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# Autoencoder Models for Accelerated Scanning Transmission Electron Microscopy Characterization of Ferroelectrics and 2D Materials

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## Abstract

Scanning Transmission Electron Microscopy (STEM) is a crucial tool for characterizing Ferroelectrics, offering high spatial resolution for studying strain, defects, and more recently, in situ responses to environmental stimuli. However, the growing capability of STEM corresponds to an exponential growth in the complexity and volume of data. This presentation focuses on leveraging non-linear machine learning techniques to handle the increasing complexity and volume of STEM data. We explore the integration of spatial transformers and regularizers into autoencoders for analyzing both Bright and Darkfield STEM images. Brightfield imaging enables rapid, high-contrast acquisition of extensive sample areas, ideal for in-situ characterization, such as monitoring domain dynamics in various environments. We develop autoencoders with Spatial Transforming layers in the latent space, enhancing awareness of periodic domain patterns and automating their classification, shown with the domain response of Barium Titanate to temperature and background gas. Additionally, L1 Regularization scheduling promotes sparsity, disentanglement, and prevents overfitting. We also investigate the Spatial Transformer's ability to interpret diffraction patterns in Darkfield imaging, providing higher spatial resolution insights into strain, domain walls, and point defects. A Cycle-Consistent Spatial Transforming Autoencoder model is developed to directly predict the transformation of diffraction patterns and yield higher resolution 2D strain maps than py4DSTEM. In the presence of noise and bias, directly predicting transformations allows the model to outperform traditional methods of finding disk positions through correlation methods or center-of-mass. These spatial transformers demonstrate robustness against noise, artifacts, and measurement bias while efficiently handling large STEM data volumes. Finally, we discuss plans for deploying these models as high-availability inference servers on Kubernetes clusters. Successful deployment onto a public platform opens the door to real-time electron microscopy analysis.

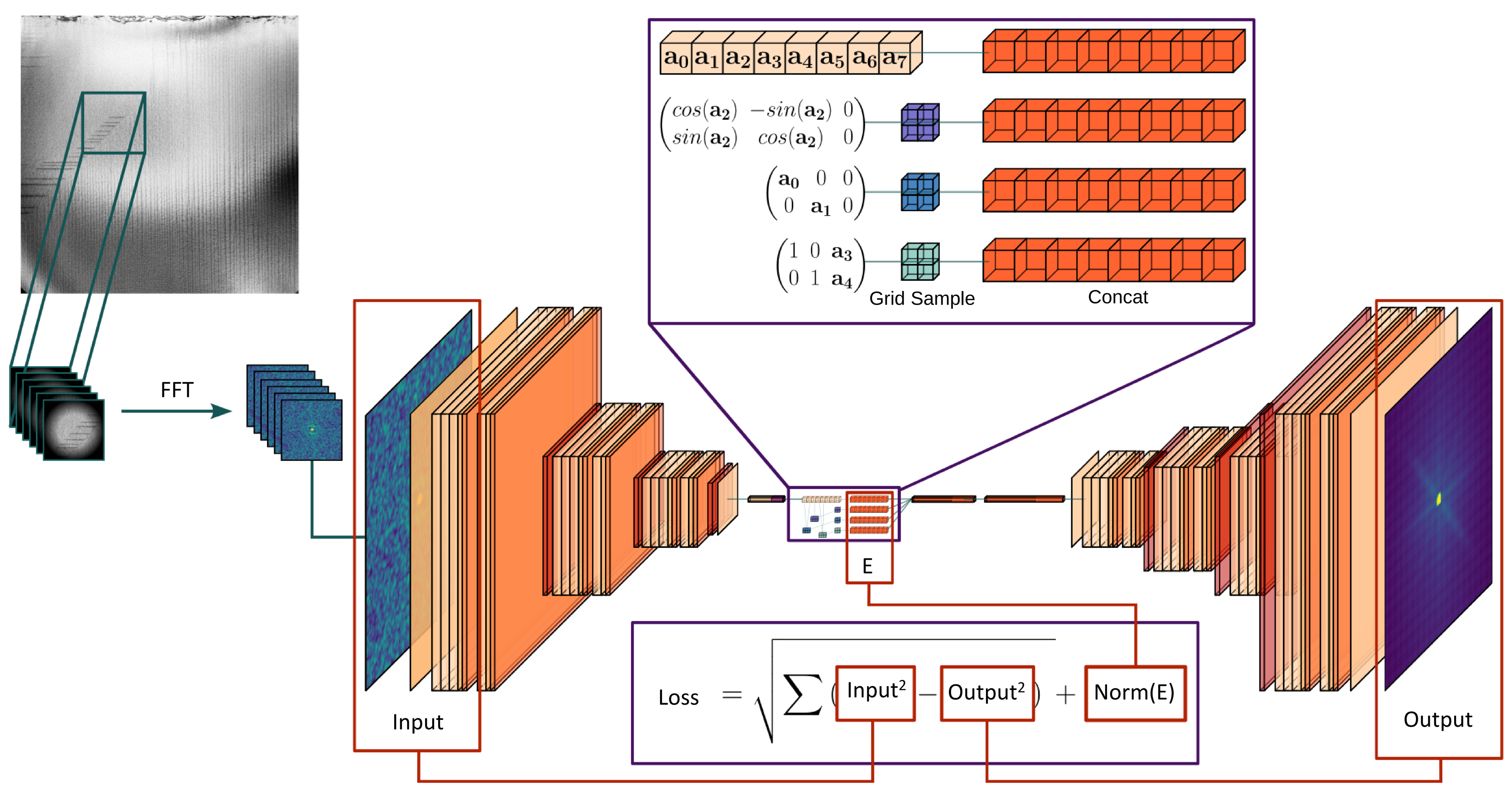
## Spatial transformers

- Classic deep learning networks (such as CNNs) are only able to disentangle translational invariance. Rotation, shear and scale is difficult to learn.
- Spatially transformed inputs are often relegated to different classes, resulting in overfitting. The results may have high accuracy, but are not physically significant.
- Efficient, parsimonious representation of Election Microscopy data relies on incorporating Spatial Transforms as learnable parameters. These transforms can represent physical features such phases, tilt, polarization, and grain orientation of the sample.

| | | | | | |
|---|---|---|---|---|---|
| Translation | $\begin{bmatrix}1 & 0 & t_x\\ 0 & 1 & t_y\end{bmatrix}$ | | Scale | $\begin{bmatrix}s_x & 0 & 0\\ 0 & s_y & 0\end{bmatrix}$ | |
| Rotation | $\begin{bmatrix}\cos\alpha & -\sin\alpha & 0\\ \sin\alpha & \cos\alpha & 0\end{bmatrix}$ | | Shear | $\begin{bmatrix}1 & k_x & 0\\ k_y & 1 & 0\end{bmatrix}$ | |

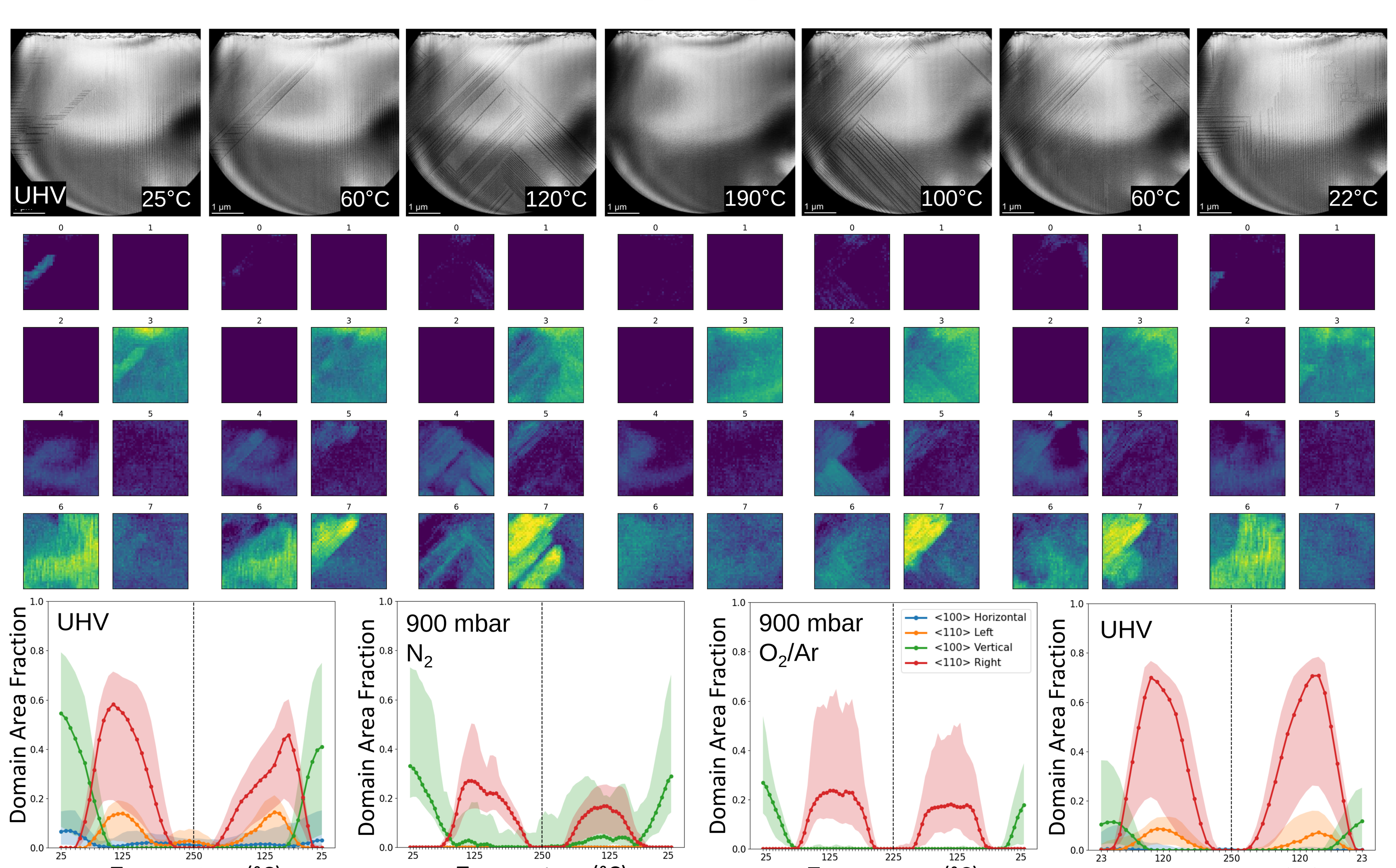
## Windowing Autoencoder

- Autoencoder model for unsupervised domain segmentation of Bright Field images of freestanding BTO
- FFTs of sliding kernel captures local information about periodicity and symmetry
- Latent space samples spatial transformation grids to append to feature vector



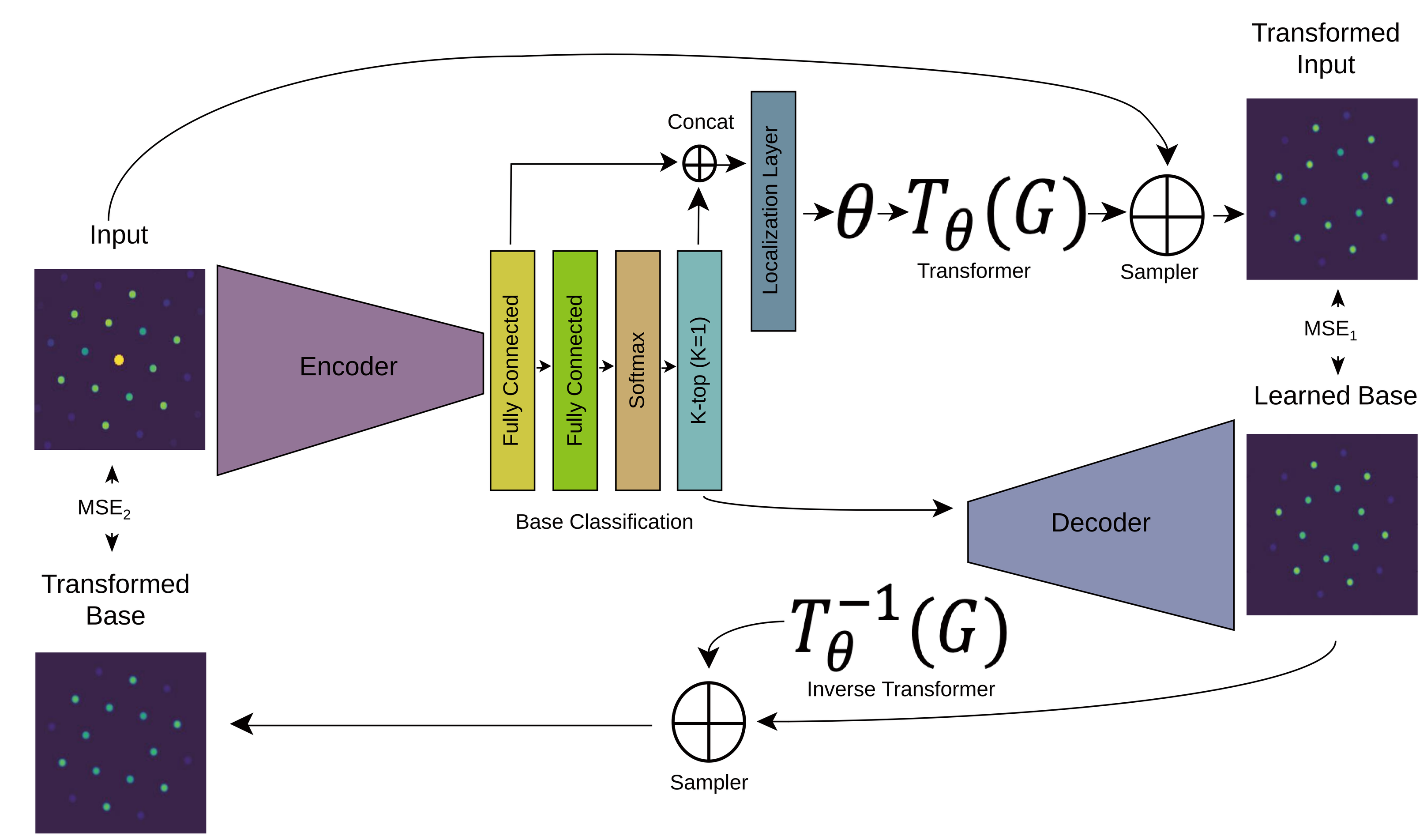

## BTO domain evolution under temperature cycling and background gas

- Feature vectors capture a-c transitioning to a-a around 60°C and completely disappear at 190°C in vacuum.
- Low SNR in gas environments due to beam interaction. Transfer learning from UVH partially resolved this.
- Domain wall formation suppressed in both $N_2$ and $O_2$ environments, and low a-a/a-c coexistence.



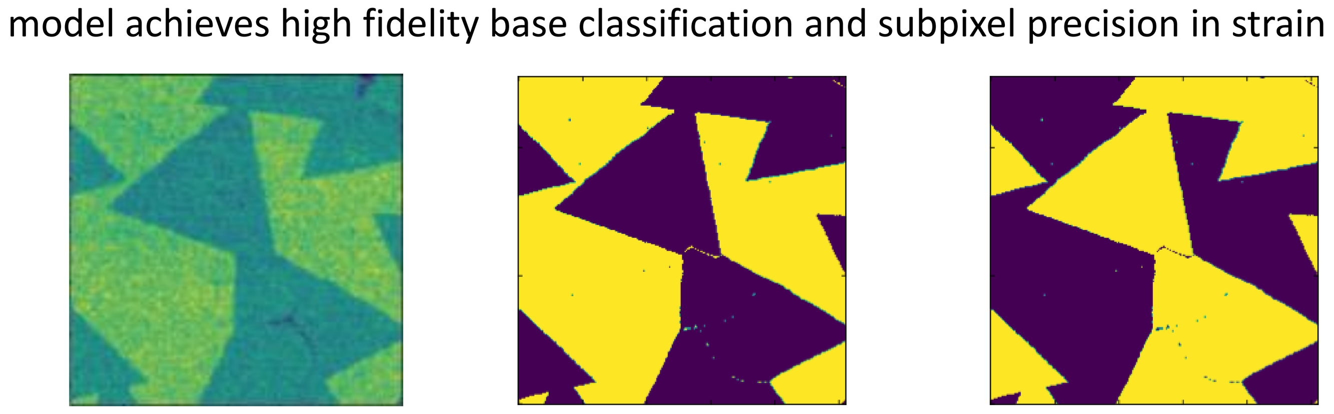

## Cycle Consistent Spatial Transforming Autoencoder (CC-ST-AE)

- ST-AE model for STEM diffraction pattern classification and strain mapping.
- Typically, strain mapping is done by finding the cross correlation with respect to a reference pattern. Bragg disk locations are labelled manually or with an algorithm like center of mass.
- This model bypasses Bragg disk labelling by directly learning the reference pattern and strain matrix.
- The model trains using two loss metrics: (1) Transform input with learned strain and compare to learned base. (2) Compare inverse transform of learned base to original input.



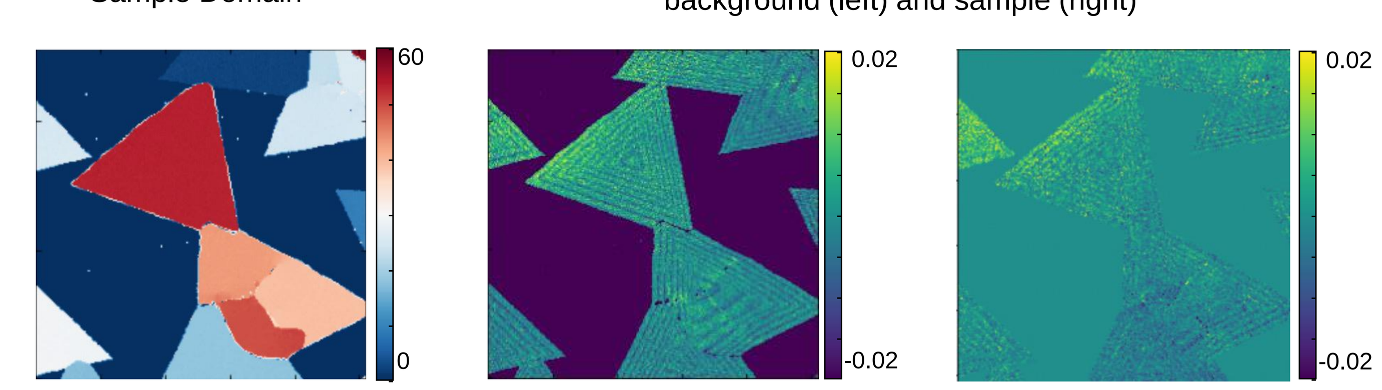

## Results on $WS_2WSe_2$

- The model achieves high fidelity base classification and subpixel precision in strain mapping



Microscopy Image of Sample Domain

Base classification using CC-ST-AE, results are base of images. background (left) and sample (right)



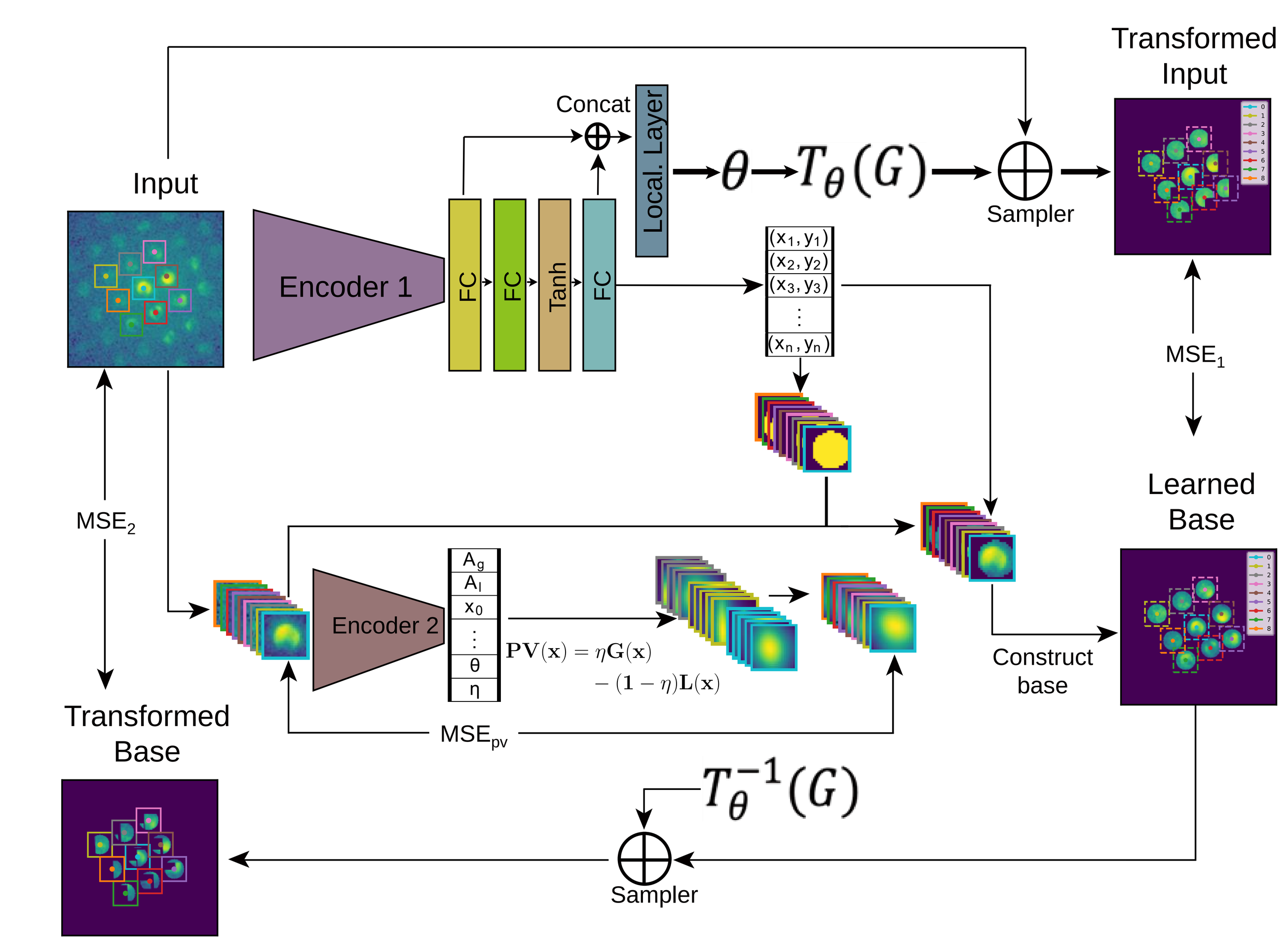

Rotation mapping using CC-ST-AE

Mapping of Strain magnitude using different methods: CC-ST-AE (left), state-of-the-art (py4DSTEM, right)

## Future Works

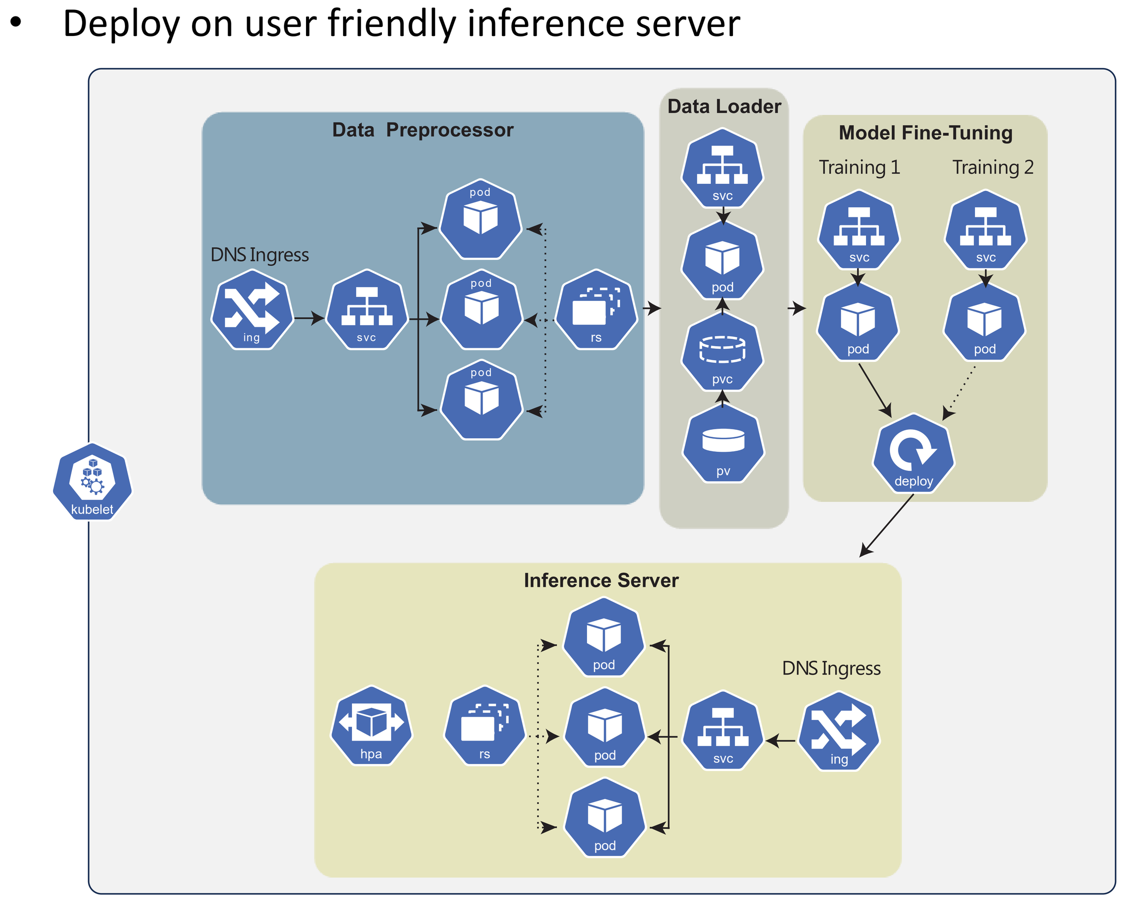
### Pseudo-Voight disk fitting

- Disentangle noise and intensity fluctuations in Bragg disks




### Model deployment on Kubernetes clusters

- Containerize model for flexibility across different operating systems
- Deploy on user friendly inference server




Check out our github:

m3learning



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