Atomic Resolution Electron Tomography

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Methods for Visualizing Atomic Structure

- X-ray crystallography can reveal the *globally*-averaged 3D atomic structure of crystals.
- Transmission electron microscopes can resolve atoms in 2D projections of 3D samples.
- Scanning tunneling and atom force microscopes can image atomic structure at surface.

Richard Feynman stated in 1959: “It would be very easy to make an analysis of any complicated chemical substance; all one would have to do would be to look at it and see where the atoms are... I put this out as a challenge: Is there no way to make the electron microscope more powerful?”

*A general imaging method that can determine the 3D positions of individual atoms in matter would have revolutionary impact in modern science and technology.*
Why Tomography?

A single projection is usually insufficient to infer the structure of a general 3D object. (New Yorkers Magazine, 1991)
Conventional Tomographic Reconstruction Method: Weighted (Filtered) Back Propagation (WBP, FBP)

(b) The missing wedge

91 projections  61 projections  37 projections  25 projections
(with a missing wedge)

Limitations for achieving atomic resolution:

(i) Aligning the projections with atomic precision is challenging.
(ii) Dynamical scattering and non-linear effects in electron microscopy.
(iii) Radiation damage limits the number of projections measurable from an object.
(iv) Specimens cannot usually be tilted beyond ±79° (a missing wedge).
Projection Misalignment in Tomographic Tilt Series

Rotation Axis 1

0°
45°
90°

Rotation Axis 2

0°
45°
90°
Achieving Atomic Precision Alignment with the Center of Mass (CM) Method

Set the CM of each projection at the origin.
An exact, invertible pseudopolar fast Fourier transform between the Cartesian and pseudopolar grid has been developed.

The lines are equally sloped ($\Delta \tan \theta$) instead of equally angled ($\Delta \theta$).

Equal Slope Tomography (EST)

\[ y = s_x x \]
\[ \Delta s_x = \frac{1}{4} \]
\[ \Delta \theta = 14.0^\circ \]

The Iterative EST Method

Free EST software and code: www.physics.ucla.edu/research/imaging/EST
Experimental STEM Tilt Series of 69 Projections Acquired from a 10 nm Au Particle
Three $0^\circ$ Projections Measured during the Acquisition of the Tilt Series
Comparison between Measured and Reconstructed Projections at 7.1°
Achieving Electron Tomography at 2.4 Å Resolution

A 3.36 Å thick central slice in the XY plane

A 3.36 Å thick slice in the ZY plane

(111)
3D Volume and Surface Renderings of the Reconstructed Au Nanoparticle
Identification of Major 3D Grains inside the Au Nanoparticle at Atomic Scale Resolution

Experimental STEM Tilt Series of 104 Projections
Acquired from a Multiply-Twinned Pt Particle
3D Reconstruction of the Pt Nanoparticle before and after Applying a 3D Fourier Filter

A 2.6 Å thick central slice in the XY plane
Comparison between 3D Fourier and 3D Wiener Filtering
Grain Boundary Comparison between Experimental and Reconstructed Projections
Reveal Atomic Steps at the 3D Grain Boundaries in the Pt Nanoparticle
Comparison between 3D Fourier and 3D Wiener Filtering on Atomic Steps across a Twin Boundary

3D Fourier filtering with a threshold of 10% (a-c) and 7% (d-f).

3D Wiener filtering with $\lambda = 3$ (g-i), $\lambda = 2$ (j-l) and $\lambda = 1$ (m-o).
3D Imaging of the Core Structure of an Edge Dislocation at Atomic Resolution

A 7.9 Å thick internal slice

Three 2.6 Å atomic layers sectioning through the slice of (b)

\[ b = \frac{1}{2}[101] \]

Edge dislocation in a simple cubic lattice
3D Imaging of a Screw Dislocation at Atomic Resolution
(A 5.3 Å Thick Internal Slice)


3D Fourier filtering codes and data sets: www.physics.ucla.edu/research/imaging/dislocations
The dislocations and the atomic steps at the twin boundaries appear to be stress-relief mechanism.
Observation of Nearly All the Atoms in the Pt Nanoparticle

www.nature.com/nature/videoarchive/nano-imaging
(Nature video with > 780,000 YouTube views)
Determining the Coordinates of Individual Atoms with a 3D Precision of ~19 pm

Tip of a tungsten needle, shown from layers 1 (dark red) to 9 (purple)  
(Number of atoms: 3,769)
3D Identification of a Point Defect and Atomic Displacements
3D Measurements of the Atomic Displacement Field and Full Strain Tensor

Xu, Chen, Wu, Scott, Theis, Ophus, Bartels, Yang, Ramezani-Dakhel, Sawaya, Heinz, Marks, Ercius, Miao, under review.
Origin of the Strain Field

Surface WC\textsubscript{x} and diffusion of C atoms
Verification of the Full Strain Tensor Using MD Simulations
Hemocyanins carry oxygen in the blood of most molluscs, and some arthropods. Similar function as hemoglobin in human.

3D model averaged from many identical copies
Comparison among EST, WBP, ART and SART Reconstructions

WBP-full
EST-full
WBP-2/3
EST-2/3

EST                         WBP
---------------------------
                         ART                        SART
Surface Renderings of a Hemocyanin Molecule Reconstructed by WBP and EST

Model

WBP-full

WBP-full denoising

EST-full

WBP-2/3

WBP-2/3 denoising

EST-2/3
Quantitative Comparison among Different Reconstruction Methods

EST improves a resolution of 5 Å over WBP, 18 Å over ART, and 21 Å over SART.

3D Reconstructions of an Intact Bacterial Cell with EST

Application of EST to X-ray Phase Contrast Imaging

- X-ray energy: 60 keV
- Detector pixel size: 92 μm
- Breast cancer sample thickness: 9 cm
- Acquisition time (2,000 projs.): ~30 minutes

Comparison Between FBP and EST Reconstructions
Identification of Detailed Features in the Breast Cancer Sample (EST 512)

1) collagen strands; 2) glandular tissue; 3) spiculations; 4) fat; 5) skin; and 6) formalin
## Blind Evaluation by Five Independent, Experienced Radiologists in Germany

<table>
<thead>
<tr>
<th></th>
<th>WBP (full)</th>
<th>EST (74% less dose)</th>
<th>WBP (74% less dose)</th>
<th>EST (90% less dose)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Overall image quality</strong></td>
<td>4.3 ± 0.9</td>
<td>4.5 ± 0.5</td>
<td>2.2 ± 0.4</td>
<td>2.7 ± 0.9</td>
</tr>
<tr>
<td><strong>Sharpness</strong></td>
<td>4.0 ± 0.7</td>
<td>4.3 ± 0.5</td>
<td>3.3 ± 0.5</td>
<td>2.2 ± 0.8</td>
</tr>
<tr>
<td><strong>Image contrast</strong></td>
<td>4.0 ± 0.5</td>
<td>4.8 ± 0.4</td>
<td>3.0 ± 0.7</td>
<td>3.4 ± 1.0</td>
</tr>
<tr>
<td><strong>Evaluation of different structure</strong></td>
<td>4.1 ± 0.6</td>
<td>4.8 ± 0.4</td>
<td>2.6 ± 0.5</td>
<td>2.9 ± 1.0</td>
</tr>
<tr>
<td><strong>Noise level</strong></td>
<td>4.2 ± 0.6</td>
<td>4.8 ± 0.3</td>
<td>1.8 ± 0.8</td>
<td>3.3 ± 0.8</td>
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“5” - the best and “1” - the worst
Low-Dose 3D Diagnosis of Human Breast Cancers in Combination of Phase-Contrast X-ray Imaging and EST

Mean Glandular Dose (MGD) for EST 512: 1.96 mGy
MGD for dual view clinical mammography: 3.4 mGy

• A CM method has been developed to align tomographic projections at atomic precision.

• EST has been developed for the 3D tomographic reconstruction from a limited number of projections with a missing wedge.

• A general electron tomography method is achieved at 2.4 Å resolution; major grains are identified inside an icosahedral multiply twinned Au nanoparticle in three dimensions.

• Atomic steps at 3D twin boundaries and the 3D core structure of edge and screw dislocations are observed in a decahedral multiply twinned Pt nanoparticle at atomic resolution.

• The 3D coordinates of thousands of individual atoms and a point defect in a material are determined with ~19 pm precision; the 3D atomic displacement field and the full strain tensor are measured.

• We expect atomic resolution electron tomography to find broad applications in materials science, nanoscience, physics, chemistry and biology.
# Collaborators

<table>
<thead>
<tr>
<th>Institution</th>
<th>Collaborators</th>
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</thead>
<tbody>
<tr>
<td>The Miao group at UCLA</td>
<td>Mary Scott, Chien-Chun Chen, Rui Xu, Jose Rodriguez, Cun Zhu, Li Wu, Matthias Bartels, Yongsoo Yang, Jihan Zhou, AJ Pryor, Marcus Gallagher-Jones, Zhifeng Huang &amp; Edwin Lee</td>
</tr>
<tr>
<td>NCEM, LBNL</td>
<td>Peter Ercius, Uli Dahmen, Colin Ophus &amp; Jim Ciston</td>
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<td>UCLA</td>
<td>Yu Huang, Chris Regan &amp; Michael Sawaya</td>
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<td>Northwestern University</td>
<td>Laurence Marks</td>
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<td>University of Birmingham</td>
<td>Wolfgang Theis</td>
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<td>Stanford University</td>
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<td>ESRF</td>
<td>Emmanuel Brun &amp; Alberto Bravin</td>
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<td>University of Akron</td>
<td>Hendrik Heinz &amp; Hadi Ramezani-Dakhel</td>
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<td>Caltech</td>
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<td>EMBL</td>
<td>Daniel Castaño-Díez</td>
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Free software, codes and data sets: [www.physics.ucla.edu/research/imaging](http://www.physics.ucla.edu/research/imaging)