Programmatic and Deep Learning Analysis Pipelines for 4D-STEM Materials Science Experiments*

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Abstract

In a traditional scanning transmission electron microscopy (STEM) experiment, a subnanometer electron probe is scanned over the sample, and at each position detectors which cover a wide angular range sum up all electron strikes. These experiments record only 1-5 values per probe position, throwing away most of the diffracted signal information. With the introduction of extremely high-speed direct electron detectors, we can now record a full image (2D data) of the diffracted electron probe scanned over the sample (2D grid of positions), producing a four-dimensional dataset we refer to as a 4D-STEM experiment. These diffraction images of the electron probe are extremely rich in atomic-scale information, such as the sample phase, orientation, deformation, ordering, composition, phonon spectra, and more. In this talk, I will discuss how 4D-STEM can be used to measure sample structure for materials ranging from metallurgical alloys to 2D material heterolayers to conductive polymers. These experimental datasets can be extremely large, and therefore require efficient software pipelines to perform the analysis. I will demonstrate various aspects of our open source py4DSTEM toolkit, which encompass numerical methods ranging from simple image correlation to deep learning. Our deep learning approach is rooted in very large-scale electron scattering simulations and open source data repositories, which we are making freely available to the research community.

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