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Extracting Local Crystallographic Structure Using 4D-STEM Datasets

<u>C. Ophus</u>¹, P. Ercius¹, M. Sarahan², C. Czarnik², J. Ciston¹ ¹National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA, ²Gatan Inc., Pleasanton, USA

Traditional scanning transmission electron microscopy (STEM) detectors are monolithic and integrate a subset of the transmitted electron beam signal scattered from each electron probe position. These convergent beam electron diffraction patterns (CBED) are extremely rich in information, containing localized information on sample structure, composition, phonon spectra, three-dimensional defect crystallography and more. Many new imaging modes become possible if the full CBED pattern is recorded at many probe positions with millisecond dwell times. In this study, we have used a Gatan K2-IS direct electron detection camera installed on an uncorrected FEI Titan-class transmission electron microscope to record 4D-STEM probe diffraction patterns on a variety of samples at up to 1600 frames per second. As an example, a 4D-STEM dataset for a multilayer stack of epitaxial SrTiO3 and mixed LaMnO3-SrTiO3 is plotted in Figure 1. Figure 1A shows a HAADF micrograph of the multilayer along a (001) zone axis. Only the A sites (Sr and La) are visible in this micrograph and the composition can be roughly determined from the relative brightness. One possible 4D-STEM technique is position-averaged convergent beam electron diffraction (PACBED) described by LeBeau et al. [1]. We can easily construct ideal PACBED patterns by averaging the probe images over each unit cell fitted from Figure 1A, which is shown in Figure 1B. By matching these patterns to PACBED images simulated with the multislice method we can precisely determine parameters such as sample thickness and composition, the latter of which is plotted in Figure 1C. For comparison, the composition has also been determined with electron energy loss spectroscopy (EELS) in a separate experiment, shown in Figure 1D. The composition range of 0-85% LaMnO3 measured by PACBED is in good agreement with the EELS measurements. In this talk we will demonstrate several other possible uses for 4D-STEM datasets.



[1] JM LeBeau, SD Findlay, LJ Allen and S Stemmer (2010). Ultramicroscopy 110, p. 118

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