3056 Microsc. Microanal. 28 (Suppl 1), 2022
doi:10.1017/S1431927622011400

Strain Mapping from Electron Diffraction Patterns using a Fourier-space Complex Neural Network

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High-speed direct electron detectors now allow us to record a full image (2D diffraction pattern) of the electron probe scanned over the sample (2D grid of positions), producing a four-dimensional measurement (4D-STEM), at the expense of generating enormous amounts of data [1]. Analysis of the increasingly large and complex data generated from these measurements needs efficient storage and data/image analysis software codes. One example is the open-source Python software py4DSTEM, which can perform many analyses such as virtual detector imaging, differential phase contrast, crystallographic classification, strain mapping, orientation mapping, and more [2]. The conventional image analysis techniques implemented in py4DSTEM, and other similar software often suffers from challenges such as sample thickness introducing multiple scattering and other experimental artifacts. Thus, there is a need for a new analysis method which is more robust against these artifacts.

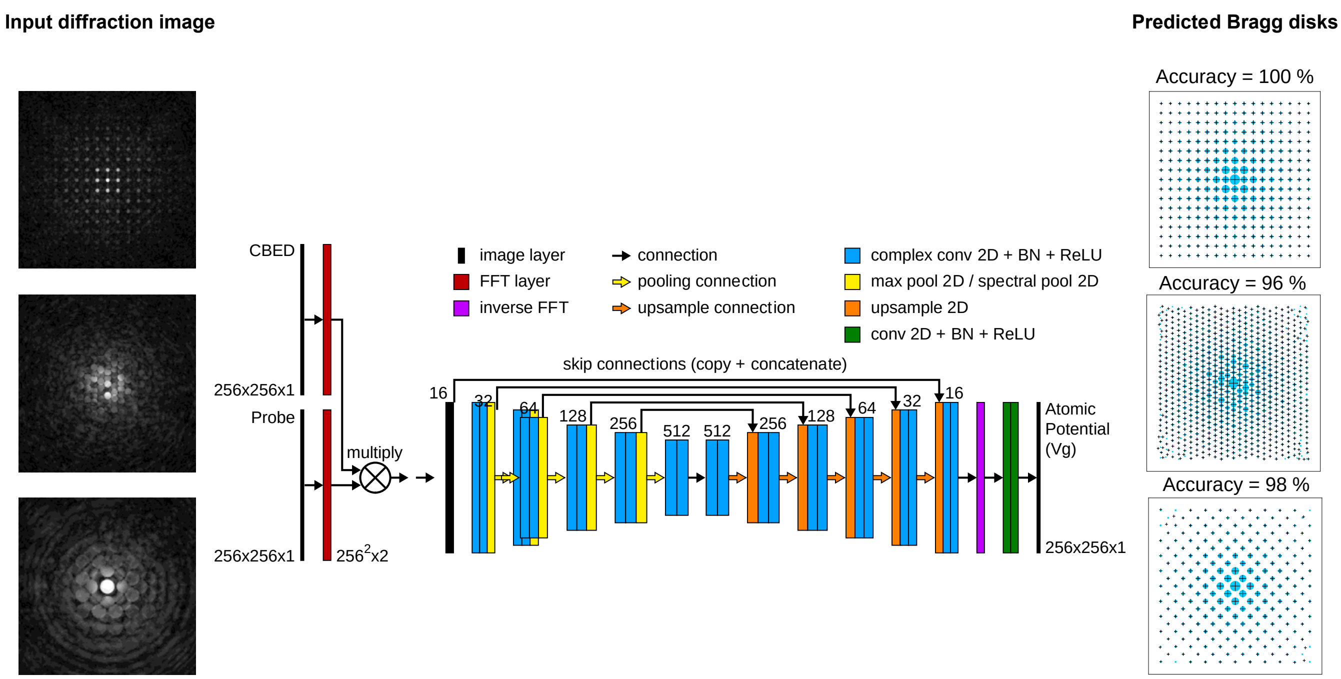

Figure 1. (left) Example diffraction (CBED) patterns from the test dataset. (right) Predicted Bragg disk positions (black) superimposed on the ground truth positions (blue). (middle) FCU-Net deep learning architecture implemented in the present work. Figures adapted from [3].

In this work, we implement a Fourier space complex U-Net (FCU-Net) deep neural network to map measured diffraction patterns to the underlying crystal structure factors for a wide range of sample thicknesses, orientations and variety of electron microscopy parameters, thus disentangling the complexity of multiple scattering and non-linear correlation between convergent beam diffraction patterns (CBED) and the structure factors. Figure 1 (middle panel) the outlines FCU-Net architecture [3]. To replace the time-consuming and error-prone manual labelling of ground truth training data from experiments, we developed a robust and automated data generation and pre-processing pipeline [4]. First, we select the structures of interest from the Materials Project database [5], shortlisted using a structural similarity measurement with crystallographic prototype systems [6]. Following the crystal system selection and manipulation using the Manipulatt toolkit, we simulate the CBED patterns and associated structure factors of the sample of interest for a wide range of sample orientations, thicknesses and microscope parameters using the Prismatic simulation code [7]. Finally, we perform physics-informed augmentation with common experimental noise, distortions, background, and artifacts using the crystal4D toolkit. We then train the FCU-Net with more than 200,000 unique diffraction images to predict the structure factors and Bragg disk positions. Bragg disk detection from the experimental diffraction pattern is the first step for many subsequent analyses pipeline such as strain mapping, automated crystal orientation mapping and others. We perform strain measurements on simulated as well as experimental 4D-STEM diffraction datasets and demonstrate improved accuracy of the FCU-Net in comparison to the traditional correlation-based approach. The trained FCU-net can be used to predict Bragg disk positions directly from experimental 4D-STEM dataset and the analysis pipeline have been fully integrated with py4DSTEM, allowing user to easily download and use the FCU-Net model [8].

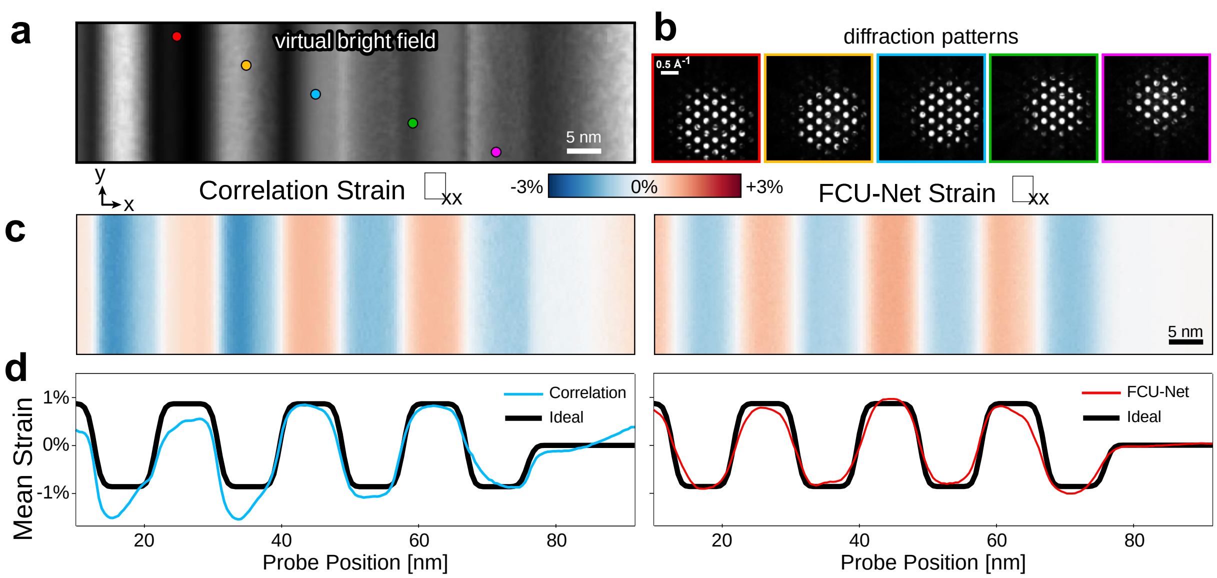

Figure 2. Strain mapping performed on simulated 4D-STEM diffraction on a twisted Si/SiGe multilayer stack. (a) virtual bright field image of the multilayer stack, (b) CBED pattern of selected probe positions as plotted with coloured dots in (a), (c) principal strain profile along x-direction using correlation approach (left) and FCU-Net (right), (d) mean strain along principal direction (x-axis) using correlation (left) and FCU-Net (right).

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https://doi.org/10.1017/S1431927622011400 Published online by Cambridge University Press

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