doi:10.1017/S1431927617001490

Microsc. Microanal. 23 (Suppl 1), 2017

Computational Methods for Large Scale Scanning Transmission Electron Microscopy (STEM) Experiments and Simulations

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Electron microscopy has become extremely data intensive in the past decade, as many imaging experiments have moved beyond single images or short image sequences towards large datasets. Examples include 3D electron tomography [1], 4D nanobeam electron diffraction (NBED) strain mapping [2], 4D ptychographic imaging [3], 4D phase plate scanning transmission electron microscopy (STEM) imaging [4], 5D time-resolved in-situ NBED [5], and also 5D scanning precession electron diffraction tomography [6]. Many of these studies have been enabled by direct electron detector technology, and all of them require highly efficient data processing pipelines and sophisticated analysis and simulation algorithms to reach their full potential. In this talk, we will provide an overview of our current next-generation detector development project, several types of 4D or higher dimension STEM experiments and their associated data processing and analysis pipelines, and our STEM simulation codes that make use of a new algorithm [7] and a parallelized GPU implementation.

Figure 1a shows the configuration of our 4D-STEM experiments, which combine a pixelated array for imaging the center of the diffraction pattern, and one or more annular rings for recording annular dark field (ADF) images. Figure 1b shows an example of an NBED experiment, where the strain in an austenitic stainless steel sample is measured from a diffraction pattern at each probe position. Figure 1c shows a simultaneously recorded annular dark field and ptychographic reconstruction of an all-inorganic halide perovskite material. The ptychographic phase image shows a much higher signal at the lighter halide atomic sites than the ADF image. Figure 2 compares the new STEM image simulation algorithm to a standard multislice simulation, showing that large speed-ups can be achieved with a negligible loss of accuracy [8].

References:

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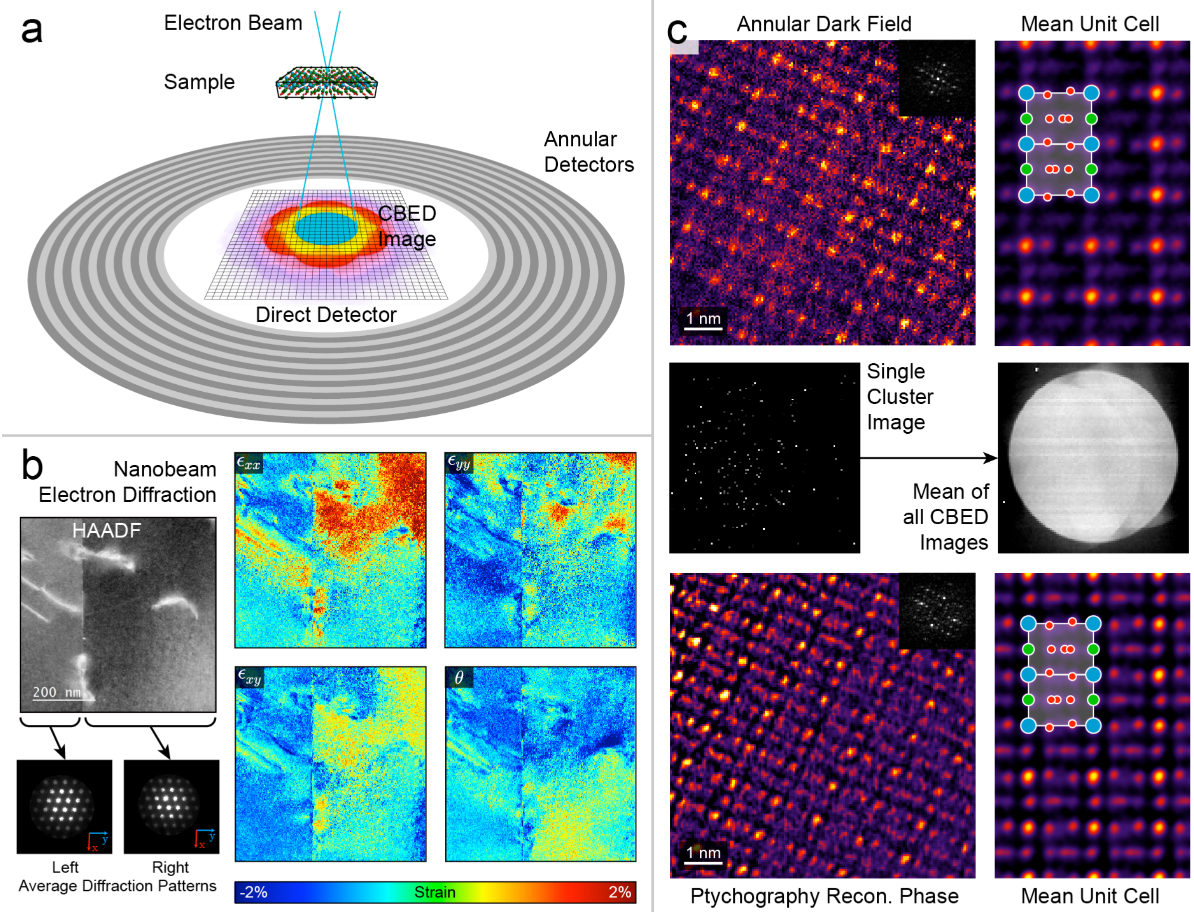

Figure 1. (a) Experimental geometry of a 4D-STEM experiment, where the full diffraction pattern is recorded, and annular detectors are used to record the highly-scattered electrons at each probe position. (b) Nanobeam electron diffraction experiment measuring strain, adapted from [2]. (c) Simultaneous ADF and ptychographic measurements of an all-inorganic halide perovskite structure. Mean unit cells show positions of heavy atoms (shown in blue and green in inset cells), while only the ptychographic image has good contrast for the lighter halide atomic site (shown in red in inset cells).

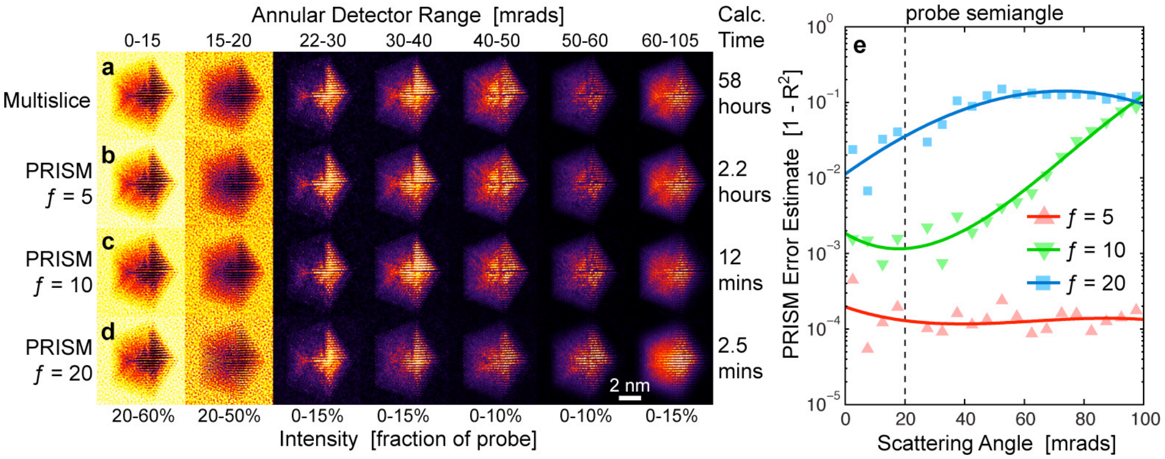

Figure 2. STEM image simulations comparing (a) the multislice method with (b)-(d) the PRISM algorithm with different interpolation factors. (e) Error estimates of (b)-(d) versus (a). Adapted from [7].