Tracking Light Atoms in 3D Ptychographic Reconstructions

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Abstract:

As semiconductor devices move to 3D nanoscale architectures, traditional 2D imaging cannot fully characterize atomic-scale defects, interface roughness, and structural transitions in buried features. Multi-slice electron ptychography (MEP) addresses this by enabling 3D visualization with sub-Ångström lateral and nanometer-scale depth resolution. This project developed a program to test the depth resolution of Scanning Transmission Electron Microscopy (STEM) MEP reconstructions, using simulated and experimental datasets of gadolinium gallium garnet (Gd3Ga5O12, GGG) sectioned into depth-dependent slices. The program tracks and optimizes atomic coordinates across each slice and plots them in 3D to reconstruct the specimen's structure, calculating integrated pixel intensity within a mask at each atom to detect the ~1 nm z-axis spacing between oxygen atoms. This 3D positional information supports accurate predictive modeling and precise defect identification needed to advance next-generation semiconductor manufacturing.

Summary of Research:

STEM datasets are collected by rastering a focused electron beam across a sample and capturing the transmitted intensity, which traditionally yields only a 2D snapshot that neglects the sample's 3D structure. To recover depth information, the Muller Group uses MEP, a computational reconstruction technique requiring 4D STEM: the electron beam is defocused onto an Electron Microscope Pixel Array Detector (EMPAD), producing an overlapping diffraction pattern with two real-space (x, y) and two reciprocal-space (kx, ky) dimensions that encode the phase and amplitude needed to reconstruct the 3D structure. The Muller Group recently achieved 2.7 nm depth resolution, sufficient to visualize individual interstitial defects (Chen et al., 2024), and is now working toward one-nanometer and eventually sub-nanometer resolution to detect a broader range of defects, dopants, and interfaces. This project's objective was to determine whether STEM-MEP reconstruction can resolve the known 12.5 Å oxygen spacing in a garnet sample, and to develop a computational method to quantitatively compare simulated and experimental depth resolution.

GGG is a suitable test material because it contains isolated oxygen columns separated by 12.5 Å along the z-axis. Resolving individual oxygens within these columns would demonstrate depth resolution better than ~1 nm. To validate the code, I first reconstructed a simulated GGG dataset from the ideal crystal structure, sectioned into fifty 3.1 Å slices to match the experimental data. Each GGG unit cell has a central alternating Gd/Ga column surrounded by eight oxygen columns. A slight planar depth offset makes four columns appear brighter and four dimmer, a pattern that switches every two slices (6.2 Å). I tracked the central Gd/Ga column across all fifty slices using the AtoMap library's position-correction tools (Gaussian fitting and center of mass), then located the eight surrounding oxygen columns by branching outward at angles calculated from a Vesta GGG visualization. Because of this depth-dependent brightness pattern, I applied a mask to each tracked position and integrated the pixel intensity within it across the image slices, enabling detection of the true oxygen positions.

The resulting simulated reconstruction reproduced the expected four-bright/four-dim lateral pattern. Along each oxygen column, the 3D intensity projection showed a blinking pattern repeating every four slices (12.4 Å), just under the true 12.5 Å oxygen spacing, confirming depth resolution better than 12.4 Å. A line trace of intensity versus depth for a single oxygen column showed peaks spaced exactly four slices apart. Analyzing the heavier Gd/Ga corner columns, where Ga atoms are spaced 6.2 Å from Gd and 12.4 Å from the next Ga, showed the same four-slice peak spacing, meaning only the larger Ga–Ga spacing was resolved,

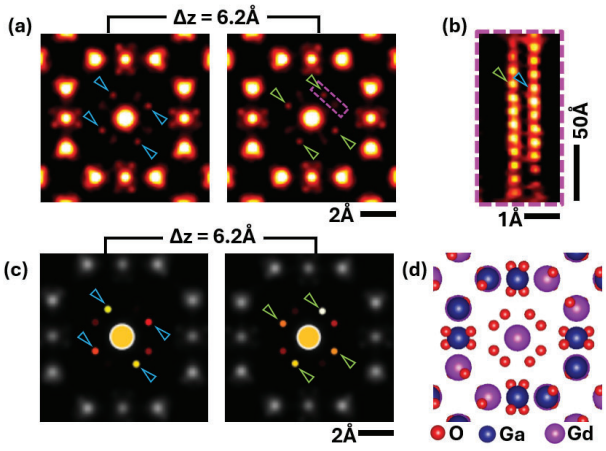

Figure 1: (a), (b), and (c) show simulated reconstructions of GGG based on the ideal crystal structure seen in (d). (a) and (c) are single 3.1 Å slices, two slices apart, from a fifty-slice stack. (a) shows the four-bright/four-dim pattern among the eight oxygen columns surrounding the central Gd/Ga column, caused by a z-axis depth offset between adjacent columns, shown in profile in (b).

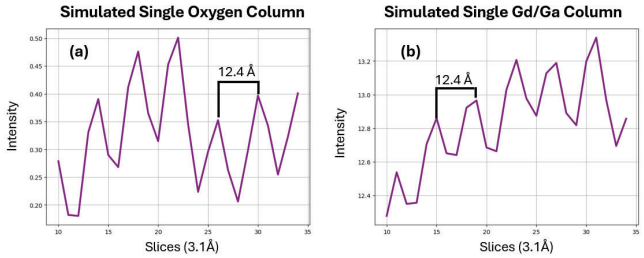

Figure 2: Integrated intensity vs. slice number for single atomic columns. (a) A single oxygen column, with peaks marking individual atoms spaced four slices (12.4 Å) apart, confirming accurate depth resolution. (b) A heavier Gd/Ga column, where only the larger Ga–Ga spacing (12.4 Å) is resolved; the smaller 6.2 Å Ga–Gd spacing is not detected.

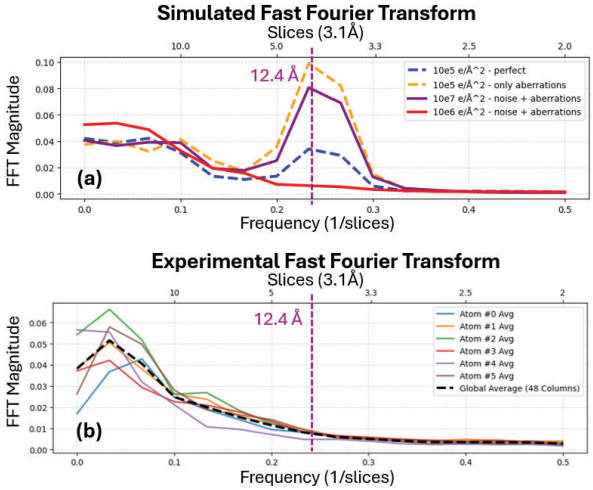

Figure 3: FFTs of oxygen column intensity traces, averaged across all eight columns per unit cell. (a) Simulated reconstruction, showing a clear 12.4 Å periodicity. (b) Experimental reconstruction, showing no corresponding periodicity.

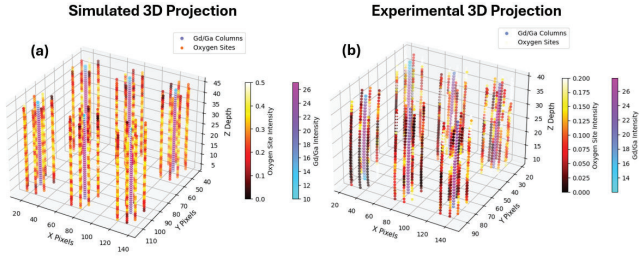

Figure 4: 3D reconstructions of atomic coordinates for the central Gd/Ga column and surrounding eight oxygen columns, from simulated (a) and experimental (b) data. Colormap indicates integrated pixel intensity within each atom's mask.

not the smaller 6.2 Å Ga–Gd spacing. This places the depth resolution between 6.2 Å and 12.4 Å. Taking the FFT of each oxygen column's line trace and averaging across all eight columns per unit cell produced a clear peak at four slices for the simulated dataset.

To identify which parameters most affect this depth resolution, I repeated this FFT analysis across multiple simulations of varying electron dose, noise, and aberrations, then overlaid the results. Most conditions still showed a 12.4 Å periodicity peak, but with varying amplitude, providing a guide to which parameters improve depth resolution.

Applying the same FFT analysis to the experimental scan showed no corresponding periodicity, indicating that the experimental reconstruction did not achieve the 12.4 Å depth resolution needed to resolve individual oxygen atoms.

Conclusions and Future Steps:

The program successfully tested depth resolution by first establishing expectations with a simulated dataset before comparing them to experimental results. This comparison showed that the experimental reconstruction did not reach the 1.24 nm depth resolution needed to resolve the oxygen sublattice in GGG. The simulation condition comparison provided valuable direction as the Muller Group continues refining STEM scan and MEP reconstruction parameters, using this program to evaluate future experimental datasets.

References:

[1] Karapetyan, S., et al. 3D atomic-scale metrology of strain relaxation and roughness in Gate-All-Around transistors via electron ptychography. Nat Commun 17, 3561 (2026).

[2] Chen, Z. et al. Imaging interstitial atoms with multislice electron ptychography. arXiv:2407.18063 (2024).