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4D-STEM Analysis with the Open Source py4DSTEM and crystal4D Toolkits

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Traditional scanning transmission electron microscopy (STEM) imaging experiments record only a few values per probe position, integrating a wide range of scattered electron momenta. However, the introduction of high-speed direct electron detectors allows us to record a full image (2D data) of the diffracted electron probe scanned over the sample (2D grid of positions), producing a four-dimensional measurement [1]. An example four dimensional-STEM (4D-STEM) experiment is shown in Figure 1 for a complex sample. Figure 1 also shows various measurements which we can extract from a 4D-STEM experiment, including virtual detector imaging, differential phase contrast or ptychography, structure classification, local sample strain, and more. However, these datasets can contain thousands or even millions of diffraction patterns, requiring efficient storage and processing software codes. To aid with 4D-STEM analysis, we have developed the open source py4DSTEM code [2]. Recently, we have expanded this code to include automated crystal orientation mapping (ACOM) [3]. This analysis allows us to determine the local phase and orientation of a crystalline sample. Figure 1 shows an ACOM example for a twisted AuAgPd nanowire sample, which includes challenging diffraction patterns such as multiple grains overlapping along the beam direction, and thick non-kinematical scattering.

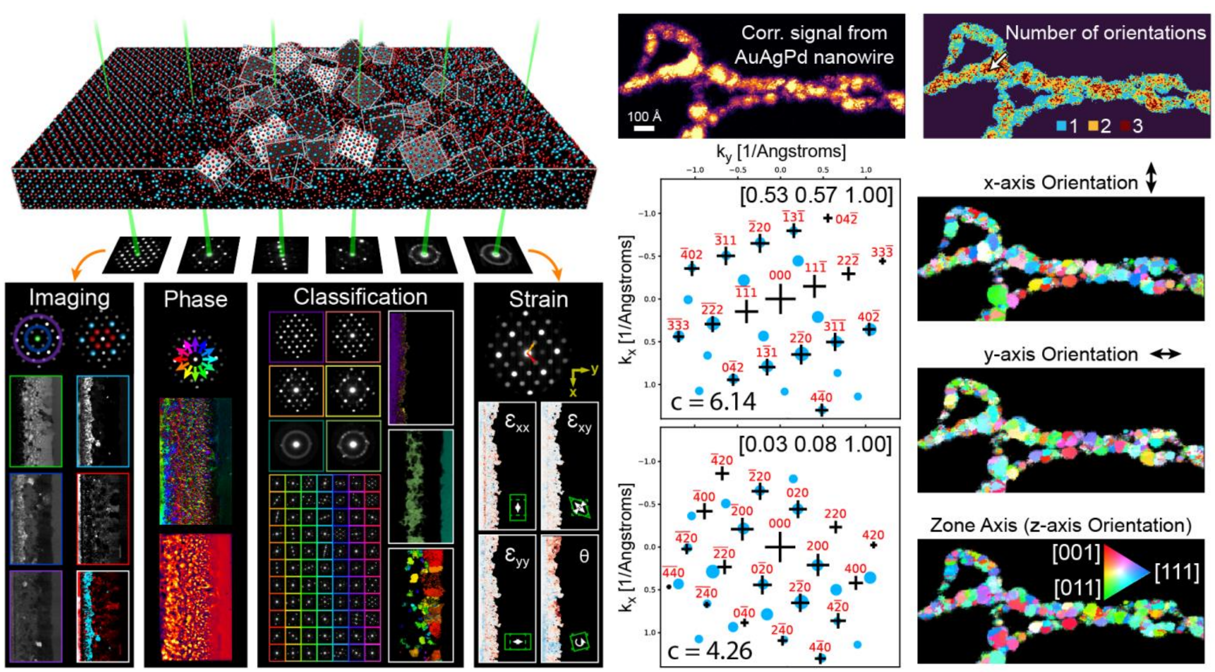

Figure 1. (upper left) Geometry of a 4D-STEM experiment for a complex sample. (lower left) Various 4D-STEM analyses of this dataset using py4DSTEM. (right) Automated crystal orientation mapping

(ACOM) workflow for a nanowire experimental dataset. Figures adapted from [2,3].

The conventional data analysis and image processing methods used in py4DSTEM work for many experiments, but often produce less accurate results when applied to real-world samples which may be thick enough to include multiple scattering of the electron beam, and other experimental artifacts. One powerful and promising modern technique to perform inversion of these complex diffraction signals is deep learning. However, deep learning methods are only as good as their training data – and labelling experimental datasets by hand is both time-consuming and low accuracy when the ground truth is unknown. Figure 2 outlines our deep learning strategy [4]. First, we select many structures of interest for a given 4D-STEM measurement, and then simulate a wide range of sample orientations, thicknesses and microscope parameters, using the Prismatic simulation code [5]. The outputs include both diffraction patterns and labeled sample property data for training. Next, we augment these simulations with dose-limited signal-to-noise ratios and common experimental distortions, backgrounds and artifacts with our crystal4D toolkit. We then train deep learning networks to predict the properties of interest such as the crystal structure factors. These deep learning image analysis pipelines have been fully integrated with py4DSTEM, allowing users to easily download the latest networks and model weights to apply to any experimental data. Additionally, all of our training simulations, experimental datasets, tutorial notebooks, and source codes are freely available online. [6]

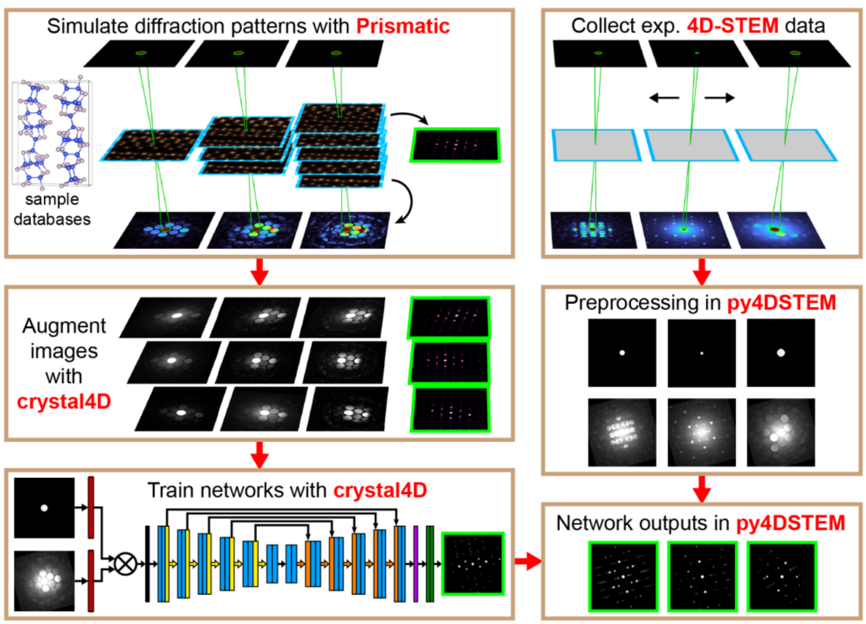

Figure 2. Deep learning analysis pipeline for 4D-STEM experiments. (left) We simulate many thousands of diffraction patterns using Prismatic. Next, we augment these images and train deep learning networks to predict the desired properties using crystal4D. (right) These trained networks can be applied to experimental datasets using py4DSTEM. Figure adapted from [4].

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