

## Reconstruction Strategies for Combined Tilt- and Focal Series Scanning Transmission Electron Microscopy

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Combined tilt- and focal series (TFS) scanning transmission electron microscopy (STEM) is a recently developed method to obtain nanoscale three-dimensional (3D) information of thin specimens [1], [2]. In this recording scheme, the specimen is tilted in relatively large angle increments, and a focal series is recorded for every tilt angle, which reduces the number of mechanical tilts. In addition, the overall tilt range is smaller than used for conventional tilt series. The computational problem of volume reconstruction from projections can be solved for this kind of data using iterative reconstruction algorithms. The first such method was the tilt-focal algebraic reconstruction technique (TF-ART), which is based on the idea of heuristic weighting and an unmatched projection/backprojection pair. But the reconstruction required high computational effort.

To address this issue, the STEM transform has been formulated as a generalization of the well-known Ray-transform for parallel illumination, taking into account the reduced depth of field (higher beam converge angle) of aberration corrected STEM compared to TEM or standard STEM. It can be shown that the STEM transform is self-adjoint, i.e.  $A_\theta^* g = p_\theta * g = A_\theta g$ , where  $A_\theta$  is the STEM transform for projection direction  $\theta$ ,  $A_\theta^*$  the adjoint,  $g$  is the image, and  $p$  is the probe function [3]. With this result, it has become possible to develop a variation of the iterative reconstruction algorithm using the adjoint operator for the backprojection. The implementation of the new algorithm exploits the fact that the convolution required to evaluate the STEM transform can be precomputed per projection direction, resulting in an efficient implementation using linear interpolation.

Another interesting result concerns the Fourier Transform (FT) of the STEM transform. In tomographic applications with parallel illumination, the Fourier slice theorem states that the FT of a projection contains exactly those 3D spatial frequencies of the volumetric function that lie on a rotated 2D plane perpendicular to the projection axis. For the STEM transform, a similar result can be derived and it can be shown that the FT of the STEM transform is non-zero in a set that corresponds to an inverse double-cone, i.e. all of Fourier space except a double cone of opening angle  $1-\alpha$ , where  $\alpha$  is the opening angle of the electron beam.

The STEM transform was thus formulated as a mathematical model applicable to STEM imaging with a convergent electron beam. It was shown that it is (1) a linear convolution, (2) a generalization of the Ray transform that contains the latter as the special case where the beam convergence semi-angle  $\alpha \rightarrow 0$ , and (3) self-adjoint, a result that facilitated a new iterative reconstruction algorithm for TFS based on a matched backprojection, which drastically improved the convergence rate, resulting in 60 times less iterations compared to previous methods. It also solved theoretical concerns about the convergence of the method, which was not guaranteed in the case of an unmatched projection/backprojection pair. This brings the combined tilt- and focal series one more step towards broad applicability by allowing the reconstruction of high resolution tomograms in feasible computation time.

References:

- [1] T Dahmen, H Kohr, N deJonge and P Slusallek *Microsc. Microanal.* **20** (2014), pp. 548–60
- [2] R Hovden *et al Ultramicroscopy* **140** (2014), pp. 26–31
- [3] T Dahmen *et al* "Matched Backprojection Operator for Combined Scanning Transmission Electron Tilt- and Focal Series" *under review Microsc. Microanal.* (2015)

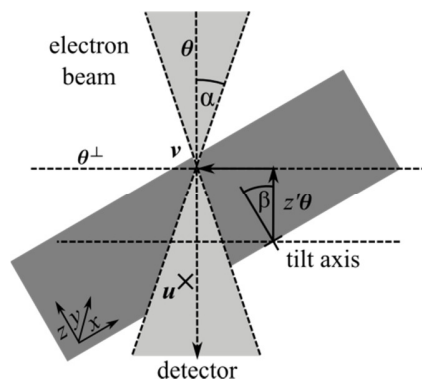


Figure 1: Parametrization of the STEM Transform. The electron beam is modeled as a double-cone, with the vertex  $v$  at the focal point. The Beam opening angle is  $\alpha$ , the beam direction  $\theta$ . By scanning the electron probe over the plane  $\theta^\perp$ , an image with limited depth of field is created.

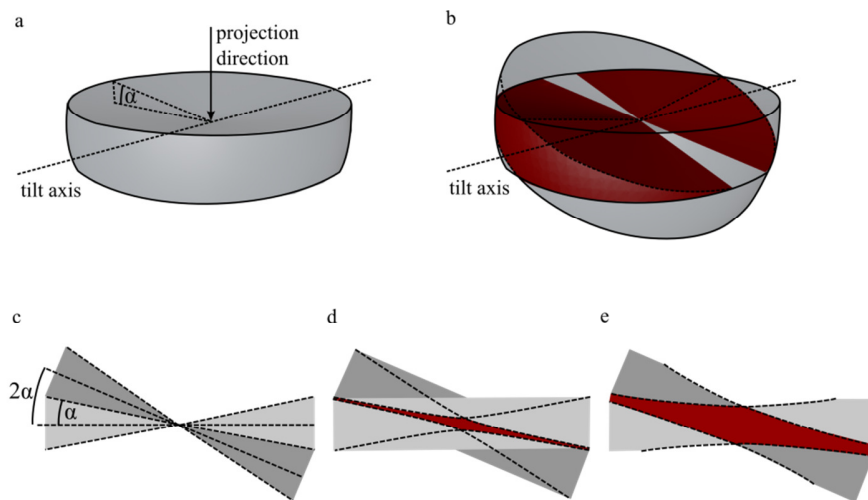


Figure 2: Geometric interpretation of the Fourier slice theorem for the STEM transform in Fourier space. a) The frequencies covered by one projection correspond to the shape of a double wedge of opening semi-angle  $\alpha$ . b) If the tilt increment is chosen as  $\Delta\beta=2\alpha$ , neighboring wedges overlap in a non-trivial shape (red). c) Considering a cross-section through the origin and perpendicular to the tilt axis, the wedges seamlessly cover the frequency space. d) A cross-section shifted along the tilt axis reveals a complex-shaped region in frequency space that contains information from more than one tilt direction. e) A cross-section even further along the tilt axis towards highest frequencies exposes that the region containing information from both tilt directions expands towards higher frequencies.