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Extremely Noisy 4D-TEM Strain Mapping Using Cycle Consistent Spatial Transforming Autoencoders

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Atomic-scale imaging of 2D and quantum materials benefits from precisely extracting crystallographic strain, shear, and rotation to understand their mechanical, optical and electronic properties. One powerful technique is 4D-STEM (4-dimensional scanning transmission electron microscopy), where a convergent electron beam is scanned across a sample while measuring the resulting diffraction pattern with a direct electron detector. Extracting the crystallographic strain, shear, and rotation from this data relies either on correlation strain measurement method (e.g., implemented in py4DSTEM) or determining the center of mass (CoM) of the diffraction peaks. These algorithms have limitations. They require manual preprocessing and hyperparameter tuning, are sensitive to signal-to-noise, and generally are difficult to automate. There is no one-size-fits-all algorithm. Recently, machine learning techniques have been used to assist in analyzing 4D-STEM data, however, these models do not possess the capacity to learn the strain, rotation, or translation instead they just learn an approximation that almost aways tends to be correct as long as the test examples are within the training dataset distribution.

We developed a novel neural network structure –Cycle Consistent Spatial Transforming Autoencoder (CC-ST-AE). This model takes a set of diffraction images and trains a sparse autoencoder to classify an observed diffraction pattern to a dictionary of learned "averaged"diffraction patterns. Secondly, it learns the affine transformation matrix parameters that minimizes the reconstruction error between the dictionary and the input diffraction pattern. Since the affine transformation includes translation, strain, shear, and rotation, we can parsimoniously learn the strain tensor. To ensure the model is physics conforming, we train the model cycle consistently, by ensuring the inverse affine transformation from the dictionary results in the original diffraction pattern.

We validated this model on a number of benchmark tasks including: A Simulated 4D TEM data of WS2 and WSe2 lateral heterostructures (noise free) with a ground truth of the strain, rotation and shear parameters. Secondly, we test this model experimental 4D STEM on 2D-heterostructures of tungsten disulfide (WS2) and tungsten diselenide (WSe2).

This model shows several significant improvements including: 1. When tested on simulated data, the model can recover the ground truth with minimal error. 2. The model can learn the rotation and strain on noisy diffraction patterns where CoM failed, and outperforms correlation strain measurement method. 3. Our model can accommodate large and continuous rotations difficult to obtain with other methods. 4. Our model is more robust to noisy data. 5. Our model can map the strain, shear and rotation; identify dislocation and ripples; and distinguish background and sample area automatically.

Ultimately, this work demonstrates how embedding physical concepts into unsupervised neural networks can simplify, automate, and accelerate analysis pipelines while simultaneously leveraging stochastic averaging that improves robustness on noisy data. This algorithmic concept can be extended to include other physical phenomena (e.g., polarization, sample tilt), can be used in automated experiments, and can be applied to other applications in materials characterization.

Primary author: QIN, Shuyu

Co-author: Prof. AGAR, Joshua (Drexel University)

Presenter: QIN, Shuyu

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