Mapping atomic scale structure using electron diffraction and imaging

Using 4D-STEM to measure the nanoscale structure of materials in 2D and 3D

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Characterizing the morphology of beam-sensitive hard and soft matter with scanning transmission electron microscopy (STEM) is challenging because these materials are often weakly scattering, and can be easily damaged by the electron dose required to resolve atomic-scale features. One of the most dose-efficient methods to study these materials is to record images of the diffracted STEM probe as a function of probe position. The resulting datasets consist of two real space and two diffraction space measurements, generating a four-dimensional array known as a 4D-STEM dataset [1]. High-speed direct electron detectors can now record thousands or even millions of diffraction patterns per experiment. To analyse this large amount of data, we have developed the py4DSTEM toolkit [2]. One of the most common 4D-STEM applications is to measure the orientation of Bragg diffracted peaks from crystalline samples using a nearly parallel electron beam, as shown in Fig. 1(a). By measuring the peak positions, we can reconstruct the morphology of beam sensitive samples [3]. Fig. 1(b) shows how the chemistry of a hierarchically ordered polymer and its chemical model can be directly connected to the resulting morphology [4]. We can also simulate diffraction patterns from crystalline materials, to measure the 3D orientation of crystalline grains through the incorporation of prior knowledge [5]. We can also boost the resolution of a 4D-STEM measurement by increasing the convergence angle until the probe size is sub-atomic, as shown in Fig. 1(c). By recording diffraction patterns of many overlapping atomic-scale probes, we can use the computational imaging method of ptychography to reconstruct the phase of the sample. Fig 1(c) also demonstrates how ptychographic measurements recorded at many sample tilts allows us to solve the structure of complex materials in 3D, for the example of a ZrTe nanowire inside a double-walled carbon nanotube (Dw-CNT) [6]. In this talk, I will describe these experiments in detail with a focus on the data analysis pipelines, and the importance of open source analysis codes and datasets.

![Figure 1](image_url)

**Figure 1.** (a) 4D-STEM experimental geometry, with reconstructed sample, adapted from [3]. (b) Orientation mapping of a polymer, adapted from [4]. (c) Ptychographic 3D tomography measurement of ZrTe nanowire in DW-CNT, adapted from [6].


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