Large-Scale 3D Atomic Resolution Phase-Contrast Imaging from 4D-STEM Measurements

Philipp M. Pelz*[2], Sinead M. Griffin[3], Alex Zettl[1], Peter Ercius[3], Mary Scott[1,3], Colin Ophus[3], Daniel G. Stroppa[4], Mingjian Wu[2]

[1]University of California, Berkeley, Berkeley, California, United States;

[2]Materials Science, Friedrich-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Bavaria, Germany;

[3]The Molecular Foundry, Lawrence Berkeley National Laboratory, The National Center for Electron Microscopy (NCEM), Berkeley, California, United States;

[4]DECTRIS AG, Villigen, Switzerland

Spurred by the development and widespread availability of fast pixelated direct electron detectors (DEDs), scanning transmission electron microscopy (STEM) is undergoing a computational imaging renaissance. Experiments envisaged more than ten years ago can finally be realized with modern detector technology and reconstruction algorithms for 4D-STEM datasets.

We show the experimental demonstration of one such experiment relying on fast DEDs: ptychographic electron tomography at atomic resolution. Using ptychographic electron tomography, we have reconstructed an atomic-resolution 3D volume of a double-wall carbon nanotube encapsulating a complex core-shell $Zr_{11}Te_{50}$ structure from 34 million diffraction patterns. From this volume, the atomic structure was determined using atom tracing methods known from annular dark-field atomic electron tomography. Ptychographic electron tomography relies on the projection approximation, such that samples have to be ~10nm or less in thickness. Multi-slice ptychographic tomography alleviates this constraint by modeling multiple scattering and allowing 3D atomic resolution phase-contrast imaging beyond the depth of focus limit. I will show first results using multi-slice ptychographic electron tomography to reconstruct samples with thickness beyond the depth of focus limit. With further technical developments, this method will be able to solve the 3D atomic structure of general TEM samples like FIB lamellas or needle specimens at atomic resolution in 3D. Finally, the limitations of current algorithms will be discussed, and developments towards imaging much larger volumes with 4D-STEM will be detailed. I will show preliminary reconstructions of a Co_3O_4 nanocube that break the depth-of-field limit of conventional electron microscopy by a factor of 3.