Segmentation of scanning transmission electron microscopy (STEM) images with unsupervised machine learning

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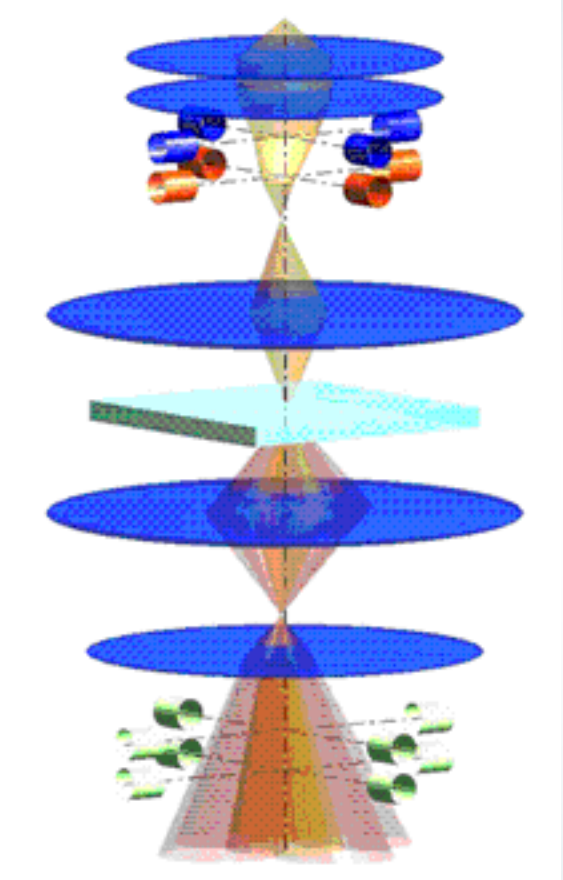
June 15, 2020

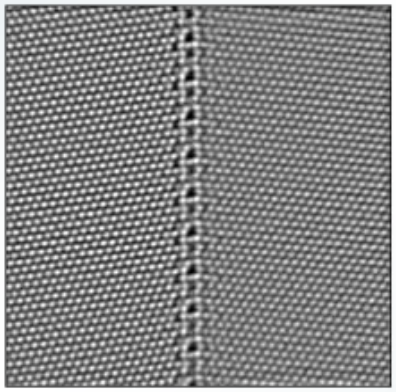
Working principle of STEM



STEM meets big data

Materials properties

Supervised,
Unsupervised,
machine learning



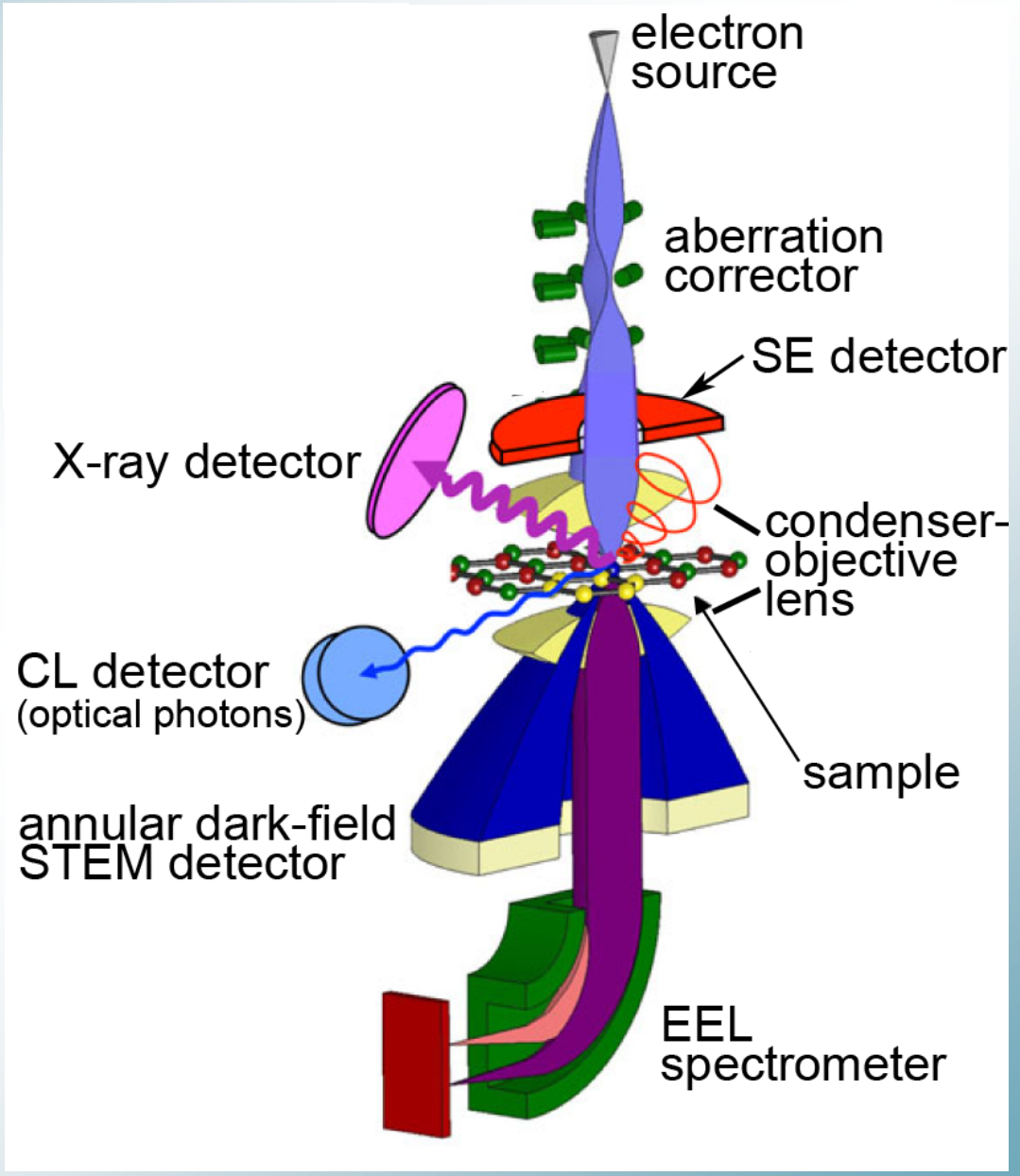
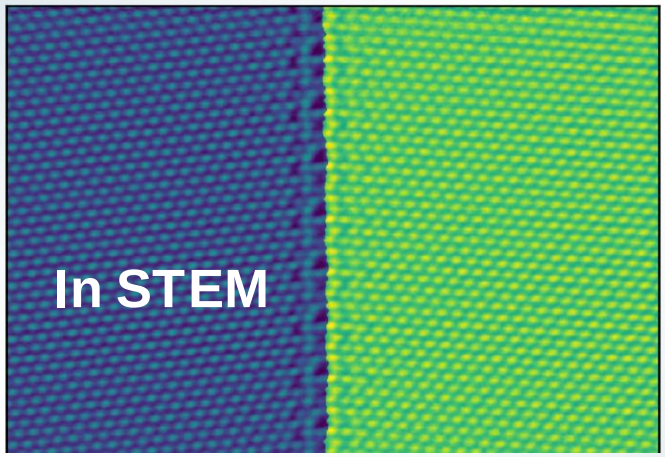


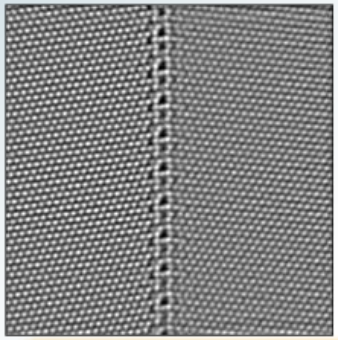
Image segmentation

https://sergioskar.github.io/Semantic_Segmentation/



HAADF-STEM image of a Cu grain boundary

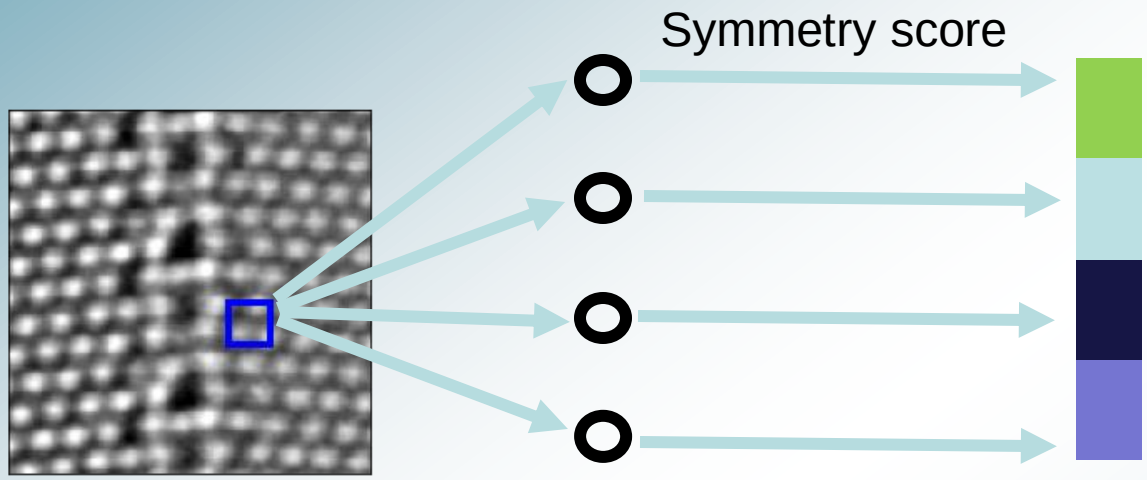
An unsupervised approach



- Free of training.
- Segmenting images according to local symmetry

HAADF-STEM images → Local-symmetry descriptors → Principal component analysis → K-means clustering

Local symmetry descriptors



Scoring symmetry:

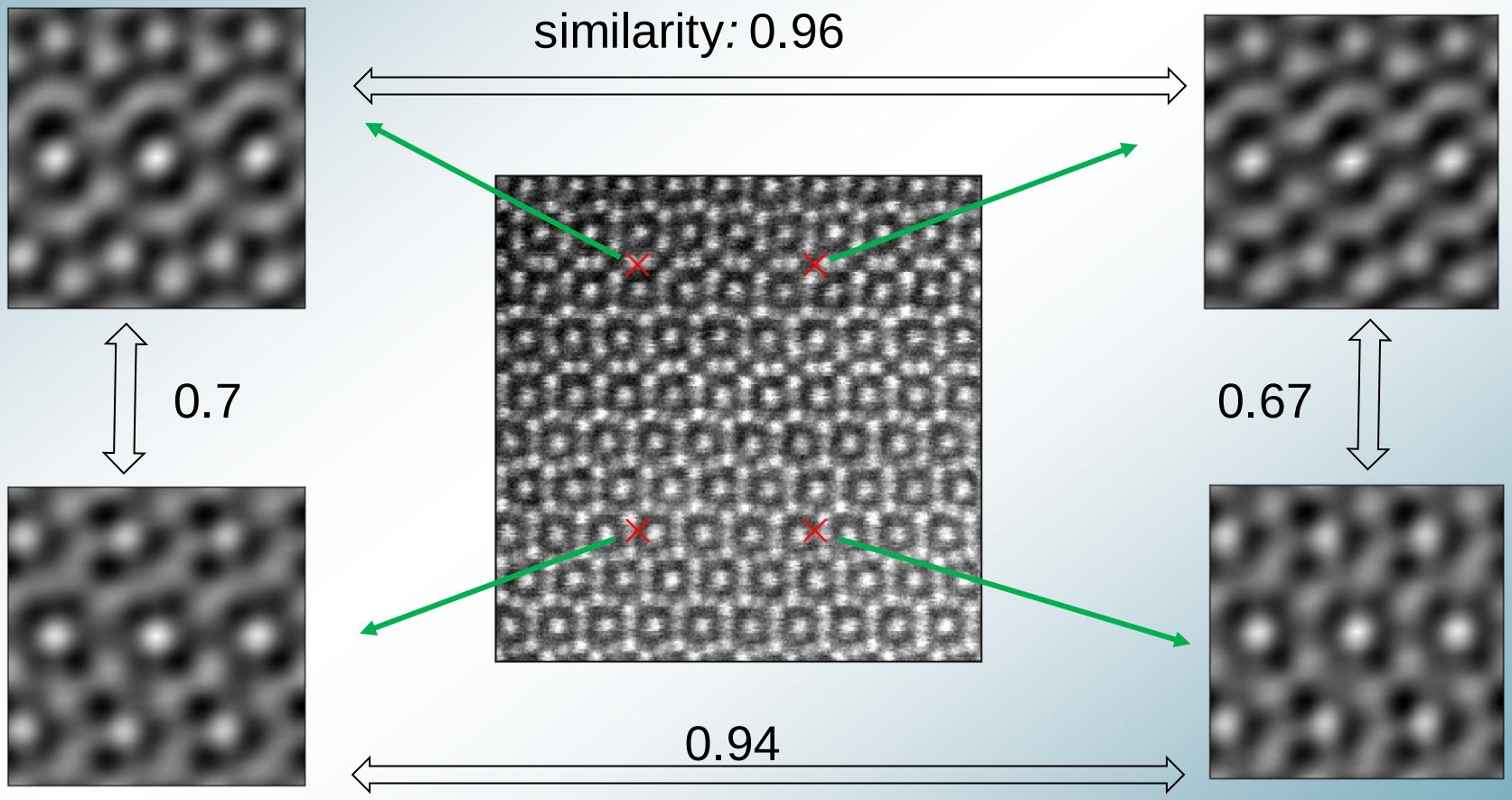
Pearson correlation coefficient

$$\rho_{XY} = \frac{\mathrm{Cov}(X, Y)}{\sigma_X \sigma_Y}$$

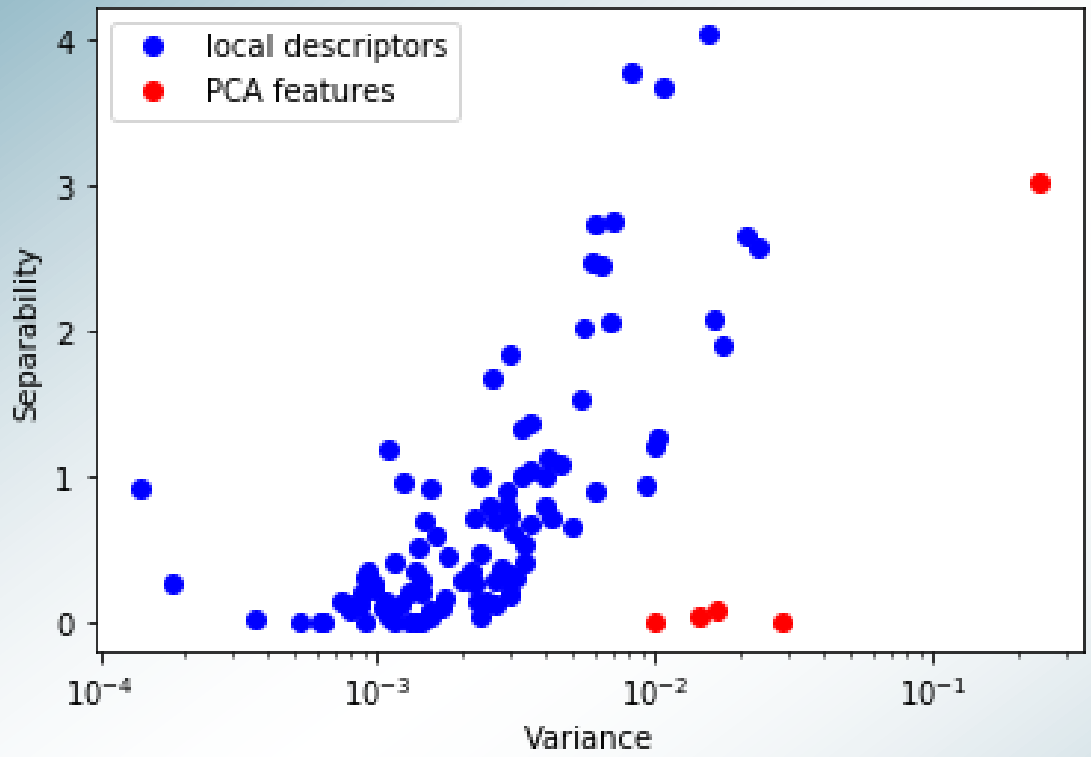
X: original patch
Y: transformed patch

Local symmetry descriptors

Pixels in same crystal pattern have *similiar* local descriptors



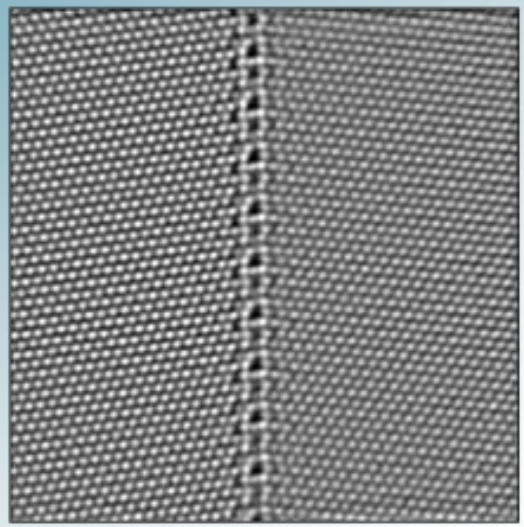
Principal component analysis



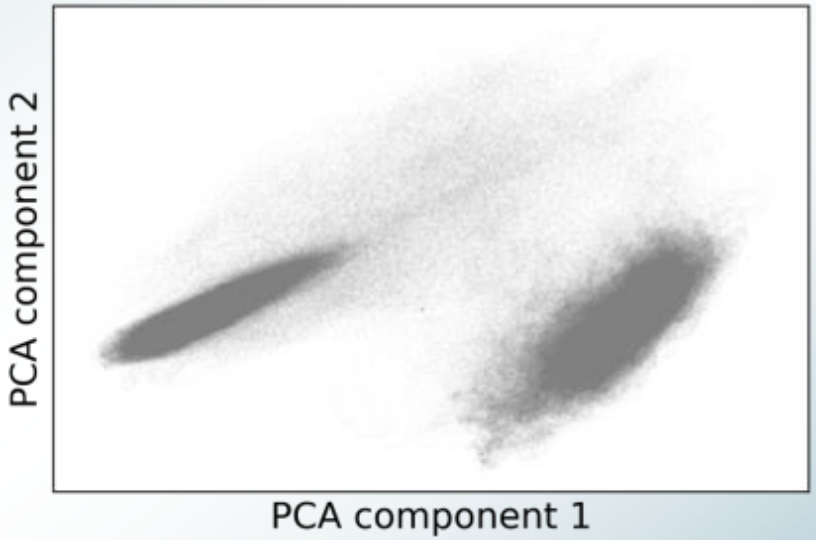
Abundance of local descriptors → PCA → A few PCA features

Principal component analysis

STEM image



Pixels projected into PCA component space

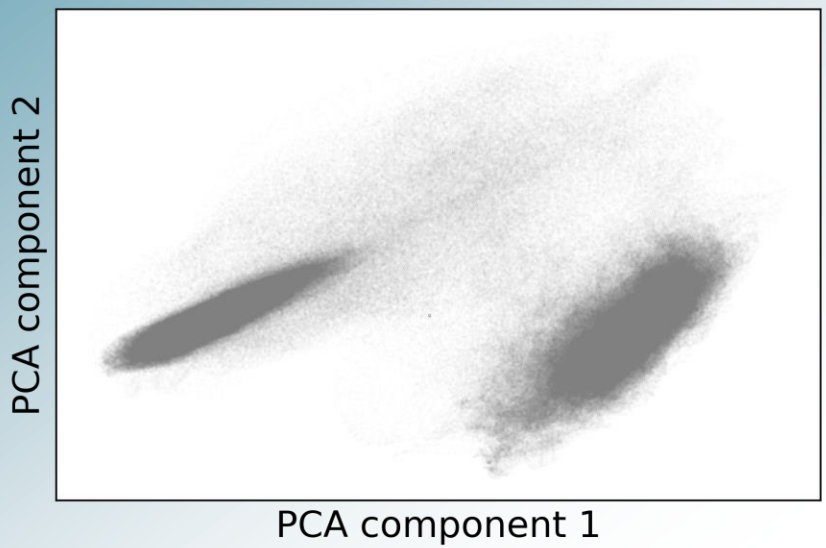


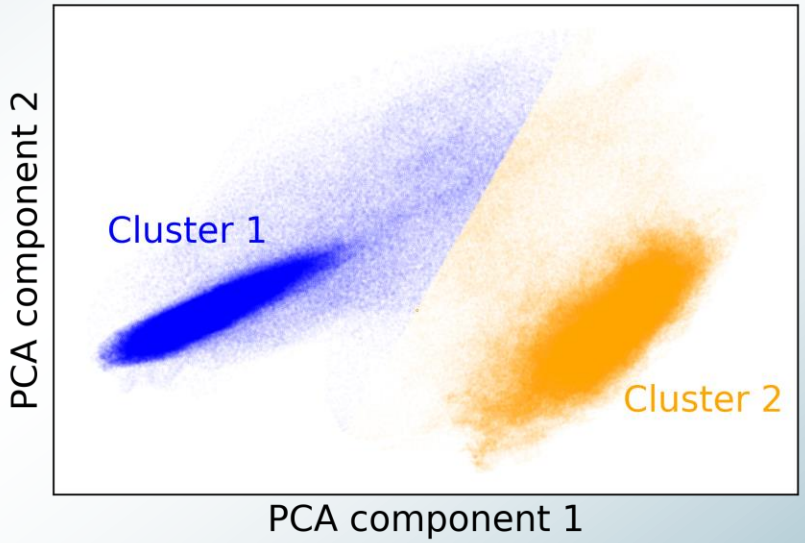
Abundance of local descriptors

PCA

A few of PCA features

K-means clustering



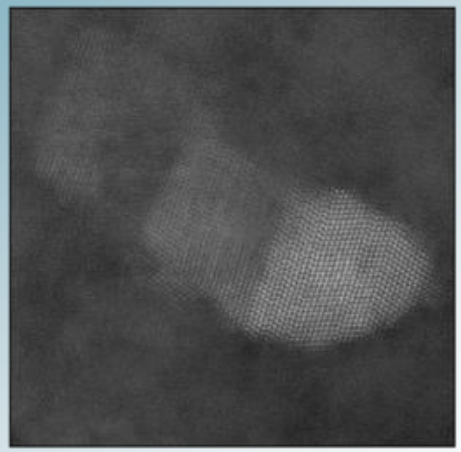


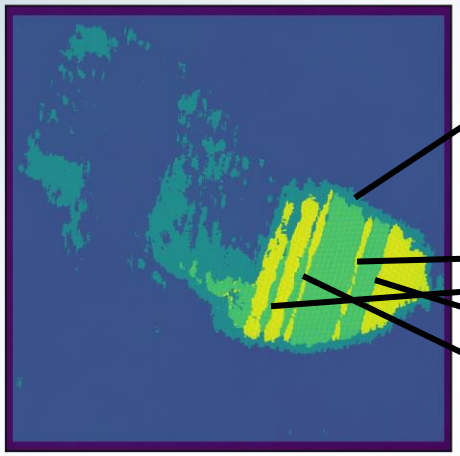
- One-to-one correspondence between crystal patterns and clusters.
- clustering module in scikit-learn is used, https://scikit-learn.org.

Applications

Raw images

Segmented images

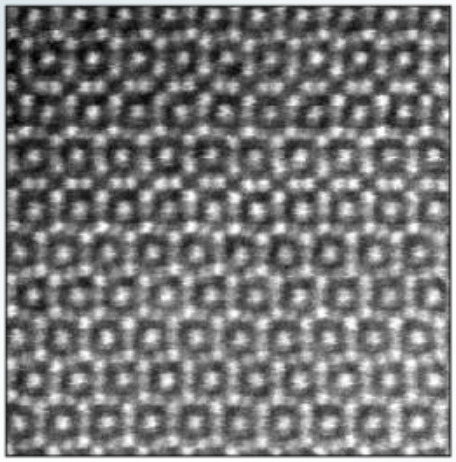


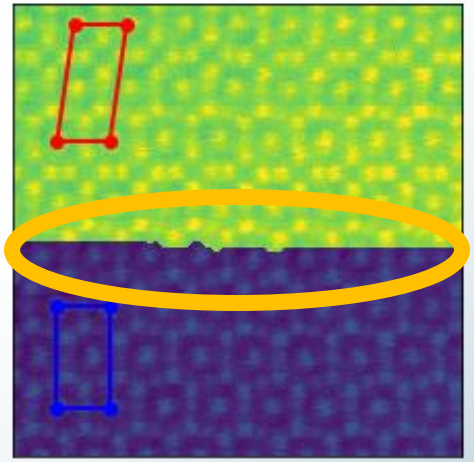


Interface between matrix and precipitate

Stacking fault

Twin boundary



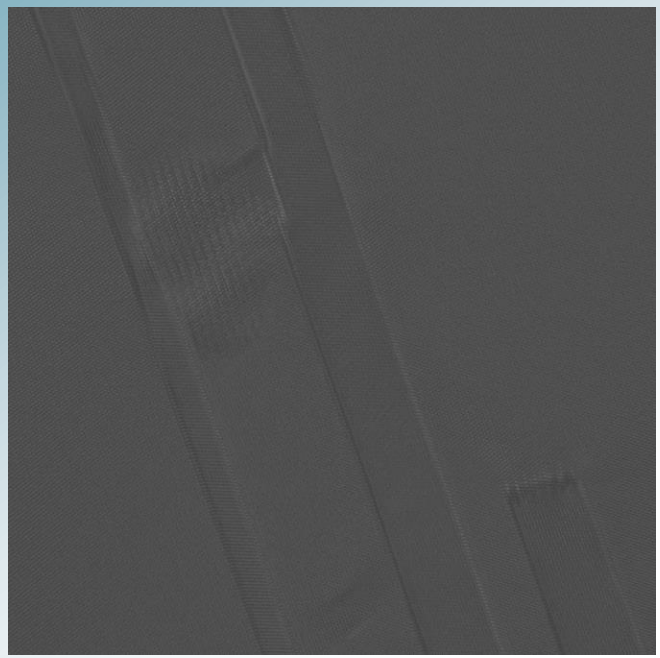


phase boundary

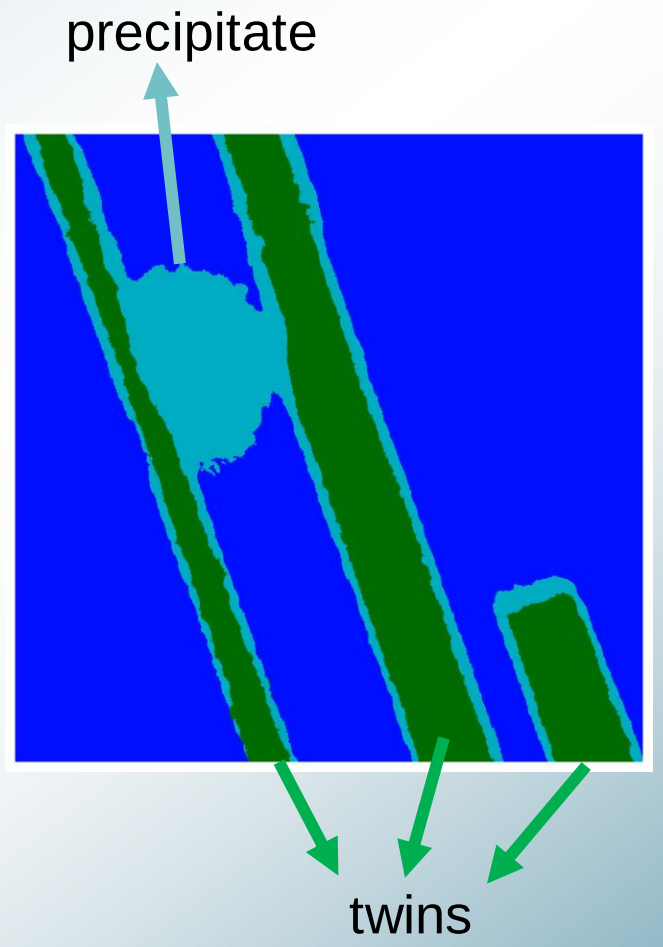
STEM image of Ni precipitate in courtesy of Spark Zhang at MPIE

Code available at:
https://pypi.org/project/pystem
https://github.com/NingWang1990/pySTEM

Applications



Segmentation



In situ experiment performed by Wenjun Lu at MPIE

Code available at:
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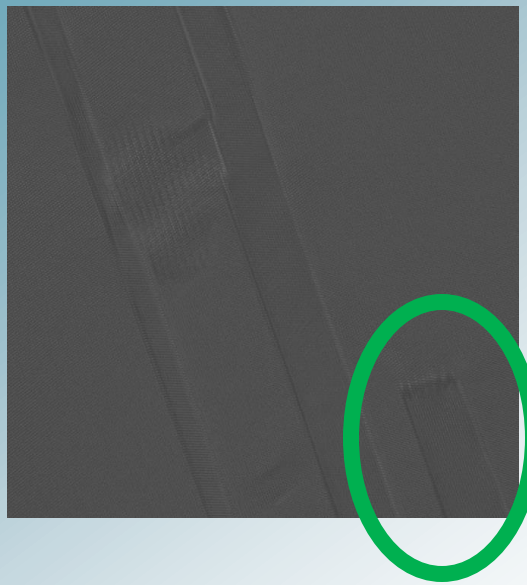
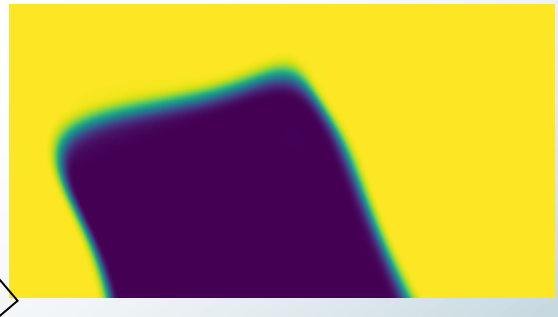
https://github.com/NingWang1990/pySTEM

Ongoing: learning dynamics



Soft segmentation

Smoothing with neural networks



Dicovering partial differential equation

$$\frac{\partial \Phi}{\partial t} = -0.43\frac{\partial \Phi}{\partial x} - 0.15\frac{\partial \Phi}{\partial y}$$

Thanks for your attention!

https://github.com/NingWang1990/Machine_learning_dynamics