Phase Retrieval of the Scattering Matrix and Aberration Retrieval from Scanning Diffraction Measurements

Philipp M. Pelz¹*, Mary Scott¹,², Colin Ophus²

¹. Materials Science and Engineering, UC Berkeley, Berkeley, USA.
². Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, USA
* Corresponding author: philipp.pelz@berkeley.edu

Ptychography provides dose-efficient phase contrast imaging at diffraction limited resolution [2, 3, 4]. The range of applications of ptychography is limited by the assumption of the projection approximation, which breaks down for all but the thinnest specimens at atomic resolution, and therefore quantitative information is lost.

Recently, it was shown that the scattering matrix (S-matrix), which fully describes an experiment in the presence of multiple scattering, can be retrieved from a series of 4D-STEM measurements [1]. In that work, it was possible to recover the projected potential from the reconstructed S-matrix since a crystalline sample was used. In the case of non-crystalline samples, previously an inverse multi-slice problem was solved to retrieve 3D information beyond the depth of focus [5].

Here we present an algorithm that inherently reconstructs the relative phases of the beams in the scattering matrix without additional symmetry constraints. The retrieved scattering matrix can then be used to compute the outcome of several different computational confocal microscopy experiments, including coherent optical sectioning and scanning confocal microscopy (SCEM). This allows retrieving 3D structural information about the sample without having to solve the multiple scattering problem explicitly.

We illustrate our method with simulations of phase contrast optical sectioning of carbon nanotubes and computational scanning confocal imaging of layered nanomaterials from the retrieved scattering matrix. We also explore the simultaneous retrieval of probe aberrations from the dataset, similar to ptychographic reconstruction algorithms [6].

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Figure 1. a) height profile of a simulated carbon nanotube sample. b) projected potential of the carbon nanotube sample. c)-e) reconstructions from a simulated 4D-STEM defocal series with half-convergence angle of $\alpha_{\text{max}}=35 \text{ mrad}$ c) reconstructed phase of the central beam of the scattering matrix at $h=0$ d) reconstructed phase of a beam at the edge of the illumination aperture at $h=(\alpha_{\text{max}}/\lambda, 0)$ e) reconstructed phase of a beam at the opposite edge of the illumination aperture at $h=(-\alpha_{\text{max}}/\lambda, 0)$. The parallax shift stemming from the different illumination angles of the top nanotube is clearly visible.