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Filling in the Missing Wedge with Aberration-corrected Electron Tomography

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Electron tomography is an underdetermined inverse problem that suffers from missing wedges of information in reciprocal space. Even with a 180° specimen tilt range, small missing wedges between each tilt restrict the 3D resolution. This theoretical limit to 3D resolution is defined by the Crowther criterion, which relates resolution to the number of projections acquired and the specimen size[1]. Developments in reconstruction methods, such as compressed sensing, are offering new limits to reconstruction quality by estimating the missing information using additional prior knowledge about the specimens [2]. It has been shown that porous materials and nanoparticles can be reconstructed reliably with fewer tilts and a limited tilt range when a sufficient amount of data is collected (e.g., 70 projections across ±70°)[3-5]. While compressed sensing has provided a better estimate of the 3D object, it does not measure additional specimen information. Compressed sensing may still fail when data is sufficiently undersampled[5], or highly directional structures are present in an object[6].

Without any prior assumptions, the small missing wedges of information can be measured using aberration-corrected STEM tomography that acquires a through-focal stack at every tilt[7]. Using a 3D linear incoherent imaging model, information is no longer mapped to a plane in Fourier (k) space, but becomes a volumetric toroid [8]. Figure shows the 3D structure of a contrast transfer function (CTF) for through focal tomography where every specimen tilt measures a toroid with petal-shaped cross-section. A remarkable feature of the 3D CTF is the overlapped regions that permit complete information collection—unachievable with conventional tomography. This breaks expected Crowther relationships and the maximum reconstructable object size is unlimited up to spatial frequency k_C. Using a massively parallelized multslice simulation[9] of aberration-corrected STEM tomography, we show atomic resolution reconstruction of large object sizes is possible. Fully quantum mechanical multislice simulation of three synthetic FePt nanoparticles spanning $(15\text{nm})^3$ was performed at incident electron energy of 200keV and convergence semi-angle of 30mrad, pixel size $(0.25\text{Å})^2$, and 1.7° specimen tilts. Tomographic reconstruction was achieved by mapping all real-space images to Fourier space and applying an inverse Fourier transform. Due to the continuum of information across the low- to mid- frequencies, a simple direct Fourier transform provides a high-quality reconstruction without aliasing.

This work discusses models for aberration-corrected electron tomography by establishing analytic descriptions for resolution, sampling and object size, using linear imaging theory and massively parallelized multislice computation. Comparisons are made with traditional measurement and compressed sensing reconstruction.

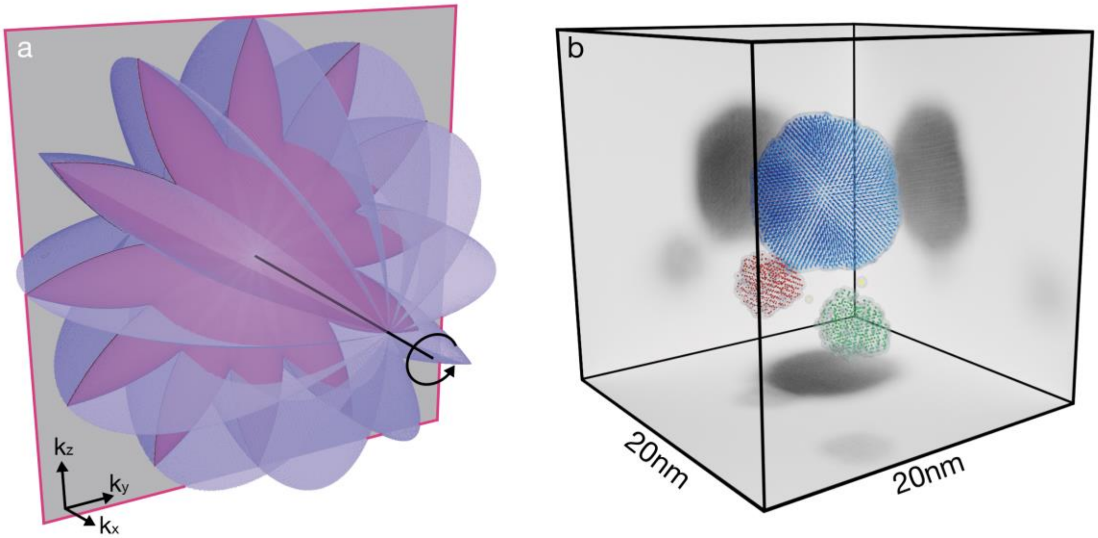

Figure 1. Aberration-corrected electron tomography enables unprecedented high-resolution of extended objects. a) 3D contrast transfer function shows no missing wedges of information is possible out to a specified spherical radius. Here aberration-corrected STEM is exaggerated to highlight key structural features (convergence semi-angle= 30 mrad, 200 keV). b) 3D atomic resolution tomography of three nanoparticles in a 20nm volume---reconstructed here from quantum mechanical scattering simulations.

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