

Uncovering Material Deformations via Cycle-Consistent Spatial Transforming Autoencoder on 4D STEM Dataset

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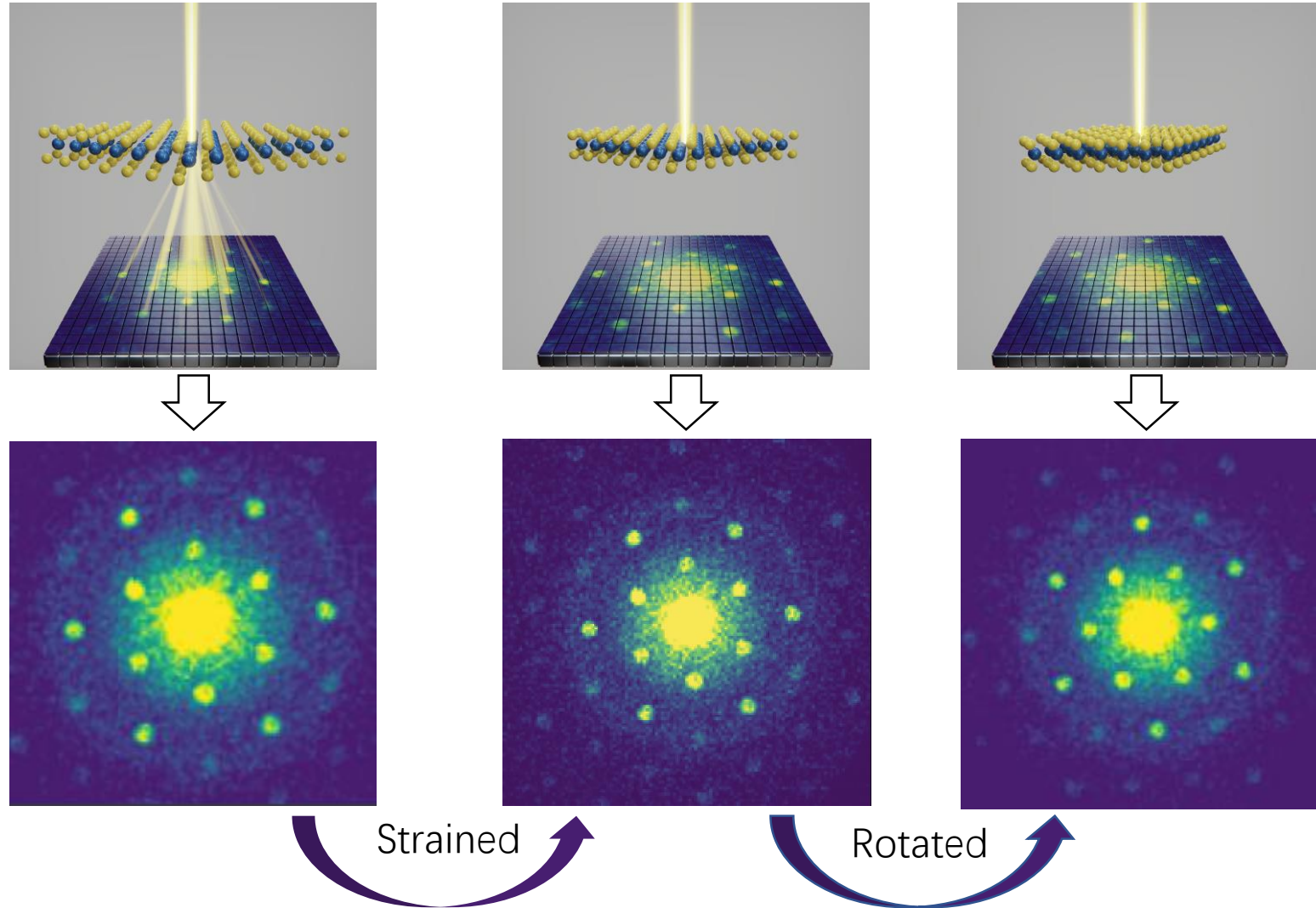
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Lehigh University

Department of Mechanical Engineering,
Drexel University



Motivation

4-Dimensional Scanning Transmission Electron Microscopy (4D-STEM)



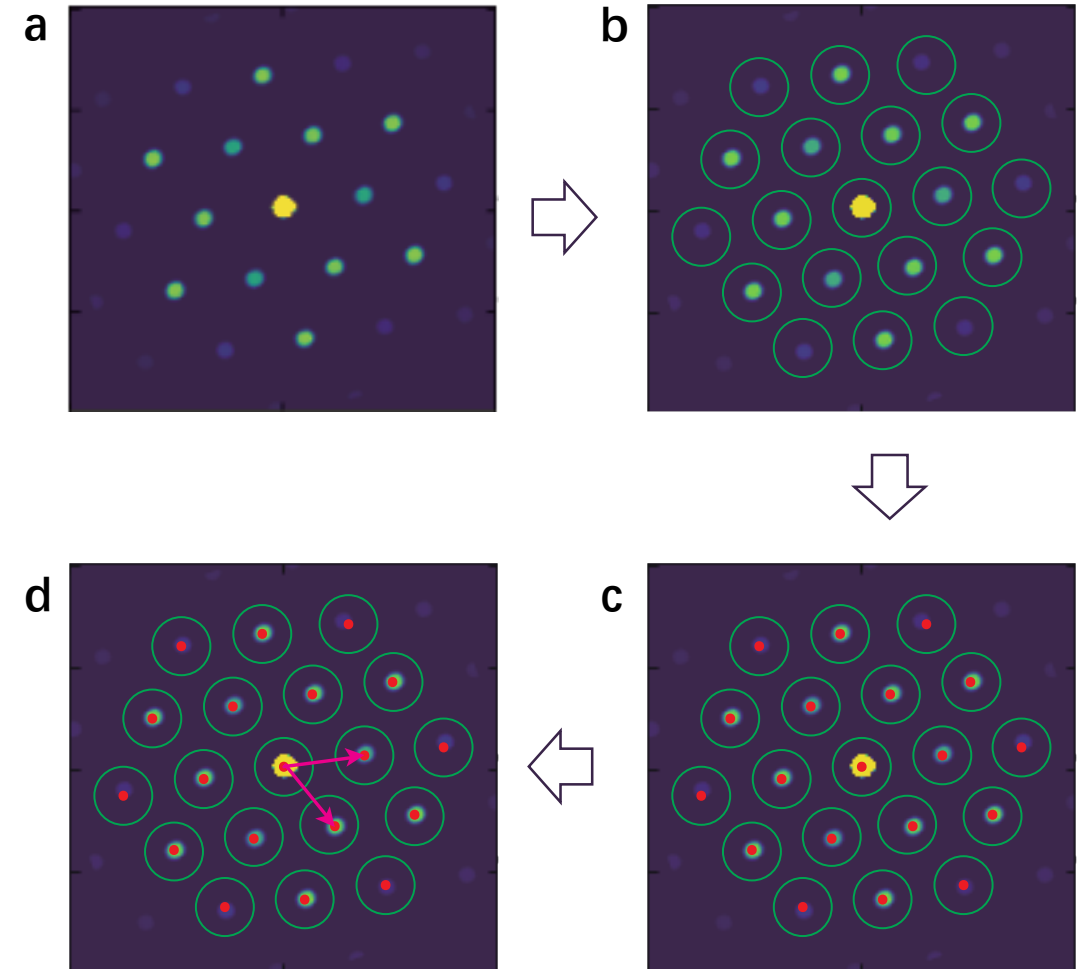
- Measure the crystal structure with sub-atomic precision
- Determine crystallographic strain, shear, and orientation
- Can correlate crystal structure to mechanical, electrical, and interfacial properties

Conventional methods

- 2D-Cross correlation strain measurement method in py4DSTEM

Strategy:

- Manually set threshold to focus on diffraction patterns (b)
- Extract the center coordinates of diffraction patterns (c)
- Calculate the strain and rotation based on 2 manually selected vectors (d)

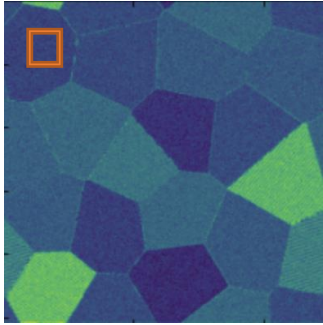


Limitation:

- Not sensitive to small scale
- Not robust on data set with background noise
- Lack of automation

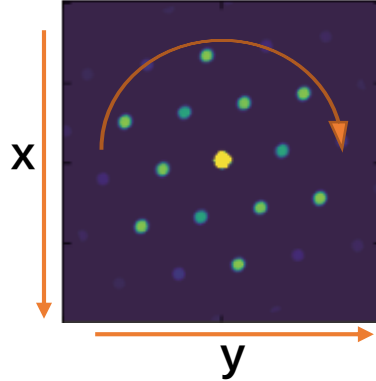
Simulated Noise-Free 4D-STEM

Sample domain image



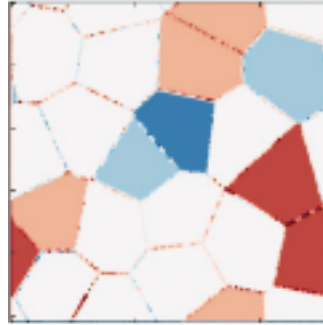
256 x 256

Random diffraction image

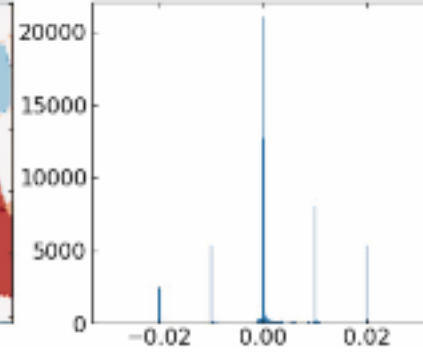


200 x 200

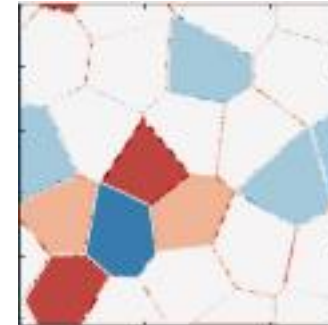
Strain x mapping



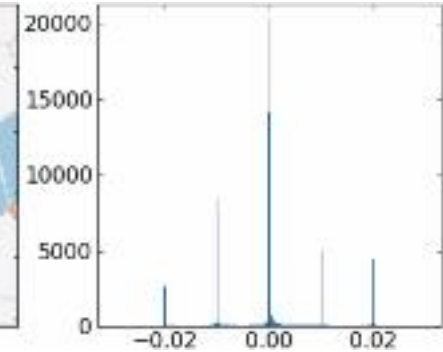
Strain x histogram



Strain y mapping

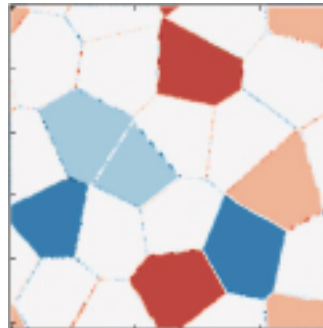


Strain y histogram

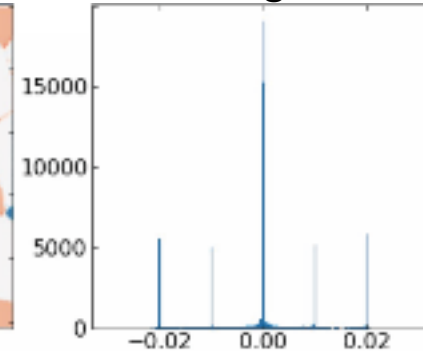


□: Reference grain:
No rotation & strain

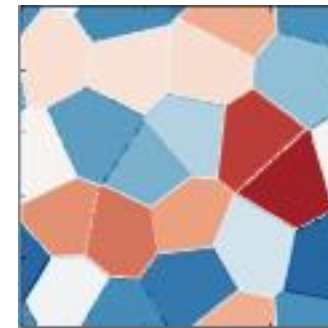
Strain xy mapping



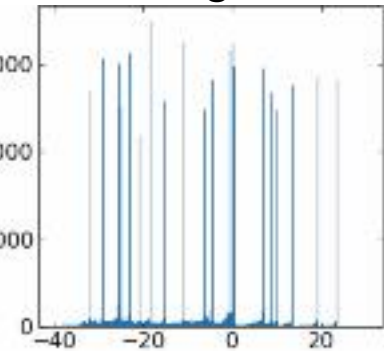
Strain xy histogram



Rotation mapping

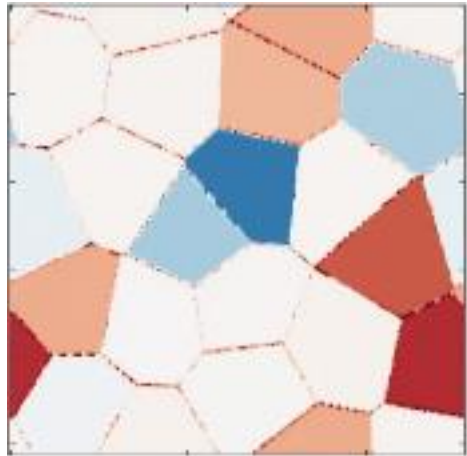


Rotation histogram

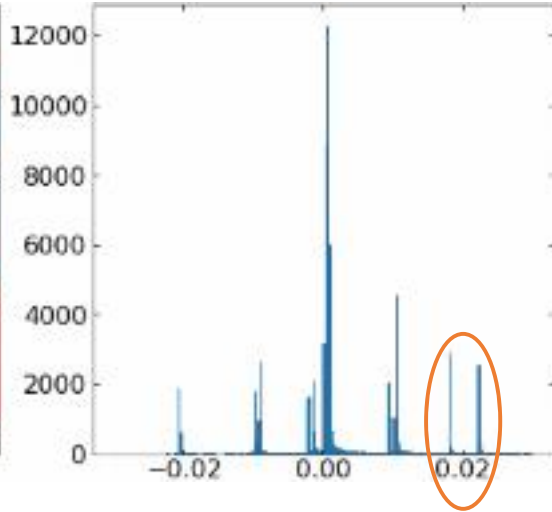


Results of py4DSTEM

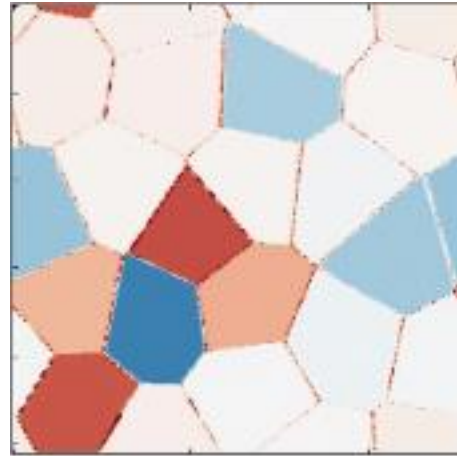
Strain x mapping



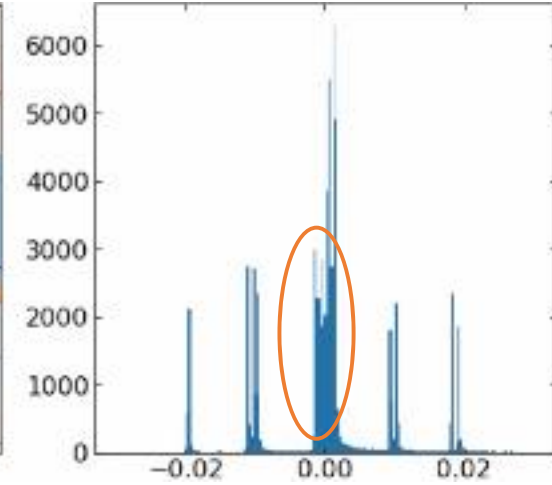
Strain x histogram



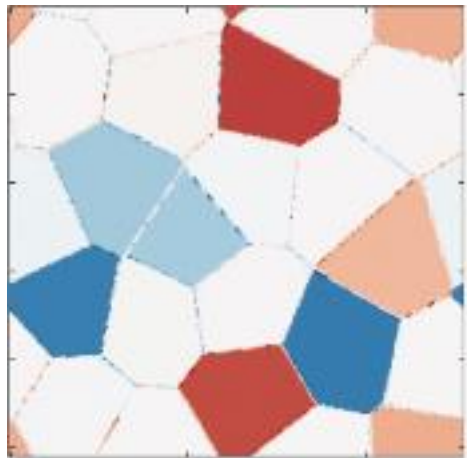
Strain y mapping



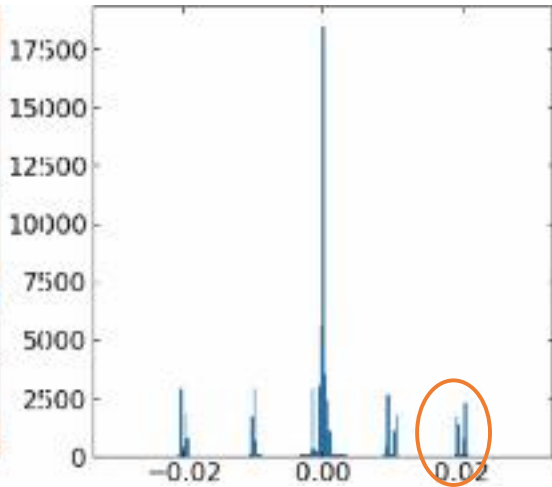
Strain y histogram



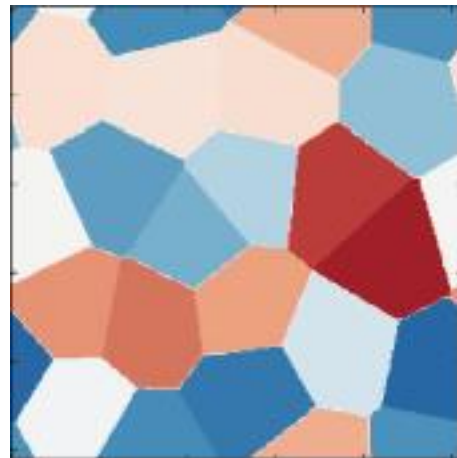
Strain xy mapping



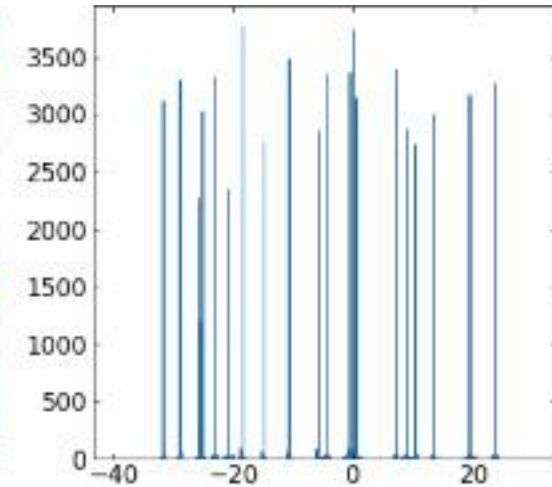
Strain xy histogram



Rotation mapping

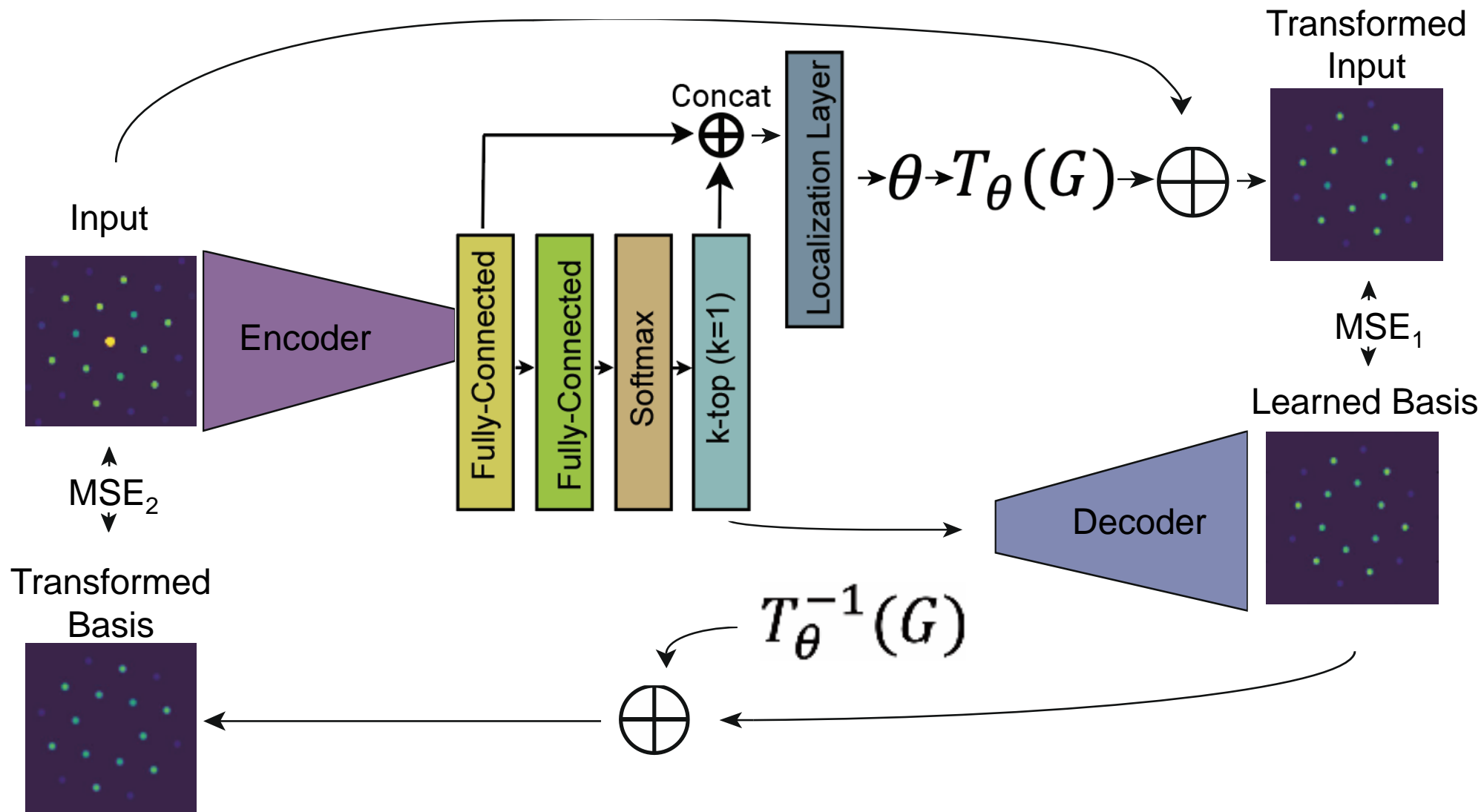


Rotation histogram

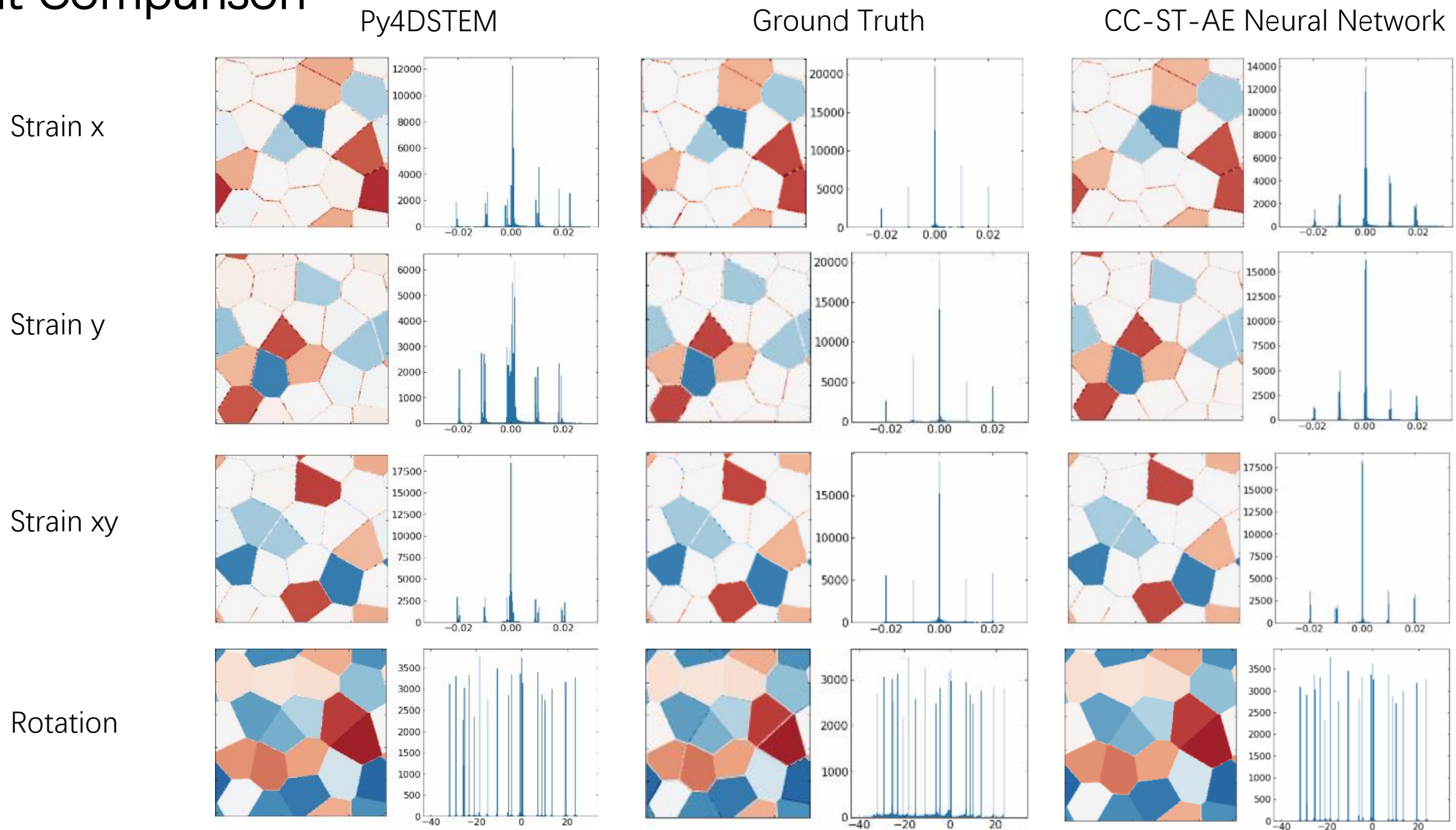


Not Perfect

Cycle-Consistent Spatial Transforming Autoencoder



Result Comparison

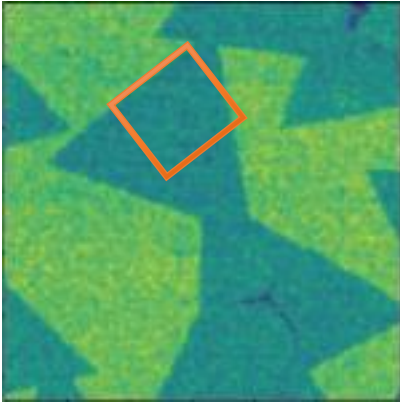


Result Comparison

Parameter	Mean Absolute Error (MAE)		Improvement
	py4dSTEM vs Ground Truth	Neural Network vs Ground Truth	
Strain X	2.0×10^{-3}	1.5×10^{-3}	25%
Strain Y	2.0×10^{-3}	1.6×10^{-3}	20%
Strain xy	9.0×10^{-4}	7.0×10^{-4}	22%
Rotation	0.8498	0.8539	-0.48%

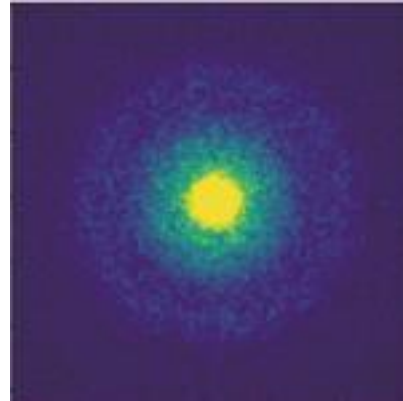
WSe₂WS₂ 4D-STEM

Sample Domain image

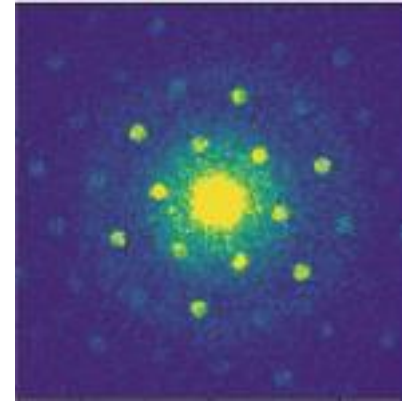


Random Diffraction image

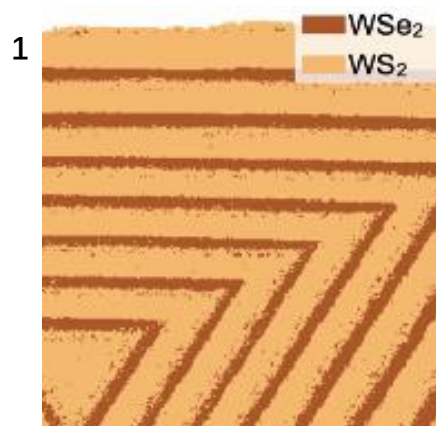
Background



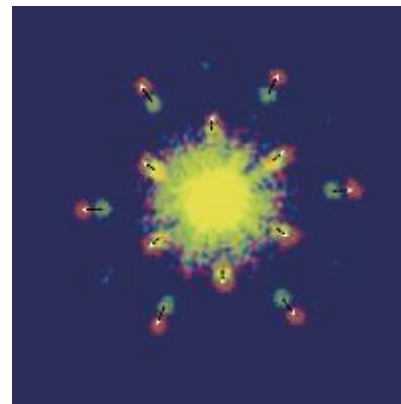
Sample



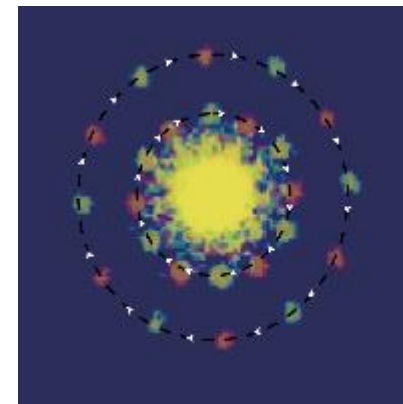
Theoretical Structure



Scale

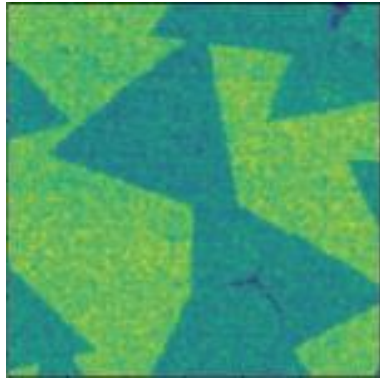


Rotation

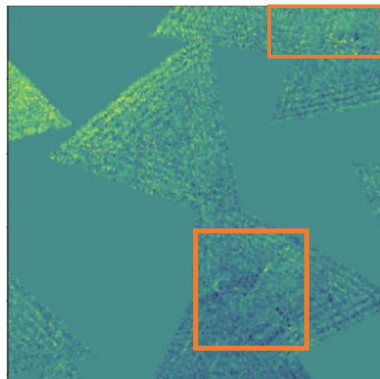


Results Comparison

Microscope Image
of Sample Domain



py4DSTEM
Strain mapping



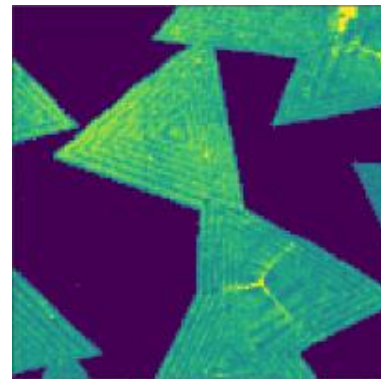
Strain failed to captured

Base Classification

Sample



Strain mapping



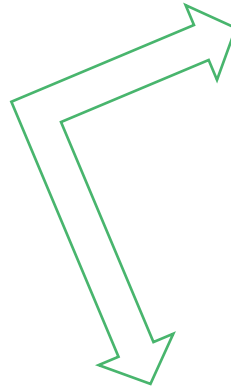
Background



Rotation



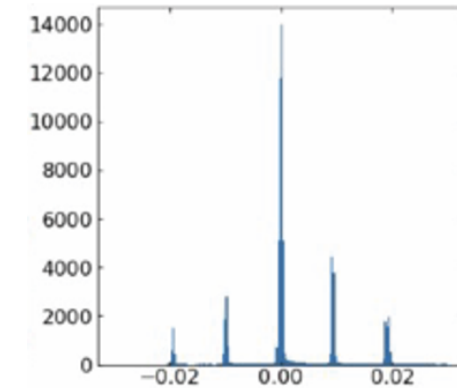
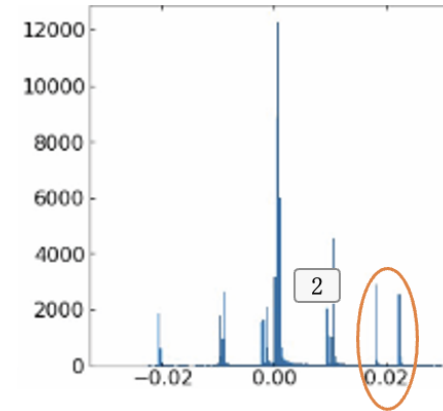
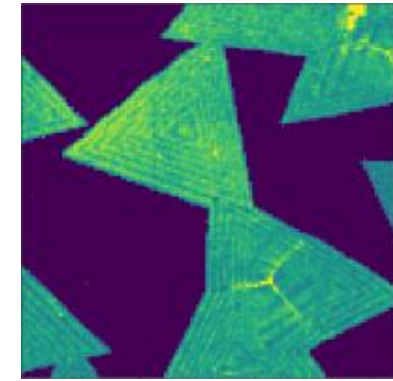
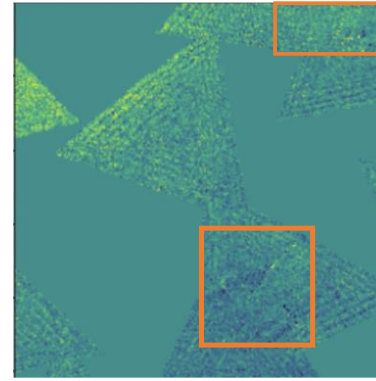
CC-ST-AE



Conclusion & Next Step

Compared with Baseline (py4DSTEM):

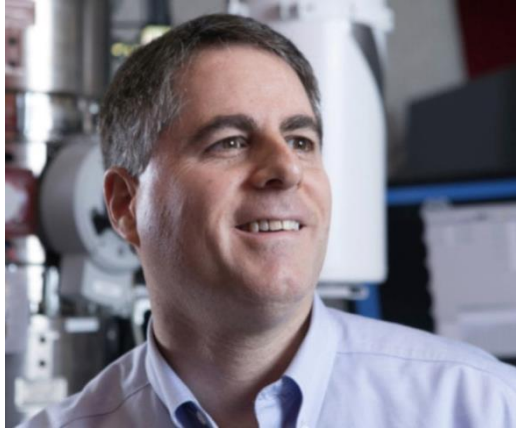
- High quality image
- Less corrupt area
- More sensitive to small scale
- Capture more accurate physics



What we do next:

- Add background noise on simulated data set
- Test the performance

Gratitude List



School of Applied and Engineering Physics, Cornell University, Ithaca, NY

Department of Materials Science and NanoEngineering, Rice University, Houston, TX

National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, CA

Thank you for your attention

Q & A