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Filling the Missing Wedge in Tomography: A Constraint-based Reconstruction Method for 3D TEM/STEM Imaging

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In (scanning) transmission electron microscopy (STEM & TEM), a 3D model of an object is obtained by acquiring its 2D projections. Experimentally, the limited and finite number of obtainable projections provides incomplete information of a 3D specimen, producing artifacts in traditional tomographic reconstructions including Weighted Back Projection and SIRT. Missing data arises from limits on the microscope's range of specimen tilts and discrete sampling. The finite number of projections governs the resolution and size of the reconstructed object—as described by the Crowther criterion [1]. However, the limited tilt range is responsible for an insidious missing wedge of information in Fourier space and causes elongation, blurring, and distracting caustics in final reconstruction.

Here, we present a new iterative constraint-based reconstruction algorithm that significantly reduces the discrepancy between the reconstruction and the true object by "filling in" the missing wedges in the Fourier data. Using constraint satisfaction problem as a guide, the algorithm searches for reconstructions that not only match the measured data, but also satisfy additional physical constraints. Ultimately, it fills in the missing information with values that satisfy these basic constraints thus providing noticeable improvements over the original information alone.

As an example, Figure 1(a) shows a slice of the 3D Fourier transform of STEM data taken from PtCu nanoparticles [2]. A continuum of information was obtained by combining through-focal imaging and specimen tilting. However, a limited tilt range provides a large missing wedge (black area). Reconstruction by the Direct Fourier method does not address the missing wedge problem—producing obvious artifacts, as shown in Figure 1(b). When the constraint-based technique is used, the missing wedge in Fourier space is filled (Figure 2a) and the image artifacts largely disappear (Figure 2b).

To recover the missing information, our algorithm starts with a random image, and then iterates back and forth between the image (real) space and Fourier space to impose the relevant constraints. In image space, it imposes a positivity constraint and zeros the image outside a support, which is iteratively refined throughout the reconstruction [3]. In Fourier space, the algorithm imposes the measured amplitudes and phases where they are known, and leaves the values in the missing wedge unchanged. A weak, total power constraint is also applied to the Fourier amplitudes at high spatial frequencies. To achieve the desired solution, we adopt the difference-map iteration [4], which has the advantage of avoiding stagnation. The algorithm is terminated when there is no discernible change in the reconstruction. The uniqueness of the reconstructed data in the missing wedge can be tested by the unconstrained mode analysis developed by Thibault et al. [5].

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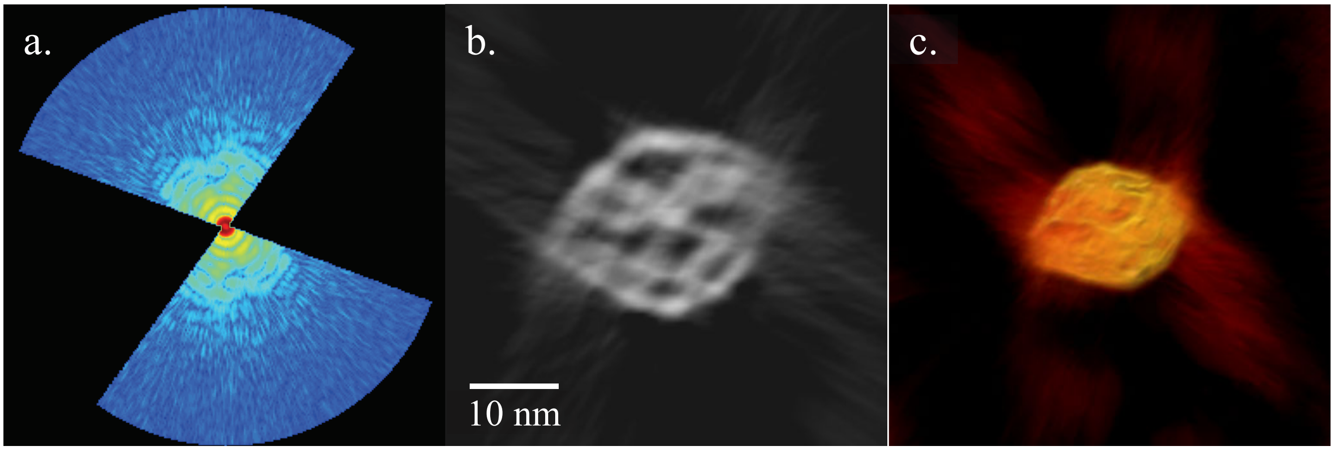

Figure 1: Reconstruction of porous PtCu nanoparticle by Direct Fourier method. The 3D object is reconstructed by mapping a combined tilt and through-focal series to Fourier space. (a) A slice of Fourier transform of the object. Since the maximum tilt range is 102 degree, there is a wide wedge of missing information. (b)&(c) Tomographic and volumetric view of the reconstructed particle. The real space image is obtained by taking inverse Fourier transform. However, due to the missing wedge, the images suffer from dramatic elongation artifacts.

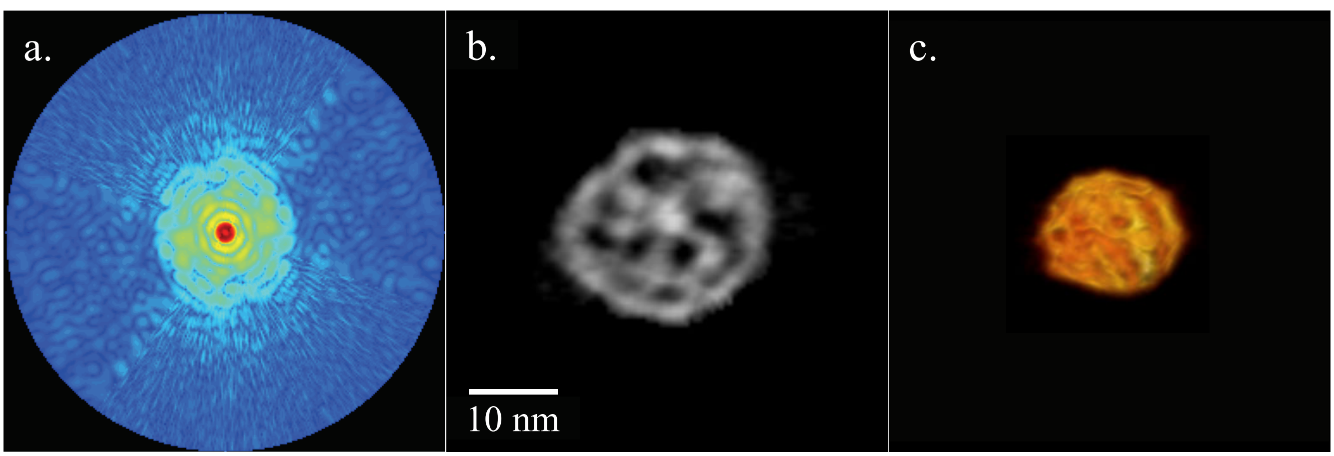

Figure 2: Reconstruction by constraint-based method. (a) A slice of Fourier transform of the reconstructed object. By solving a constraint satisfaction problem, our algorithm retrieves the information in the missing wedge. (b)&(c) Tomographic and volumetric view of the reconstructed particle. Now, with the missing wedge being filled, the shape and inner structure of the particle is much clearer.

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