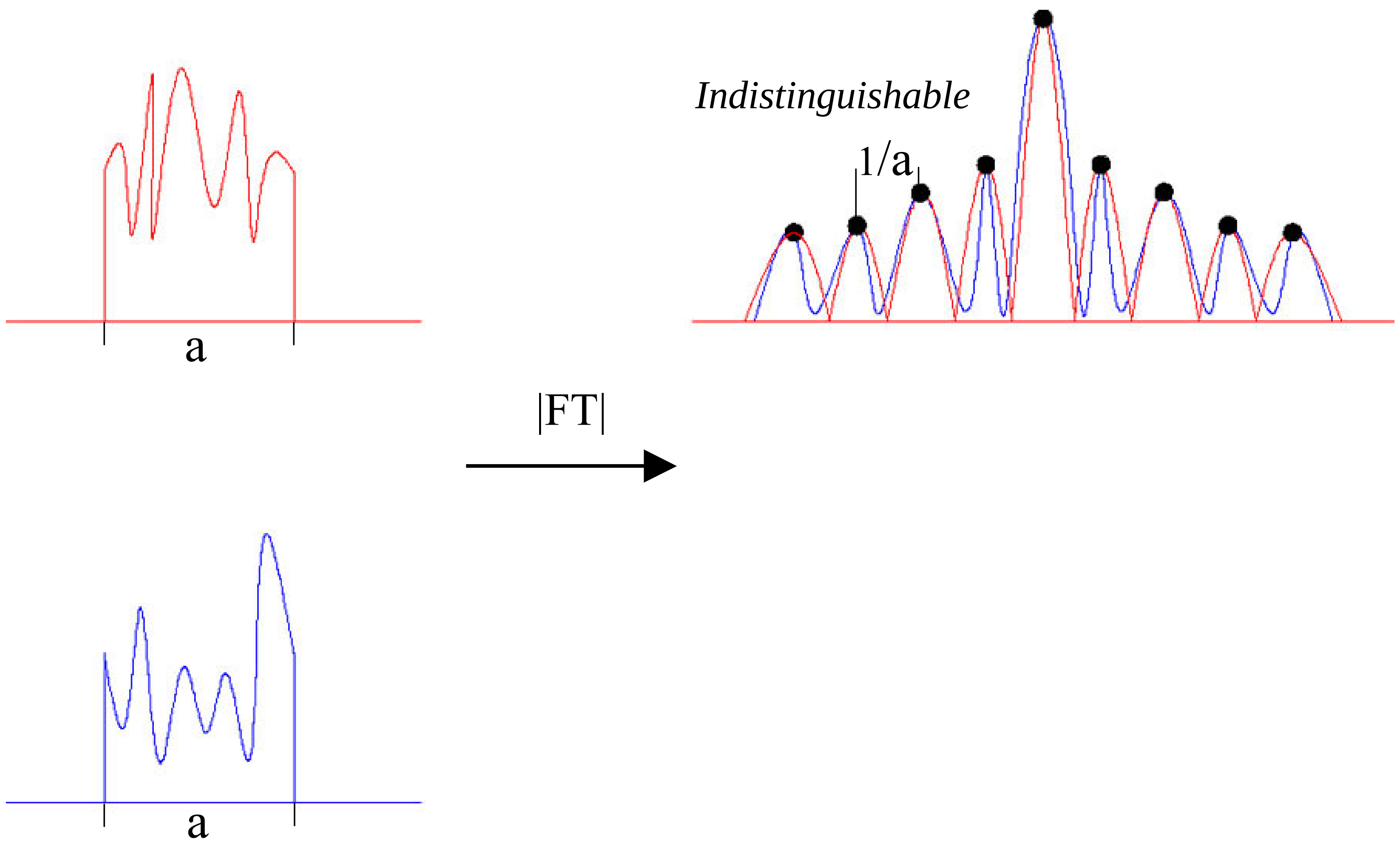


Shannon Sampling vs. Bragg-peak Sampling

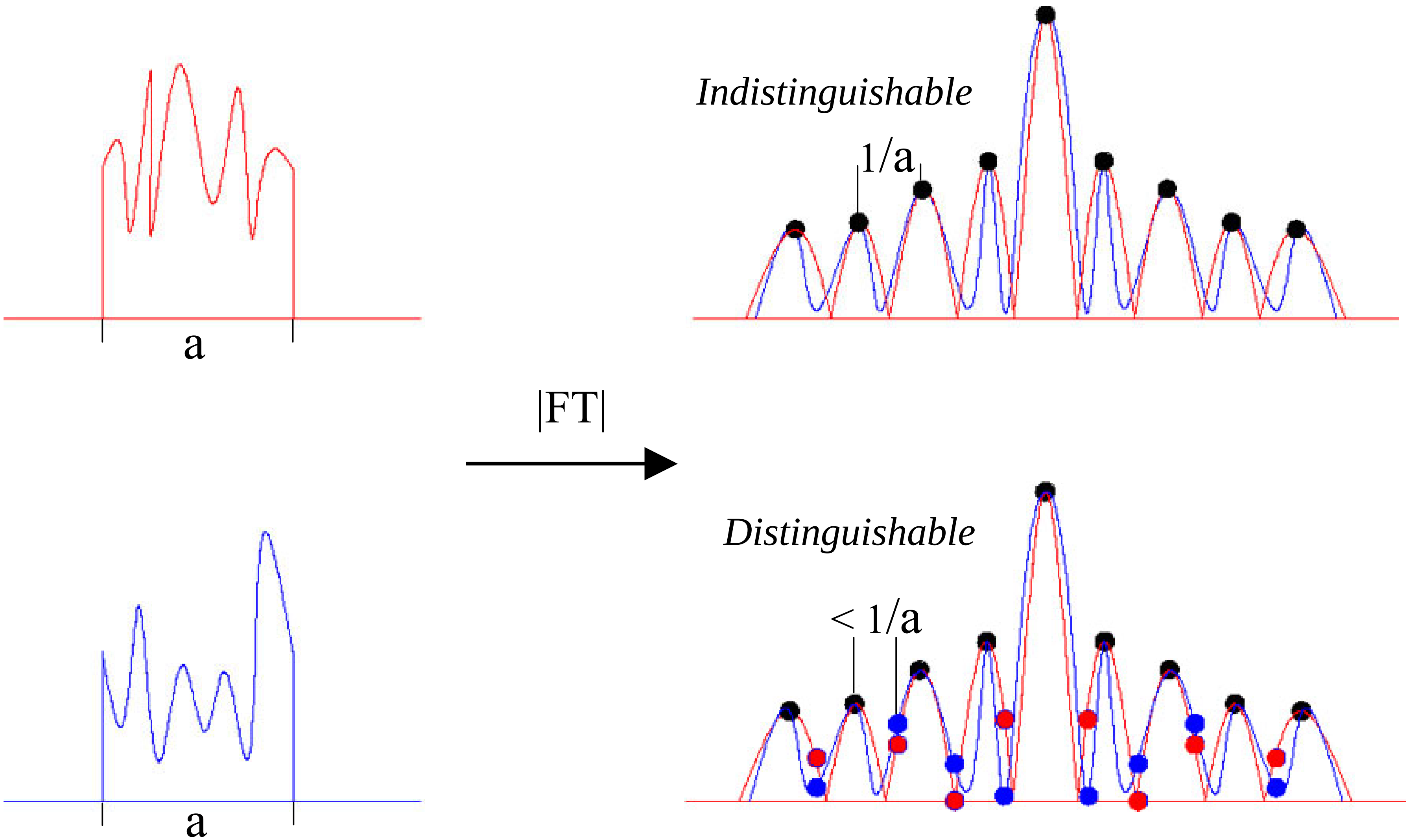




Bragg-peak Sampling vs. Oversampling

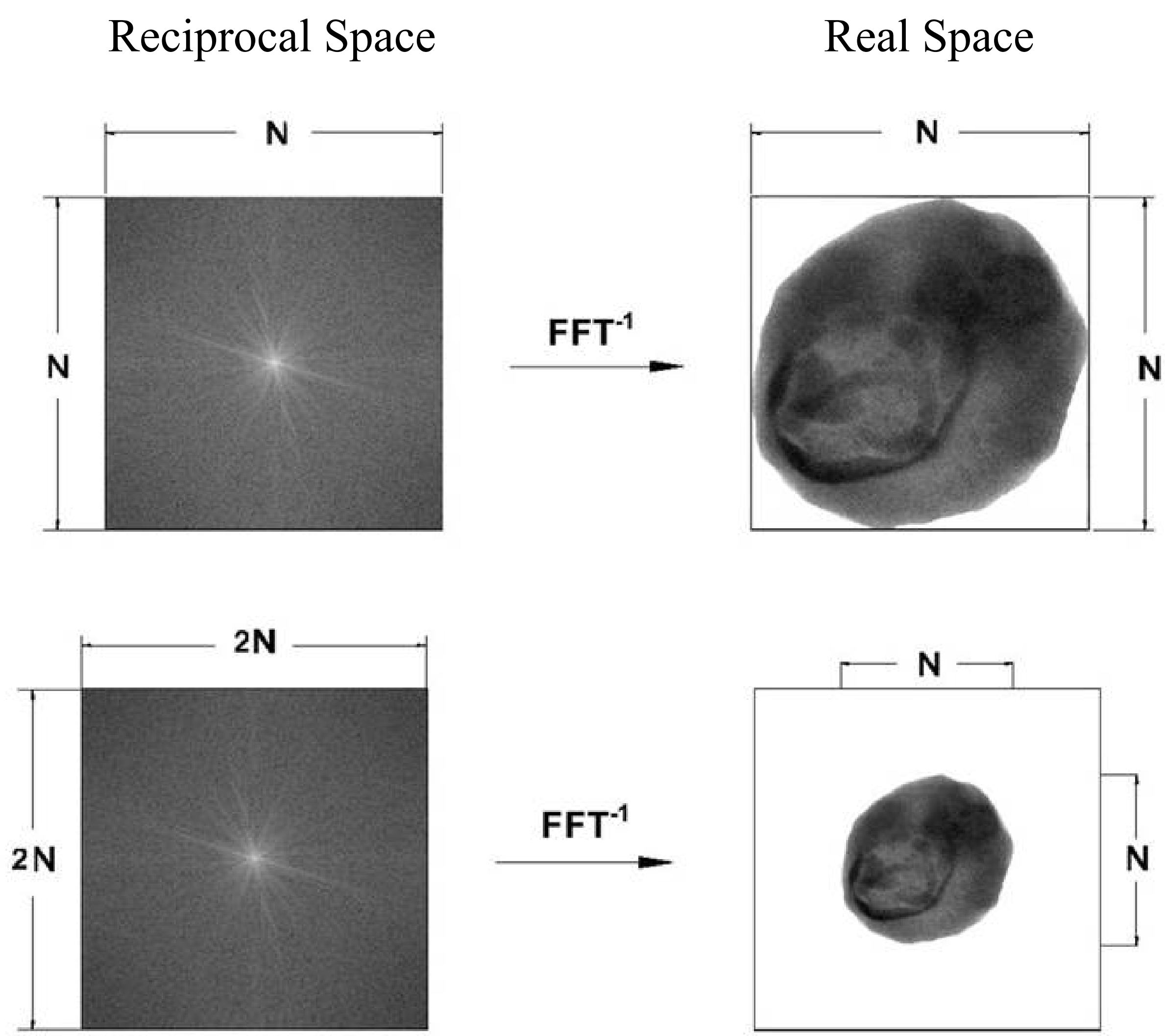


Bragg-peak Sampling vs. Oversampling



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

A Pictorial Representation of the Oversampling Method



An Iterative Algorithm

Real Space | Reciprocal Space

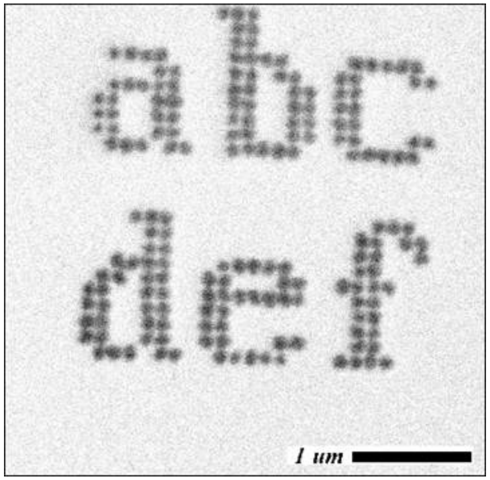
$$
\begin{tikzcd}
\rho_j^{'}(\mathbf{r}) \arrow[d, "\mathbf{B}"] & & F_j^{'}(\mathbf{k}) \arrow[ll, "FFT^{-1}"'] \\
\rho_j(\mathbf{r}) \arrow[rr, "FFT"] & & F_j(\mathbf{k}) \arrow[u, "\mathbf{A}"']
\end{tikzcd}
$$

A: $$F_j^{'}(\mathbf{k}) = \left| F_{\exp}(\mathbf{k}) \right| \times e^{\varphi_{j-1}(\mathbf{k})}$$

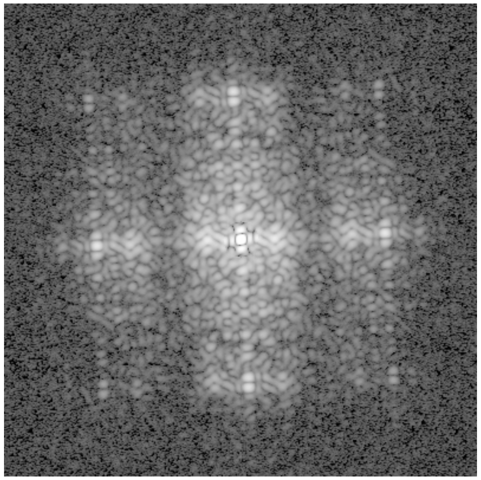
B: $$\rho_j(\mathbf{r}) = \begin{cases} \rho_j^{'}(\mathbf{r}) & if\ \mathbf{r} \in S\ \cap\ \rho_j^{'}(\mathbf{r}) \geq 0 \\ \rho_{j-1}(\mathbf{r}) - \beta \times \rho_j^{'}(\mathbf{r}) & if\ \mathbf{r} \notin S\ \cup\ \rho_j^{'}(\mathbf{r}) < 0 \end{cases}$$

Fienup, *Opt. Lett.* 3, **27** (1978).

The First Experimental Demonstration



(a) A SEM image



(b) An oversampled diffraction pattern (in a logarithmic scale) from (a).

(c) An image reconstructed from (b).

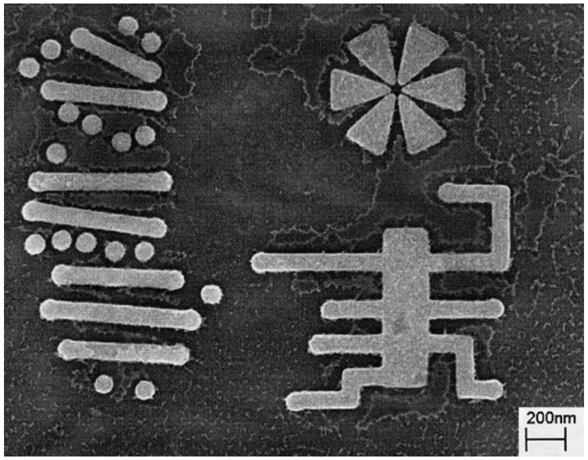
Miao *et al.*, *Nature* **400**, 342 (1999).

Current Detectors for Coherent X-ray Diffraction Microscopy

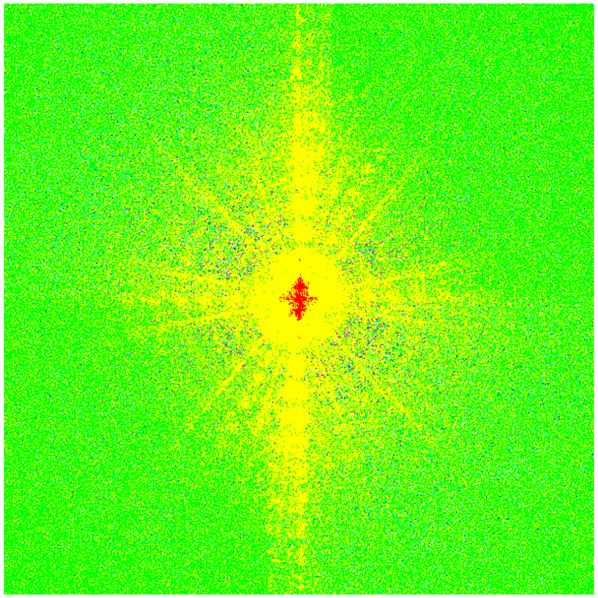
Direct-illuminated CCD cameras.

- High quantum efficiency: ~ 80%.
- Low dynamic range: ~ 10^2 photons/pixel.
- Slow read-out: ~ 1s.
- Pixel size: ~ 20 x 20 μm^2.
- Number of pixels: 1K x 1K
- Good linearity and sensitivity.
- Very low noise with LN cooling

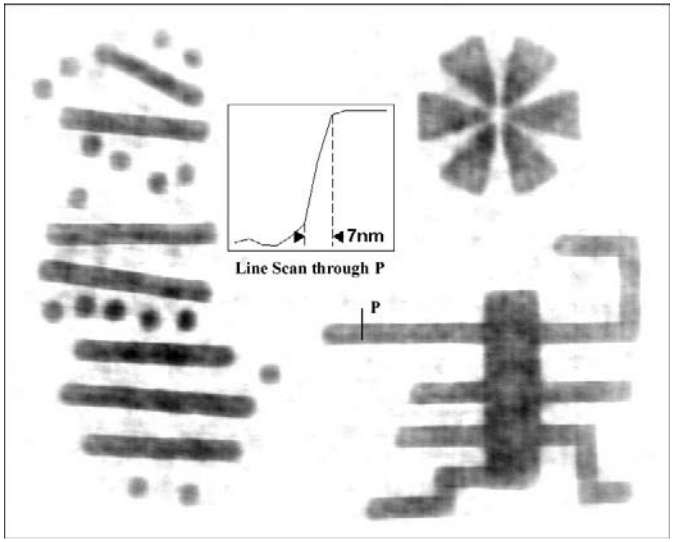
Imaging Nanostructures at 7 nm Resolution



(a) A SEM image of a non-crystalline sample made of Au

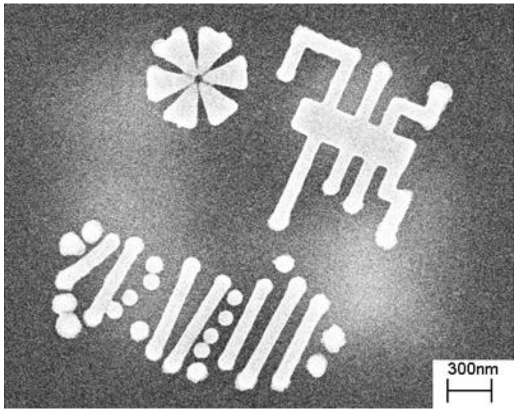


(b) A coherent diffraction pattern from (a) (the resolution at the edge is 7 nm)

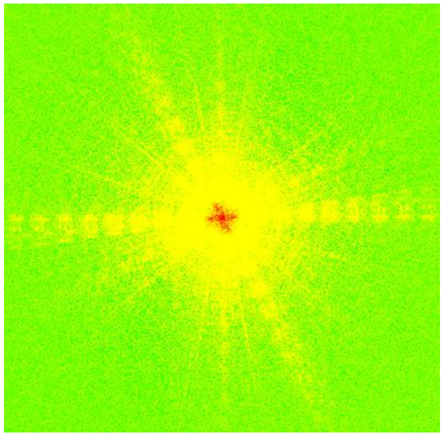


(c) An image reconstructed from (b)

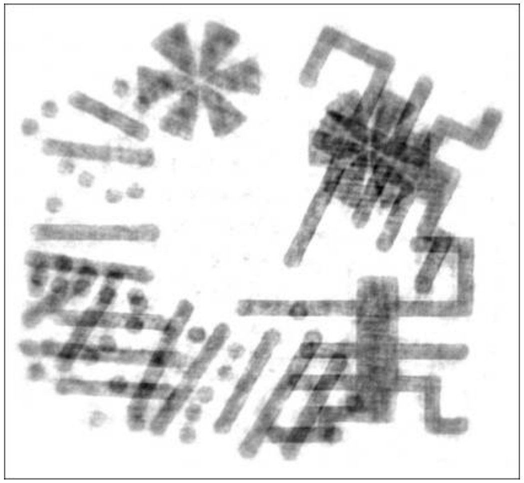
3D Imaging of a Nanoscale Material



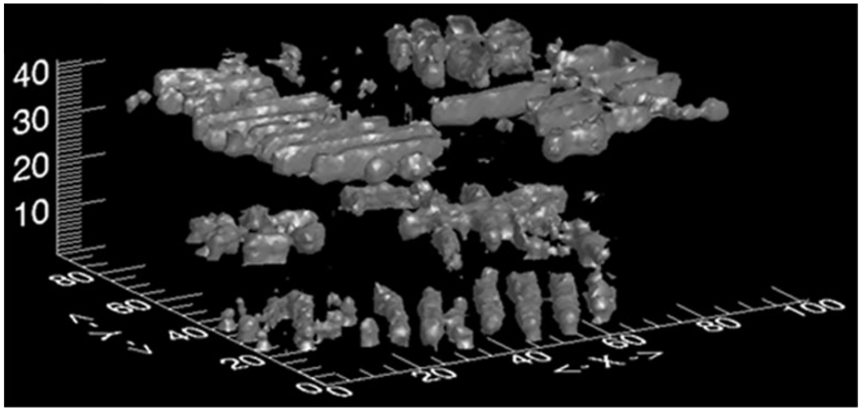
(a) A SEM image of a double-layered sample made of Ni (~2.7 x 2.5 x 1 μm^3)



(b) A coherent diffraction pattern from (a)



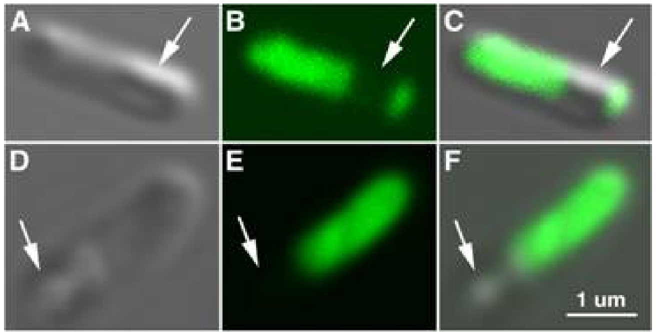
(c) An image reconstructed from (b)



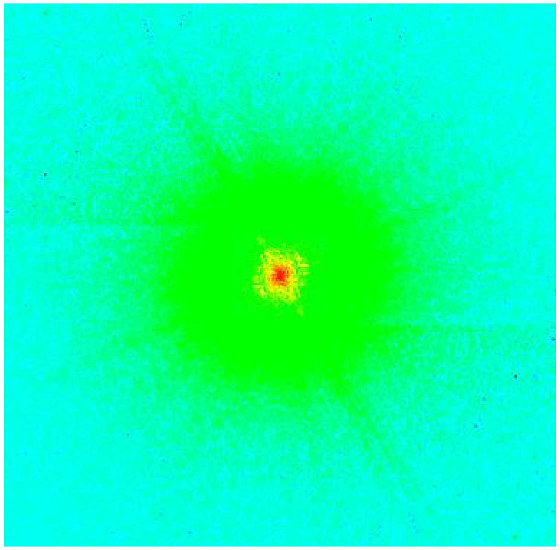
(d) An iso-surface rendering of the reconstructed 3D structure

Miao *et al*., *Phys. Rev. Lett.* **89**, 088303 (2002).

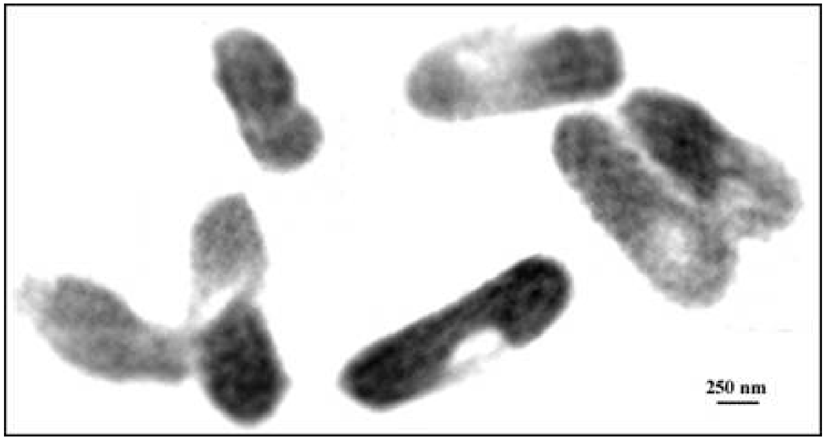
Imaging *E. Coli* Bacteria



(a) Light and fluorescence microscopy images of *E. Coli* labeled with manganese oxide



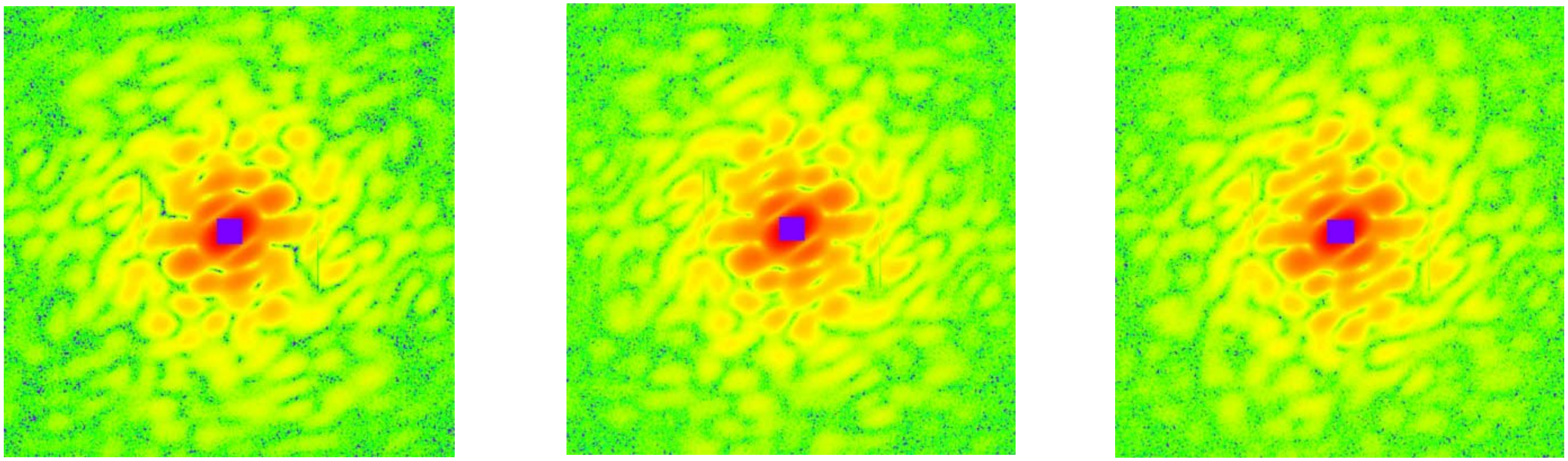
(b) A coherent X-ray diffraction pattern from *E. Coli*



(c) An image reconstructed from (b).

Miao *et al*., *Proc. Natl. Acad. Sci. USA* **100**, 110 (2003).

Quantitative Image Reconstruction of a Single GaN Quantum Dot from Oversampled Diffraction Intensities Alone

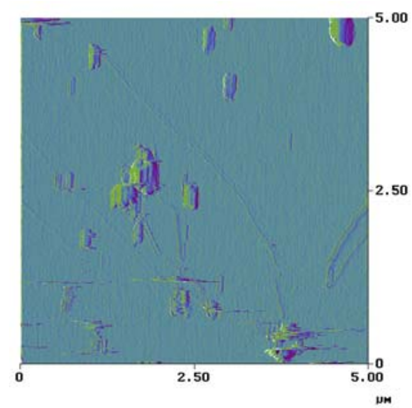


-7° 0° 7°

Diffraction patterns from a single GaN quantum dot at different orientations

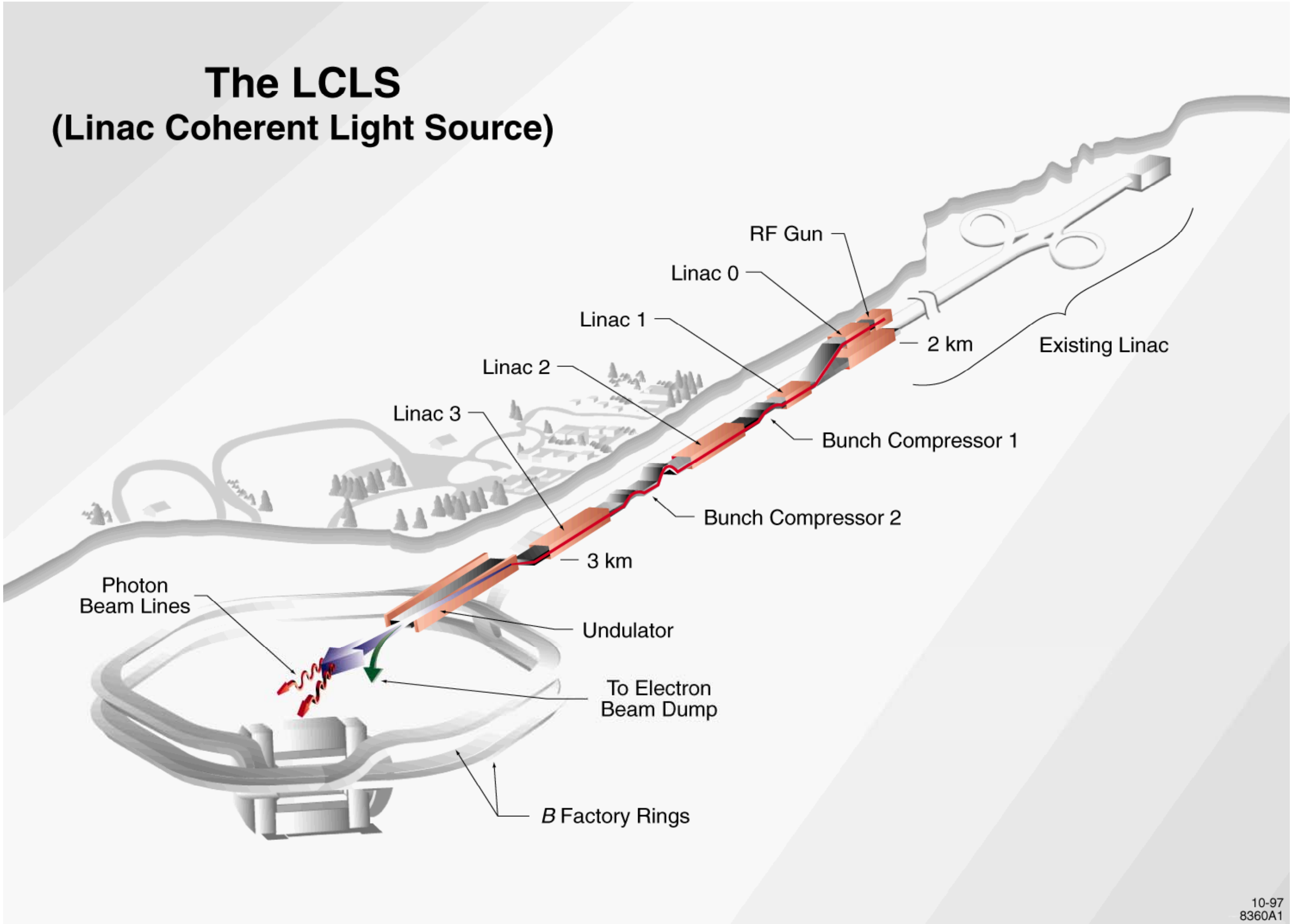
-7° 0° 7°

Image reconstruction of the diffraction patterns



An AFM Image of GaN quantum dots
Risbud, UC Davis

X-ray Free Electron Lasers



Two Major Challenges

Radiation Damage

Solemn & Baldwin, *Science* 218, 229 (1982).

Neutze *et al.*, *Nature* 400, 752 (2000).

When an X-ray pulse is short enough (< 10 fs), a 2D diffraction pattern could be recorded from a molecule before it is destroyed.

Orientation Determination

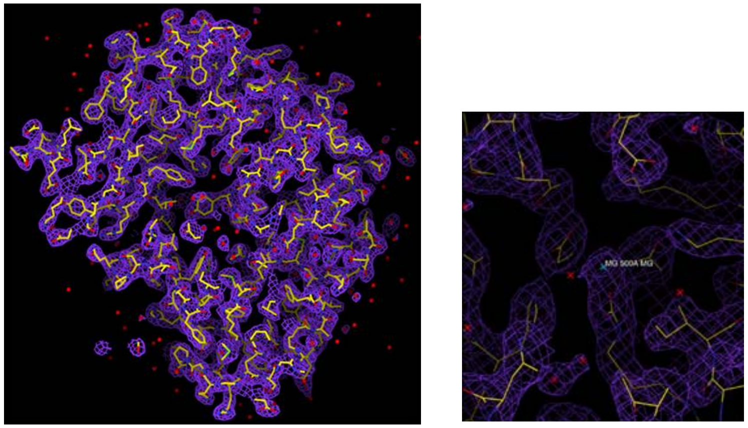
Use the methods developed in cryo-EM to determine the molecular orientation based on many 2D diffraction patterns.

Crowther, *Phil. Trans. Roy. Soc. Lond.* B. 261, 221 (1971).

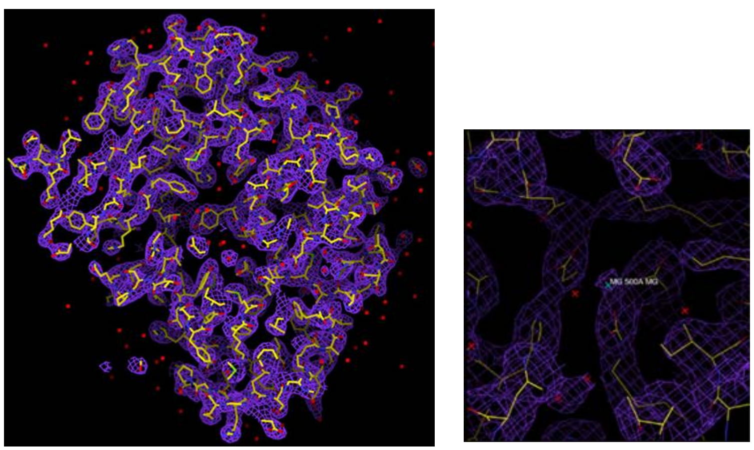
Use laser fields to physically align each molecule.

Larsen *et al.*, *Phys. Rev. Lett.* 85, 2470 (2000).

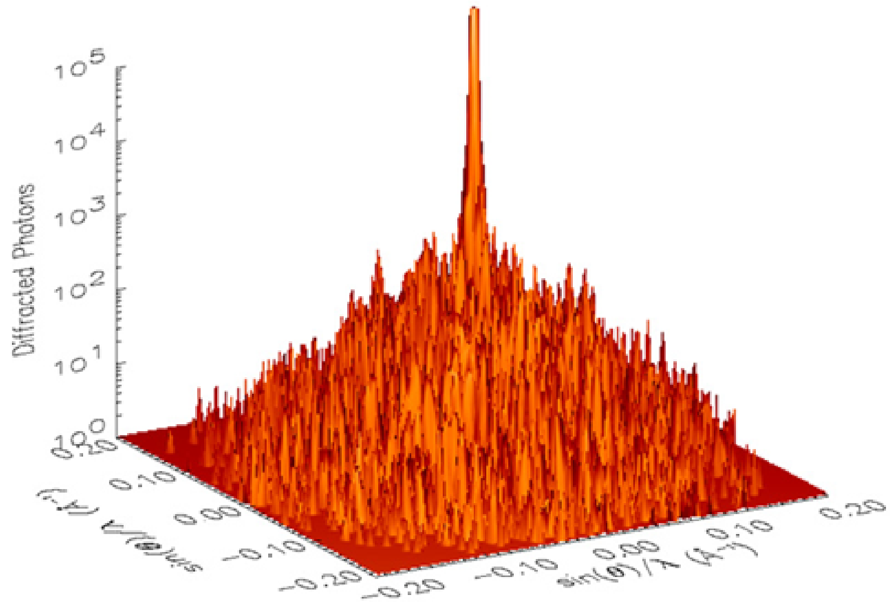
Potential of Imaging Single Molecule



(a) The 3D electron density map of a rubisco molecule and its active site (from PDB)



(c) The reconstructed 3D electron density map



(c) A section of the oversampled 3D diffraction pattern with Poisson noise, assembled from 3 x 10^5 simulated 2D diffraction patterns.

Miao, Hodgson, Sayre, *Proc. Natl. Acad. Sci. USA* 98, 6641 (2001).

Future Detectors for Coherent X-ray Diffraction Microscopy

- High quantum efficiency: > 90%.
- High dynamic range: > 10^4 photons/pixel.
- Fast read-out: ~ ms.
- Pixel size: 50 x 50 μm^2 – 100 x 100 μm^2.
- Number of pixels: ≥ 2K x 2K
- Sensitivity: Single photon counting
- Very good linearity

Pixel Array Detectors!

Summary

- Oversampling the diffraction intensities $\Rightarrow$ the phase information.
- Methodology of x-ray crystallography has been extended to image non-crystalline specimens.
- Imaged nanostructures and biological samples in two- and three-dimensions with a highest resolution of 7 nm.
- Future: 3D imaging of single particles at near atomic resolution in a combination of brighter X-ray sources with pixel array detectors.

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C. Larabell, *UC San Francisco and LBNL*

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B. Lai, *Argonne National Lab*

J. Amonette, *Pacific Northwest National Lab*

O. Terasaki, *Stockholm University*