Cycle-Consistent Spatial Transforming Autoencoders

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Department of Mechanical Engineering and Mechanics

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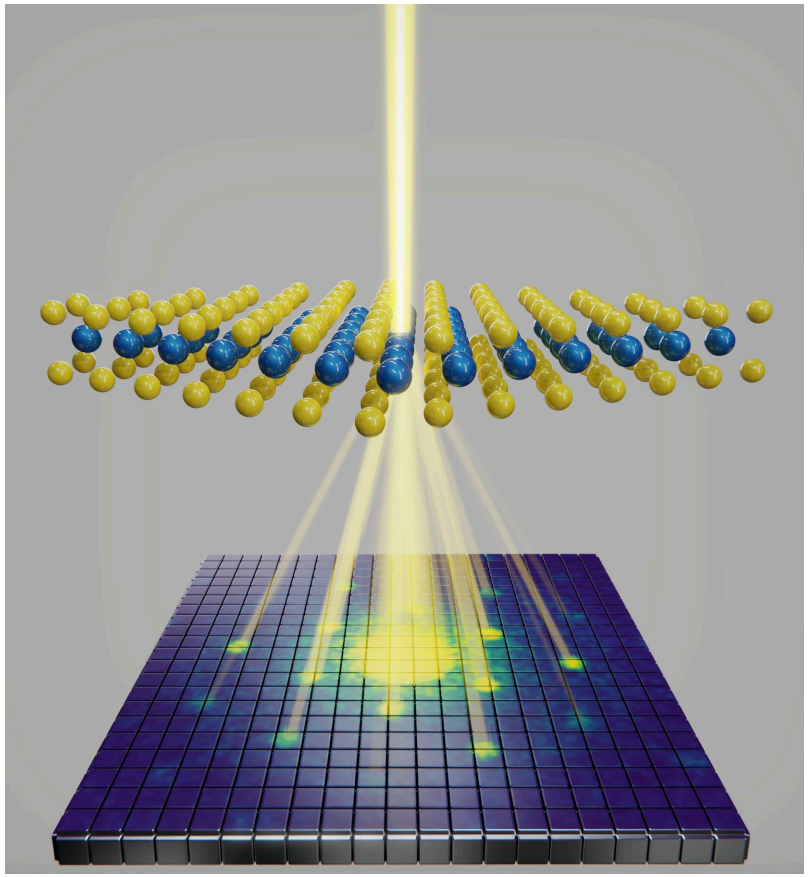
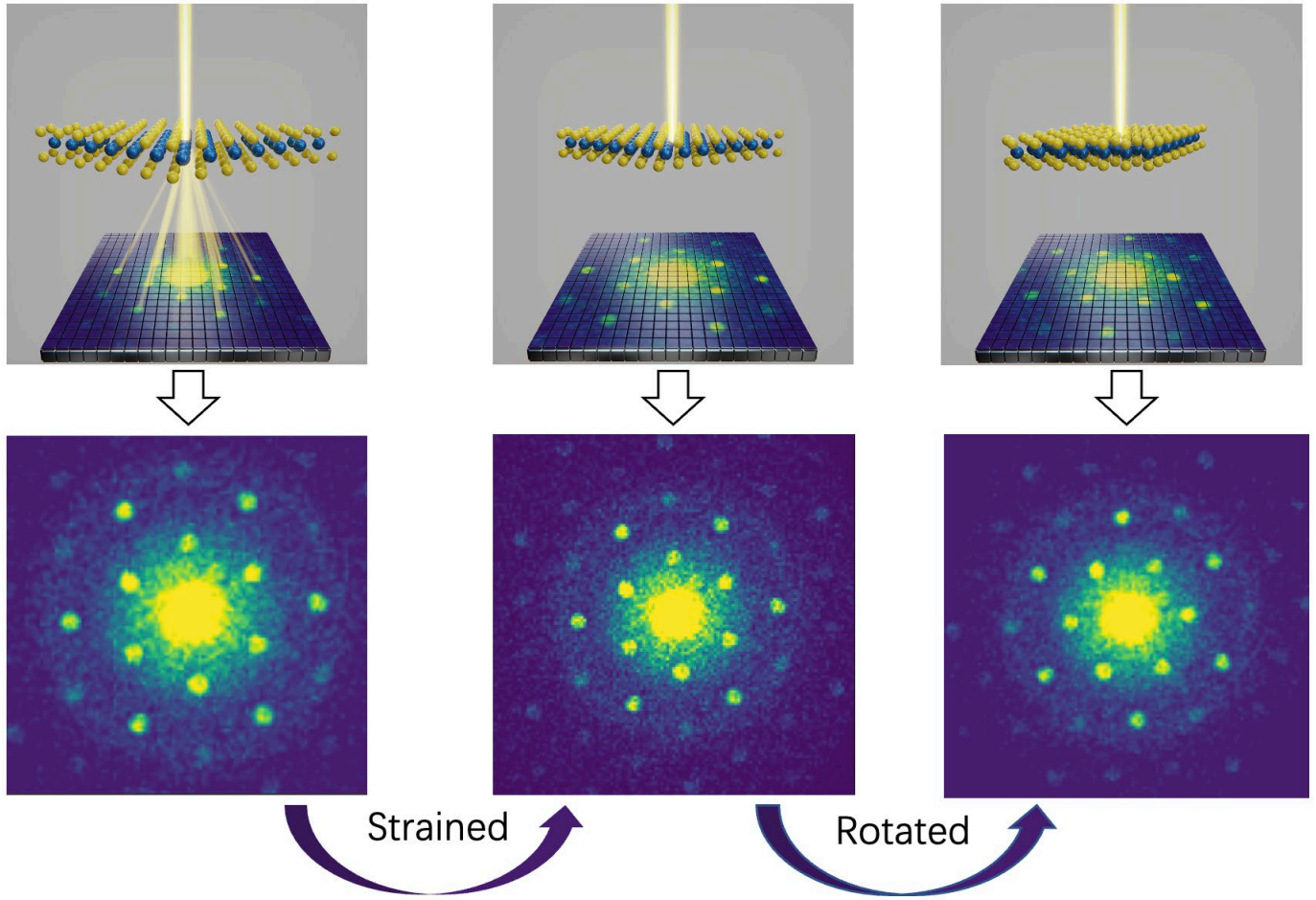
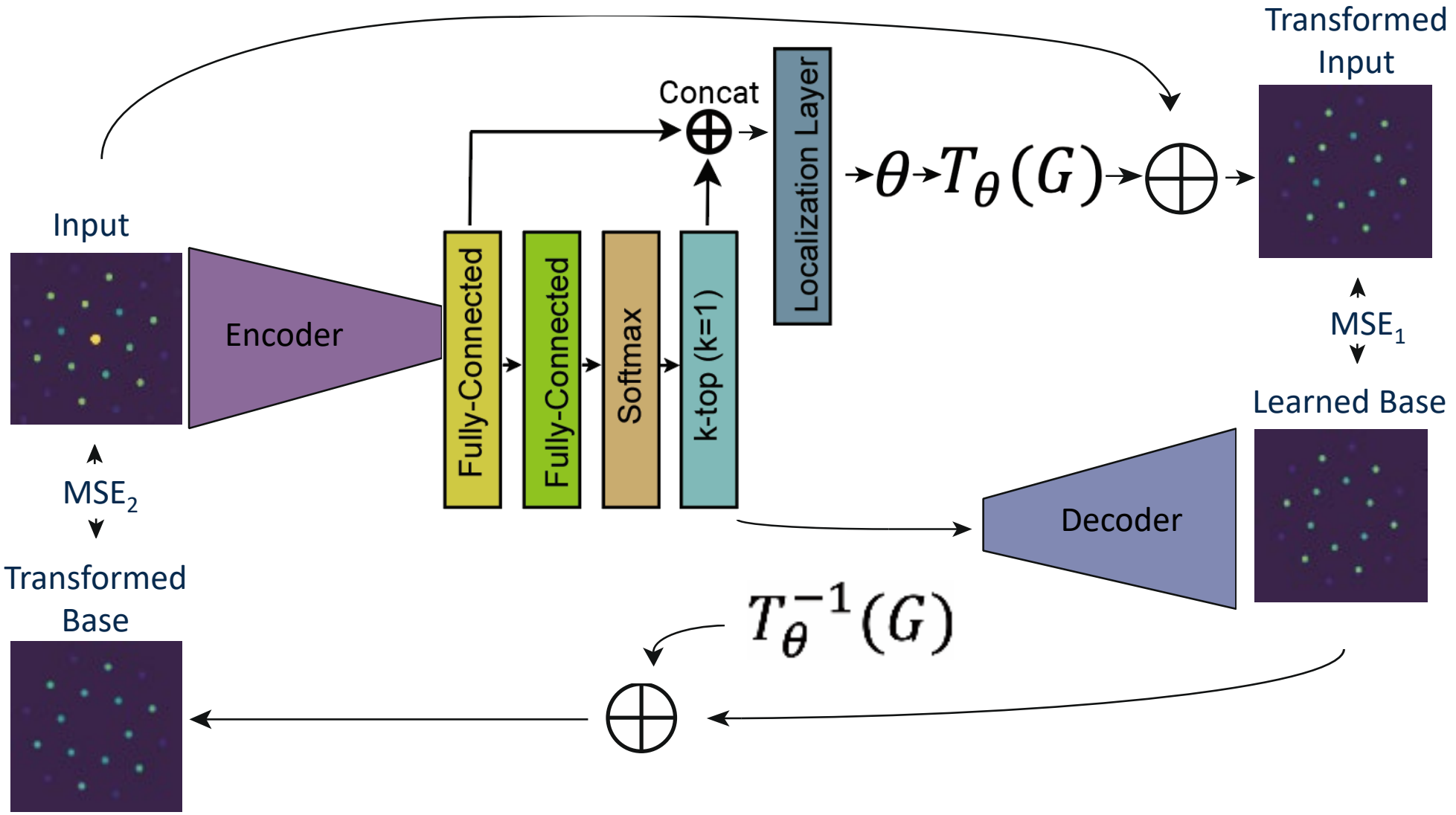
Parsimonious Machine Learning



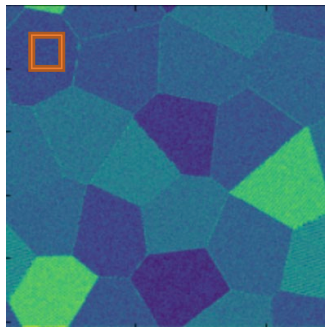


Cycle-Consistent Spatial Transforming Autoencoder



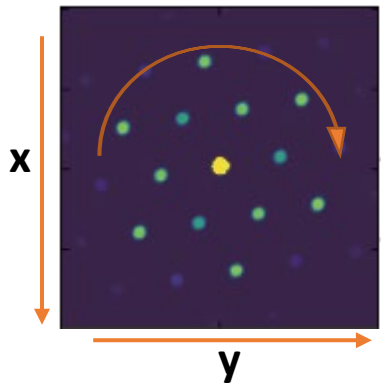
Simulated Noise-Free 4D-STEM

Sample domain image



256 x 256

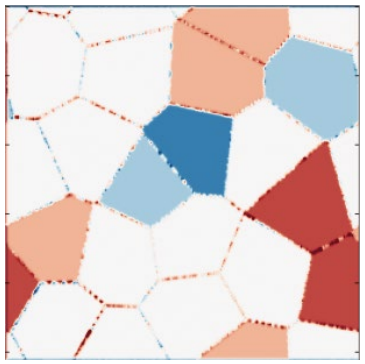
Random diffraction image



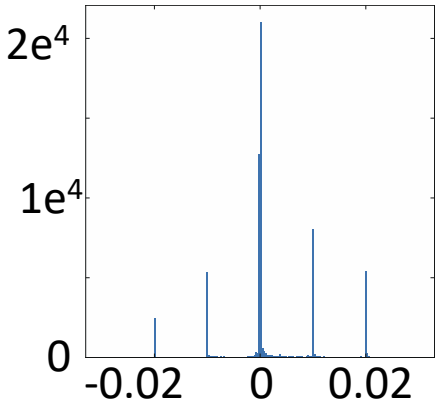
200 x 200

: Reference grain:
No rotation & strain

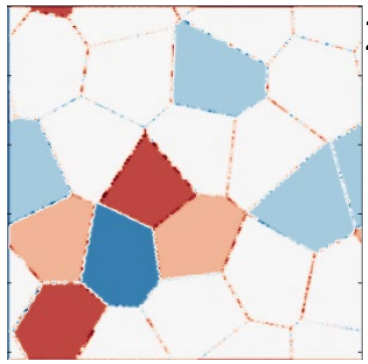
Strain x mapping



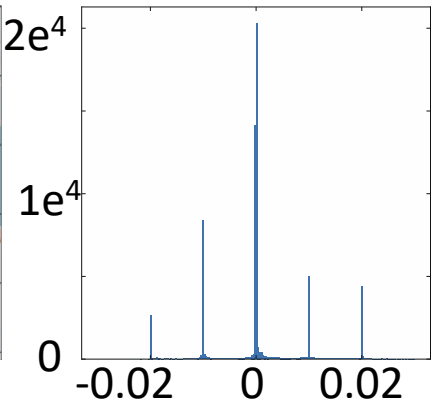
Strain x histogram



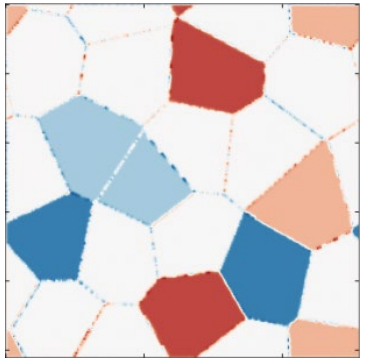
Strain y mapping



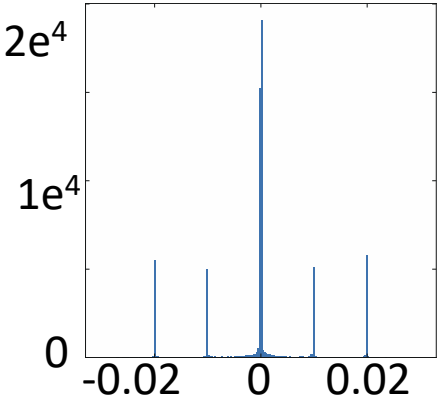
Strain y histogram



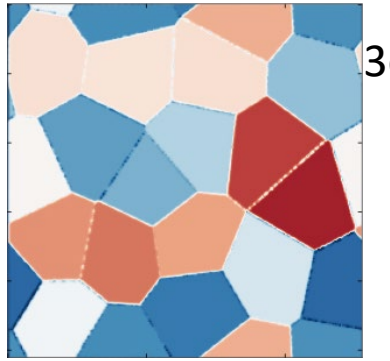
Strain xy mapping



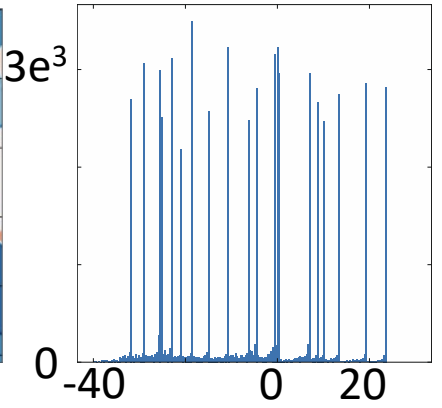
Strain xy histogram



Rotation mapping

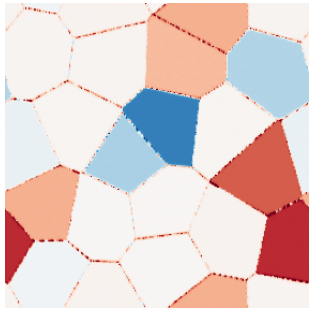


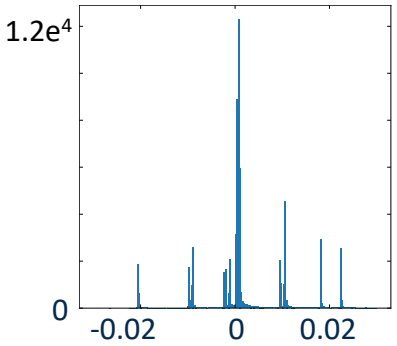
Rotation histogram

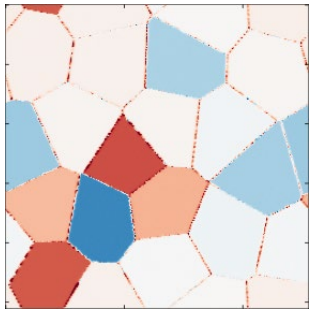


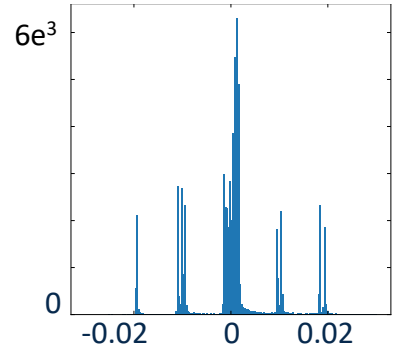
Comparison of py4DSTEM (Clean Data strain map)

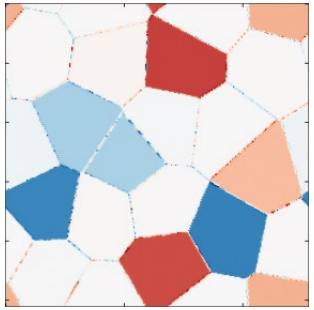
py4DSTEM

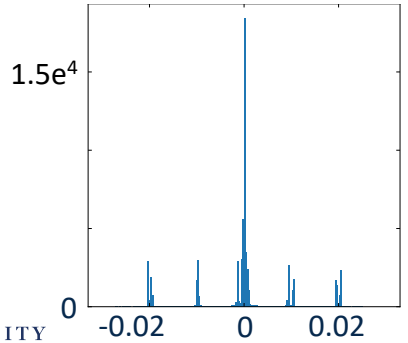




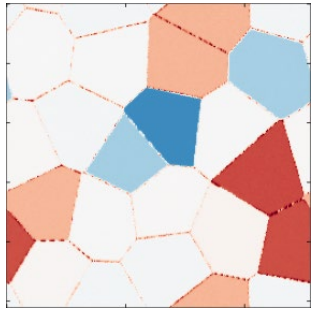


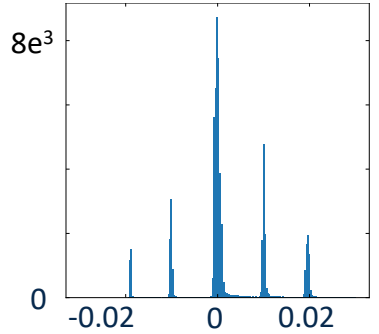


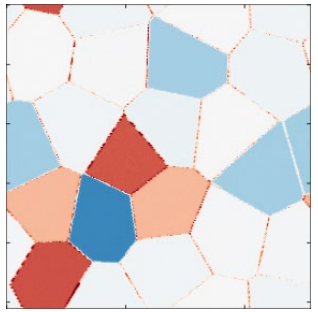


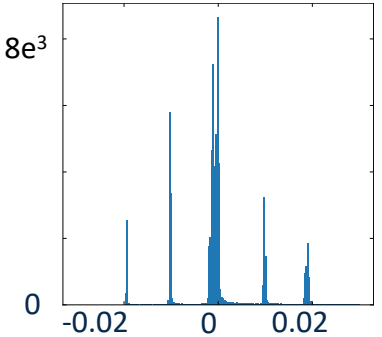


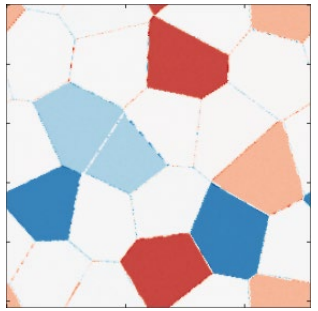
Neural Network

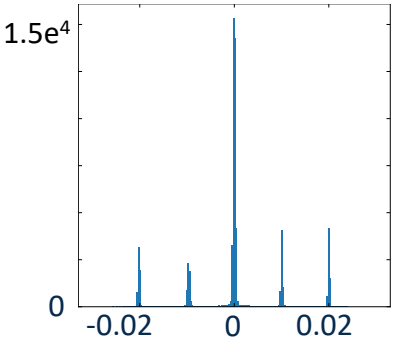












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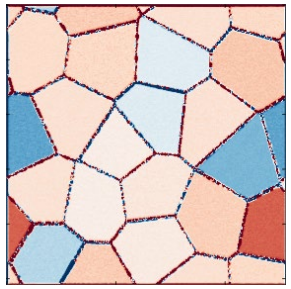
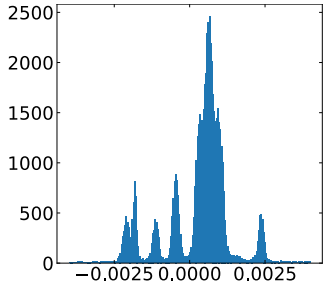
Visualize difference with Label (Map & Histogram)

py4DSTEM

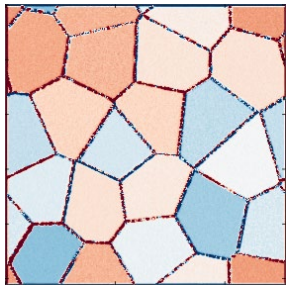
Strain X



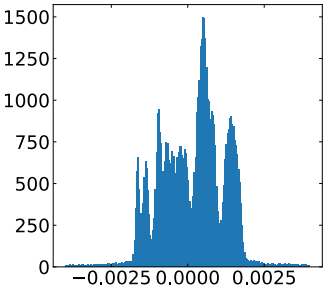
MAE: 0.0020



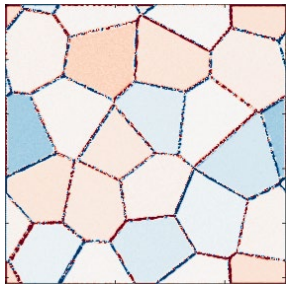
Strain Y



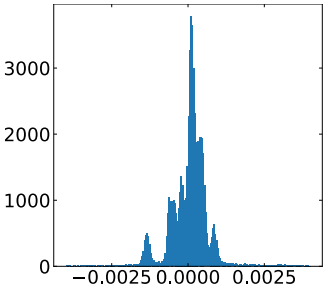
MAE: 0.0020



Shear

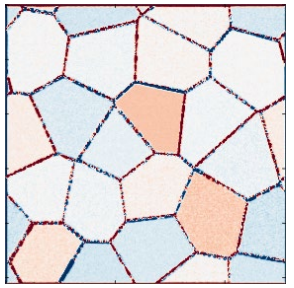


MAE: 0.0009

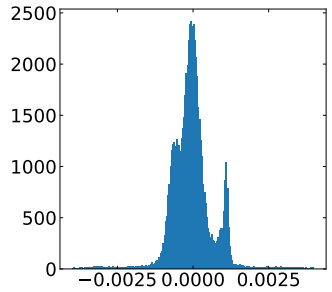


Neural Network

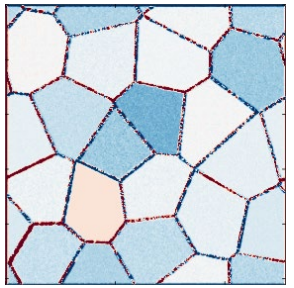
Strain X



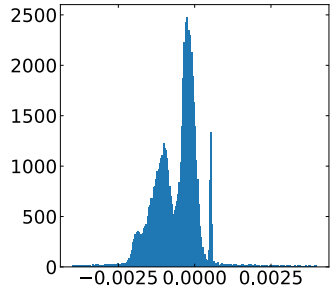
MAE: 0.0015



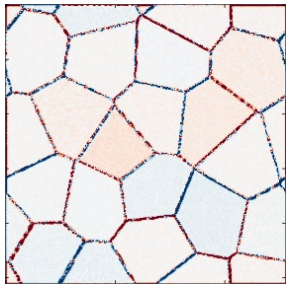
Strain Y



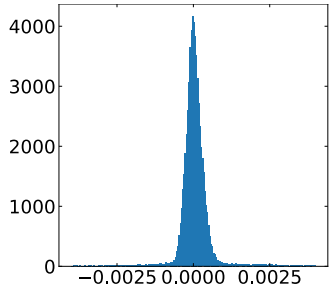
MAE: 0.0018



Shear



MAE: 0.0007



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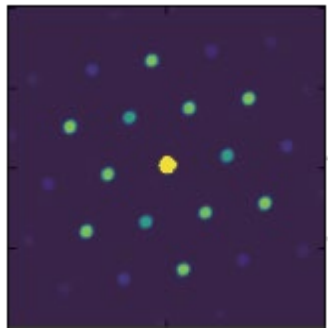
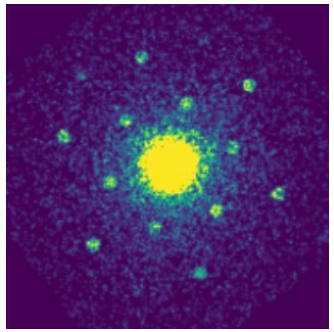
Comparison of py4DSTEM (Add 25% Background Noise)

Noise-Free



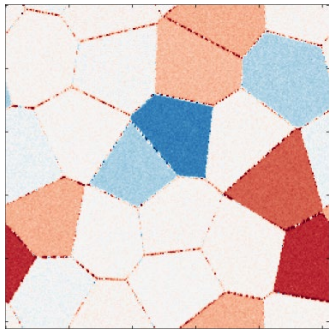
Add Noise

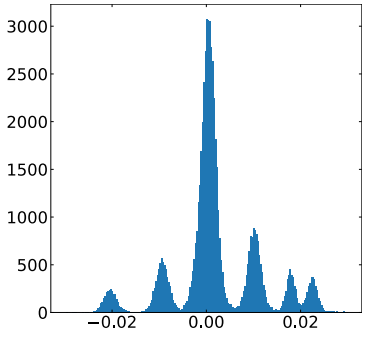


Add 25% Poisson Background Noise to each Diffraction Image

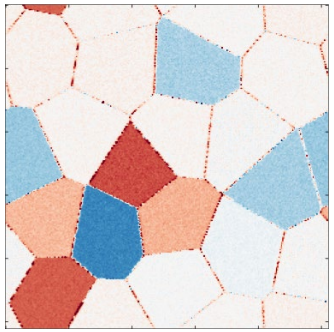
py4DSTEM

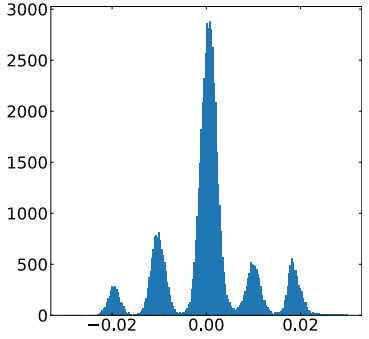
Strain X



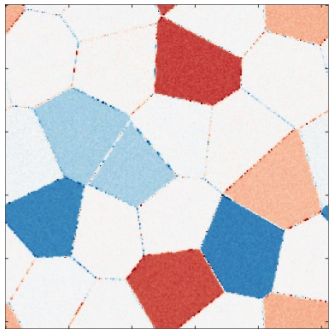


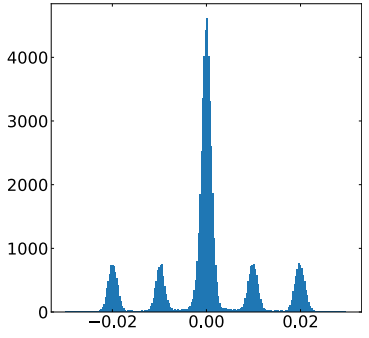
Strain Y





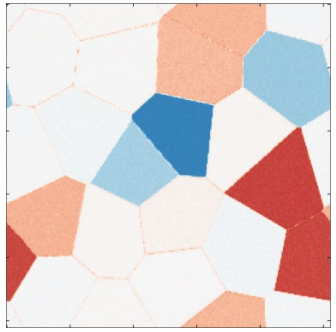
Shear

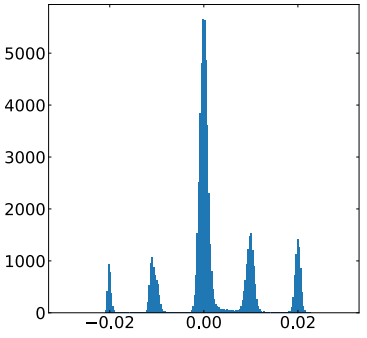




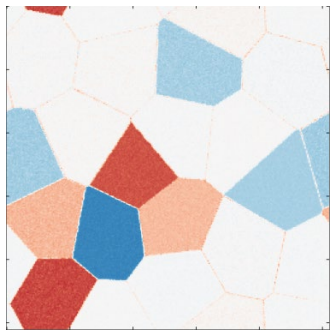
Neural Network

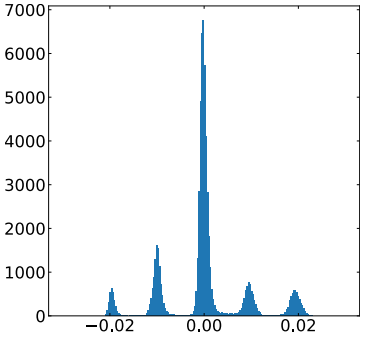
Strain X





Strain Y





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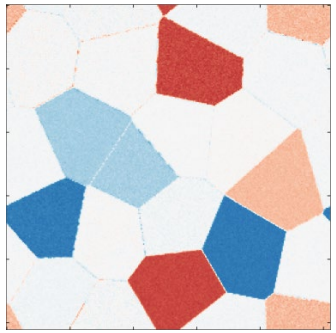

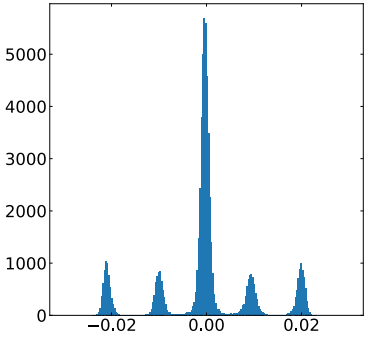

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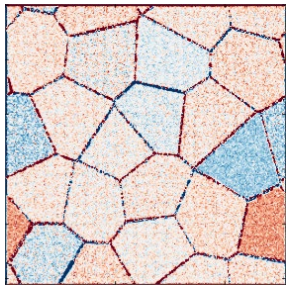
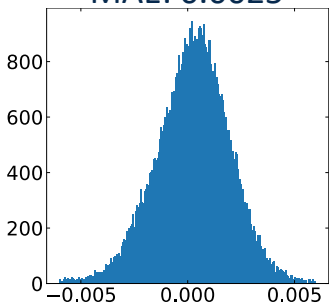
Visualize difference with Label (Map & Histogram)

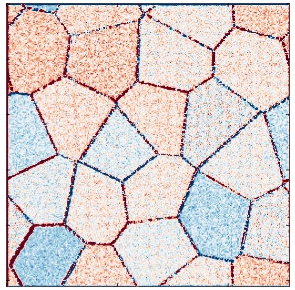
py4DSTEM

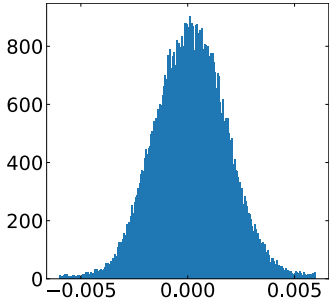
Strain X



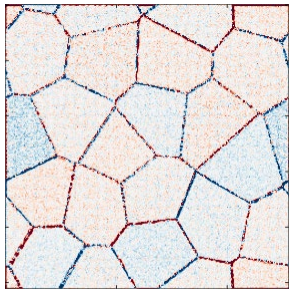


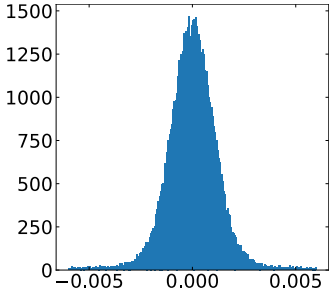
Strain Y





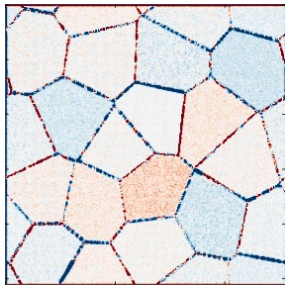
Shear

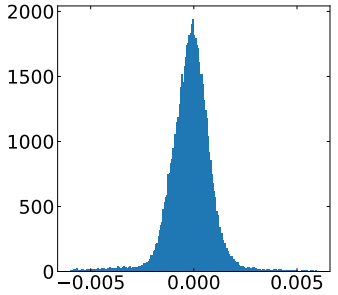




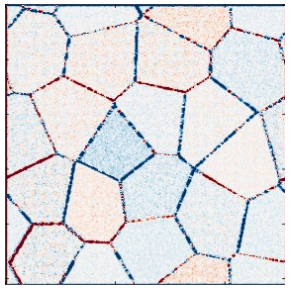
Neural Network

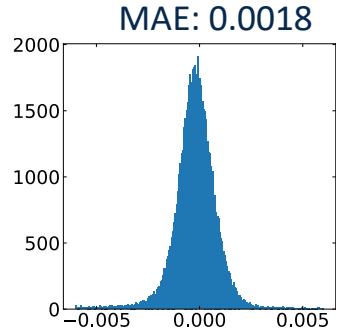
Strain X



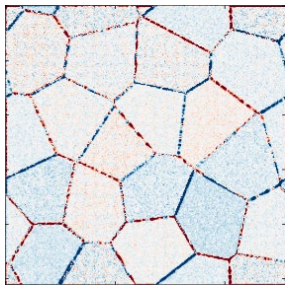


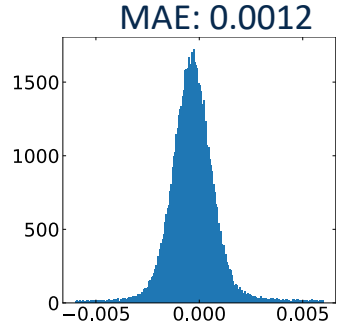
Strain Y





Shear



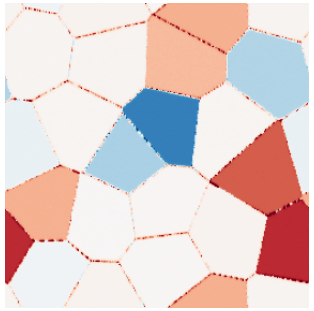


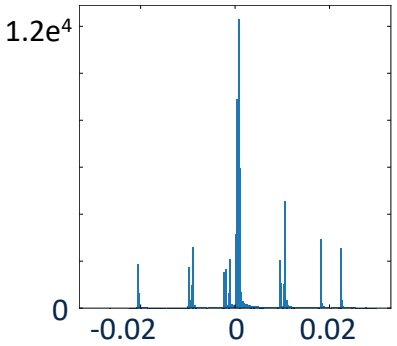
Noise Benchmark

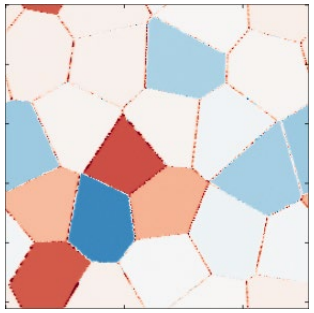
BKG noise intensity /Percentage	Strain X (MAE with Label) *1e-3		Strain Y (MAE with Label) *1e-3		Shear (MAE with Label) *1e-3	
	py4dstem	CC-ST-AE	py4dstem	CC-ST-AE	py4dstem	CC-ST-AE
0	2.0	**1.5**	2.0	**1.8**	0.9	**0.7**
5%	2.3	**1.5**	2.4	**1.6**	1.2	**1.2**
10%	2.3	**1.5**	2.4	**1.6**	1.3	**1.0**
15%	2.3	**1.6**	2.4	**1.7**	1.3	**0.9**
20%	2.4	**1.7**	2.5	**1.7**	1.4	**1.0**
25%	2.5	**1.6**	2.5	**1.9**	1.4	**1.1**
30%	2.5	**1.6**	2.6	**1.7**	1.4	**1.2**
35%	2.6	**1.8**	2.7	**1.8**	1.5	**1.1**
40%	2.7	**1.7**	2.7	**1.8**	1.6	**1.3**
45%	2.8	**1.8**	2.9	**2.0**	1.7	**1.2**

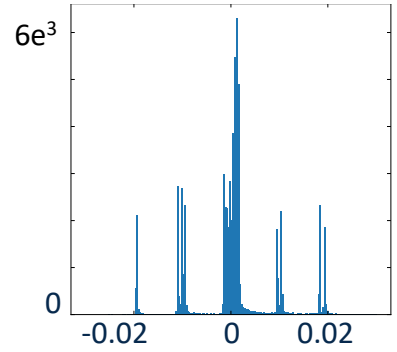
Comparison of py4DSTEM (Add 60% strain map)

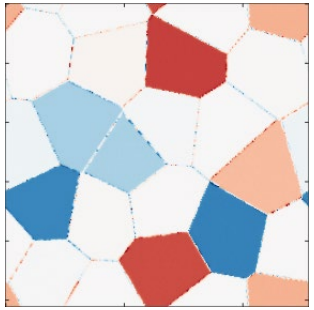
py4DSTEM

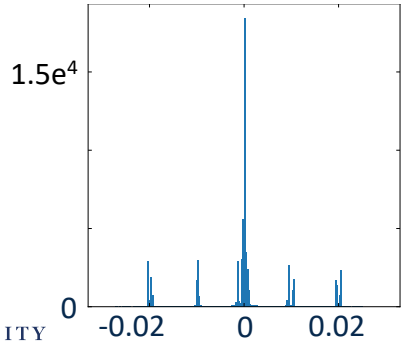




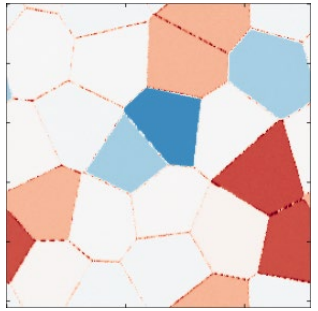


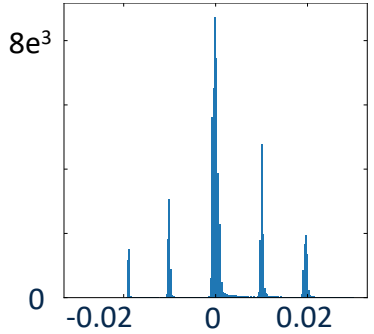


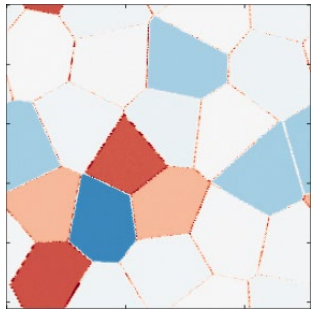


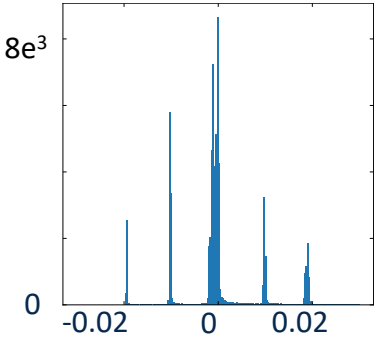


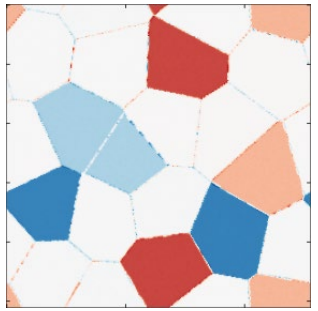
Neural Network

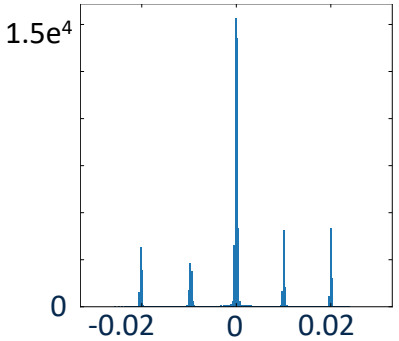












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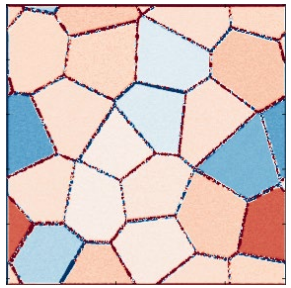
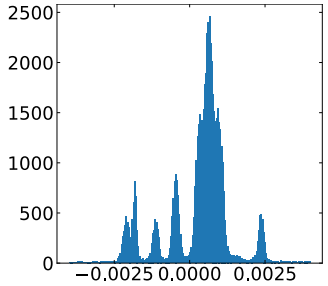
Visualize difference with Label (Map & Histogram)

py4DSTEM

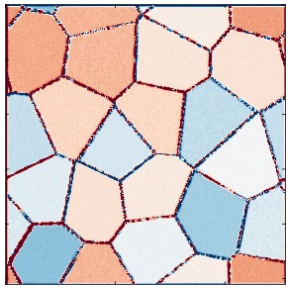
Strain X



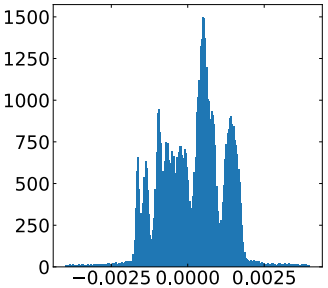
MAE: 0.0020



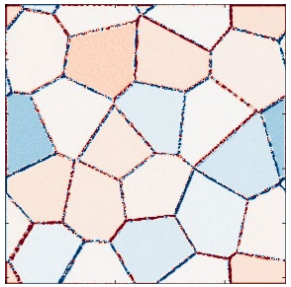
Strain Y



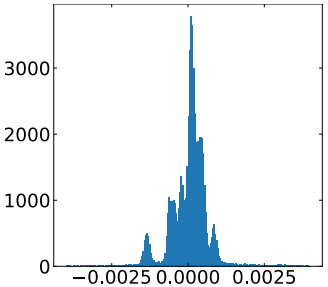
MAE: 0.0020



Shear

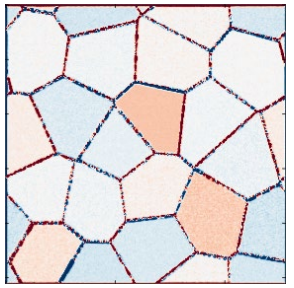


MAE: 0.0009

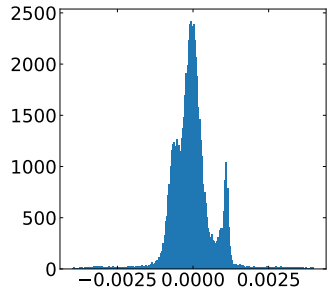


Neural Network

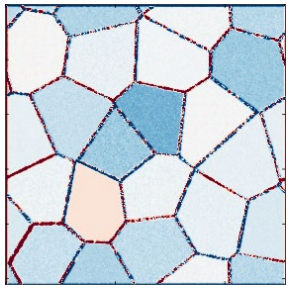
Strain X



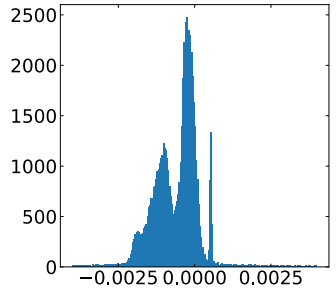
MAE: 0.0015



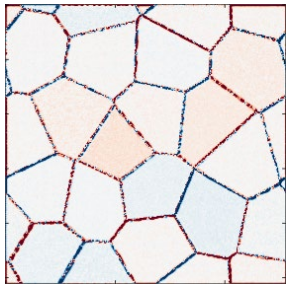
Strain Y



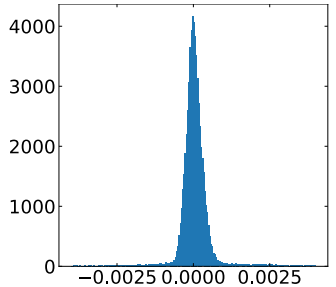
MAE: 0.0018



Shear



MAE: 0.0007



Experimental Dataset: WSe_2WS_2 4D-STEM

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Strain Mapping of Two-Dimensional Heterostructures with Subpicometer Precision

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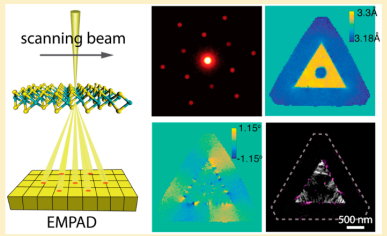
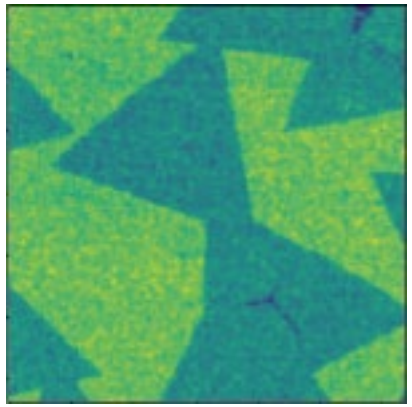
Supporting Information

ABSTRACT: Next-generation, atomically thin devices require in-plane, one-dimensional heterojunctions to electrically connect different two-dimensional (2D) materials. However, the lattice mismatch between most 2D materials leads to unavoidable strain, dislocations, or ripples, which can strongly affect their mechanical, optical, and electronic properties. We have developed an approach to map 2D heterojunction lattice and strain profiles with subpicometer precision and the ability to identify dislocations and out-of-plane ripples. We collected diffraction patterns from a focused electron beam for each real-space scan position with a high-speed, high dynamic range, momentum-resolved detector—the electron microscope pixel array detector (EMPAD). The resulting four-dimensional (4D) phase space data sets contain the full spatially resolved lattice information on the sample. By using this technique on tungsten disulfide (WS_2) and tungsten diselenide (WSe_2) lateral heterostructures, we have mapped lattice distortions with 0.3 pm precision across multimicron fields of view and simultaneously observed the dislocations and ripples responsible for strain relaxation in 2D laterally epitaxial structures.



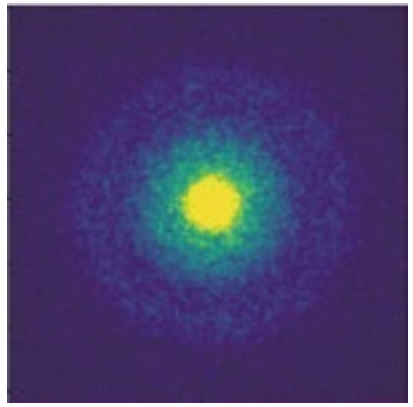
KEYWORDS: *EMPAD, STEM, 2D lateral heterostructure, strain, dislocation, ripple*

Sample Domain image



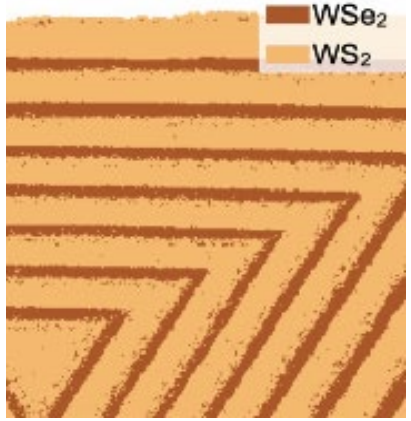
Random Diffraction image

Background

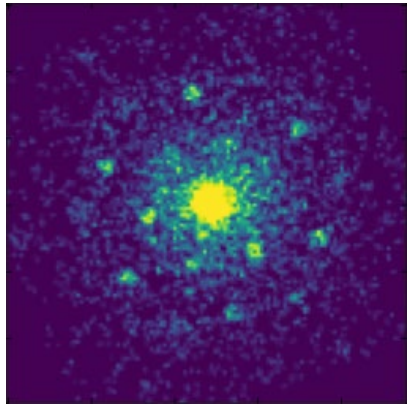


theoretical Structure

1



Sample

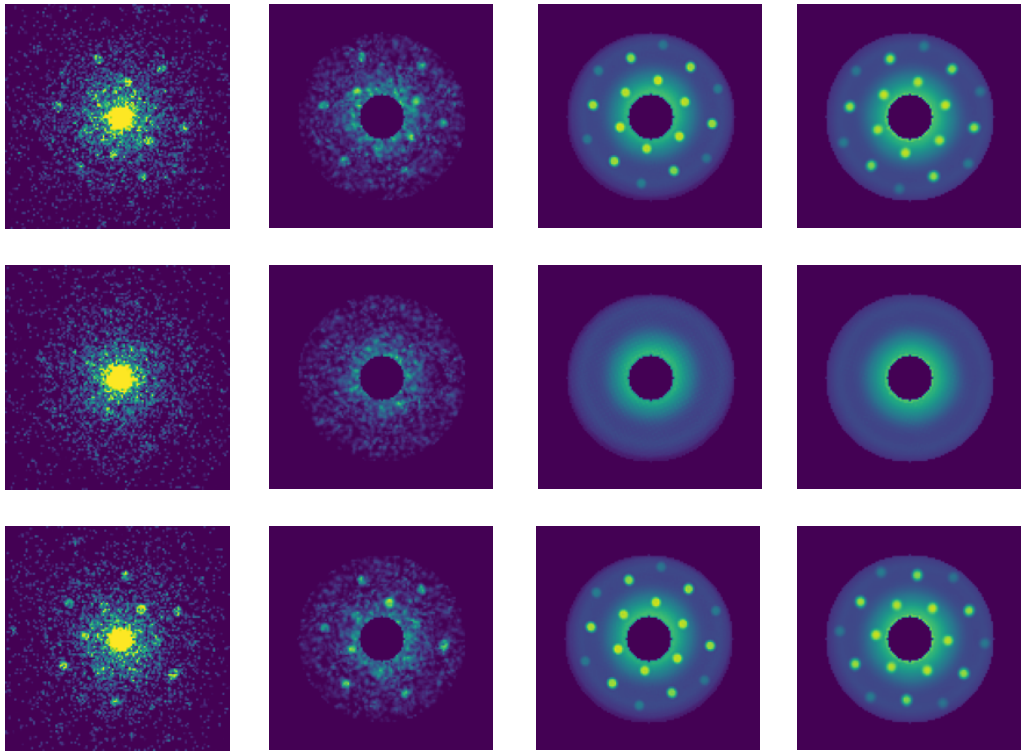


1. Uncovering Material Deformations via Machine Learning Combined with Four-Dimensional Scanning Transmission Electron Microscopy

CC-ST-AE Training Results

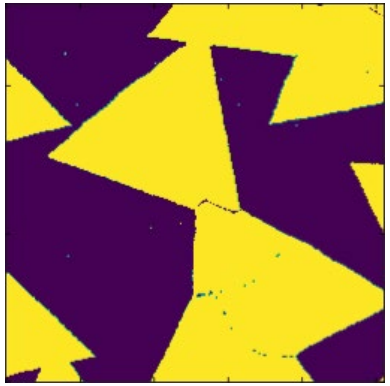
Random Example

Input image | After affine transformation | Generated base | After inverse affine

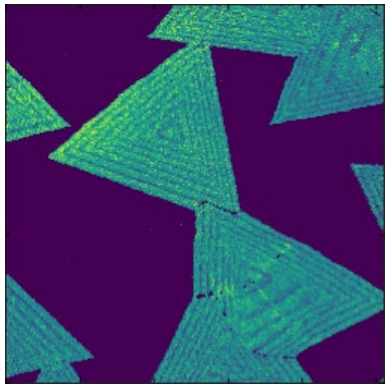


Classification & Strain map

Sample region



Magnitude Map



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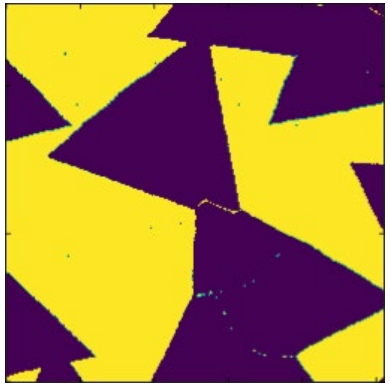

Histogram