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
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

X-rays, electrons or lasers → An object → Diffraction intensities

Solving the phase problem
The Shannon Sampling Theorem

Shannon Sampling Theorem, 1949

Without Phases
The Oversampling Method

Indistinguishable

\[ \frac{1}{a} \]

\[ |\text{FT}| \]
The Oversampling Method

Indistinguishable

Distinguishable

$\frac{1}{a}$

$< \frac{1}{a}$
Experimental Implementation of the Oversampling Method

Reciprocal Space

Real Space

\[ \text{FFT}^{-1} \]

\[ \text{FFT}^{-1} \]
The Physical Explanation to the Oversampling Method

Better coherence ⇒ More correlated intensity points ⇒ Phase information

The Guided Hybrid Input-Output Algorithm

(i) Started with 16 independent reconstructions.

(ii) For each reconstruction:

Real Space \[ \xrightarrow{\text{FFT}} \] Reciprocal Space

\[ \xleftarrow{\text{FFT}^{-1}} \]

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

\[
R = \sum \left| F_{\text{exp}} - \alpha F_{\text{cal}} \right| \sqrt{\sum F_{\text{exp}}(k_x,k_y)}
\]

(iv) \[
\rho_{new}^i = \sqrt{\rho_{seed} \times \rho_{old}^i}
\]

\[ i = 1, 2, \ldots, 16 \]
An oversampled diffraction pattern from a single GaN quantum dot at 0°.

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

Coherent X-ray Diffraction Pattern from a Single GaN Quantum Dot Nanoparticle
Image Reconstruction Using the gHIO Algorithm

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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

(a) (b) (c) (d)

200 nm

200 nm
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

“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.”


Reconstruction of a simulated vesicle by using conventional tomography (27 projections ranging from -69 ° to +69 °)
Pseudo-Polar Fast Fourier Transform (PPFFT)

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

Conventional tomographic reconstruction

\[ F_\theta (R, Z) \xrightarrow{\text{PPFFT}^{-1}} \xrightarrow{\text{PPFFT}} \rho(x, y, z) \]

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

3D Imaging of Hemocyanin Molecules Using Equally Sloped Tomography
Summary

• Oversampling the diffraction intensities ⇒ the phase information.

• Coherent (i.e. lensless) imaging ⇒ structure determination of nanomaterials and biological samples in two- and three-dimensions.

• Application of coherent imaging: materials science, nanoscience and biology.

• Equally sloped tomography ⇒ 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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