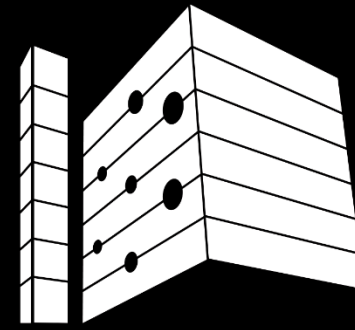


**MOLECULAR
FOUNDRY**



Programmatic and Deep Learning Analysis Pipelines for 4D-STEM Materials Science Experiments

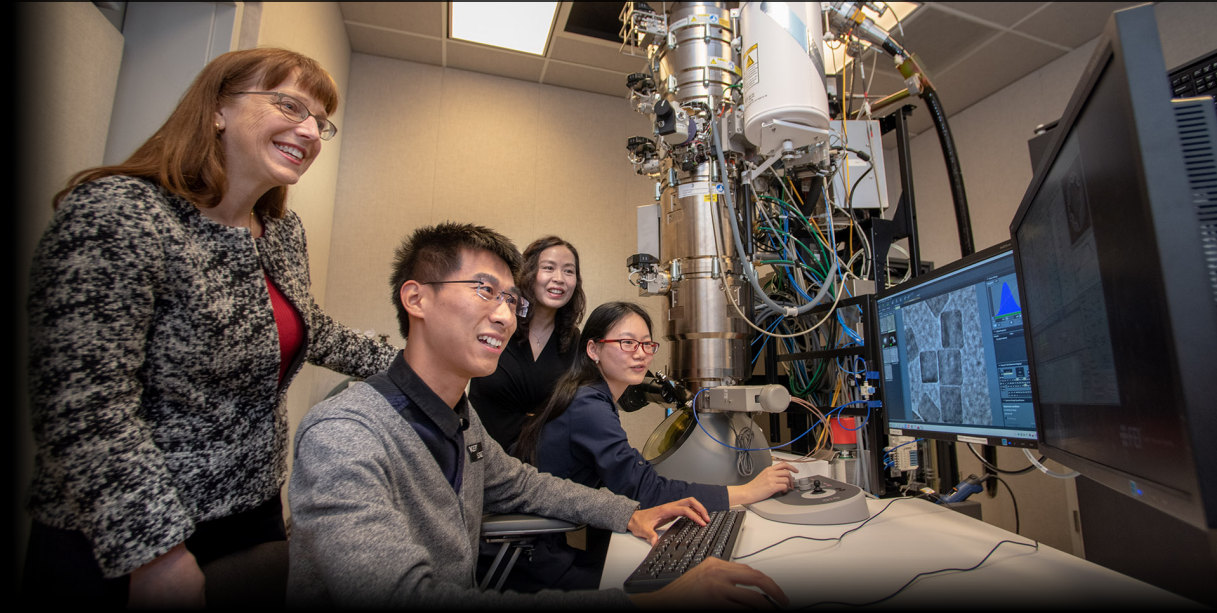
Colin Ophus

NCEM, Molecular Foundry, Lawrence Berkeley National Laboratory

2023 June 21 – Thursday 15:00

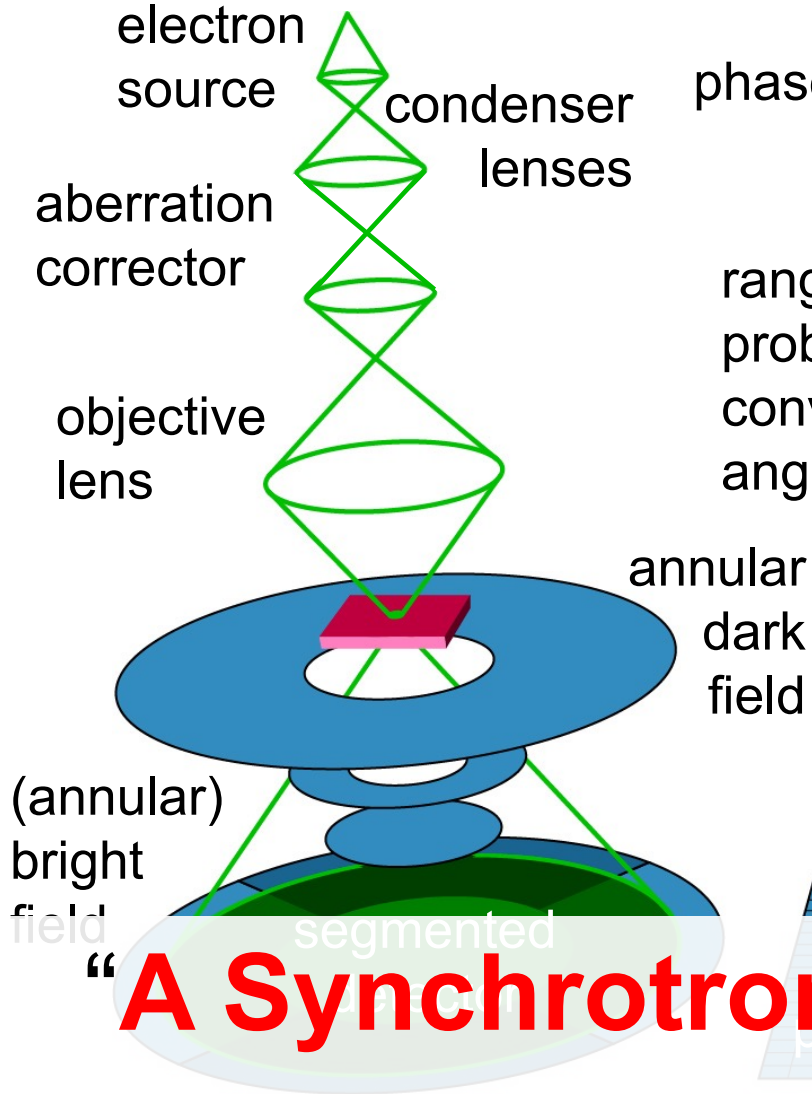
University of Maryland – AI for Scattering Workshop

Open Call for Proposals – September 2023 – foundry.lbl.gov

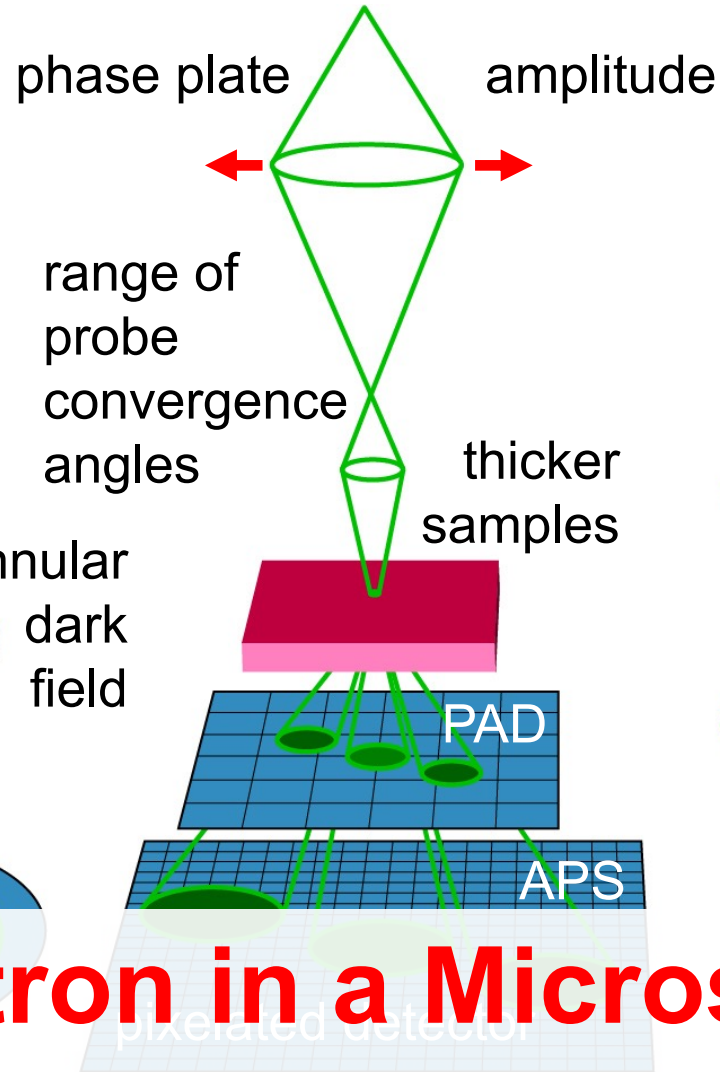


Scanning Transmission Electron Microscopy

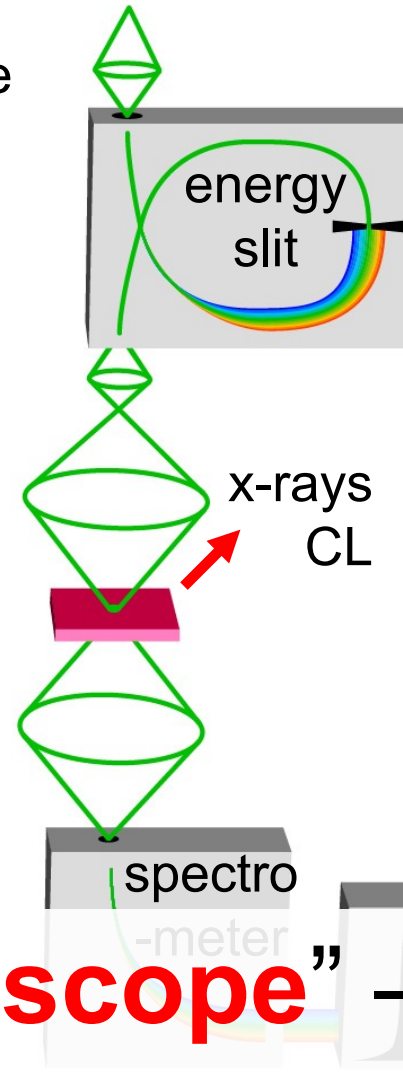
Imaging



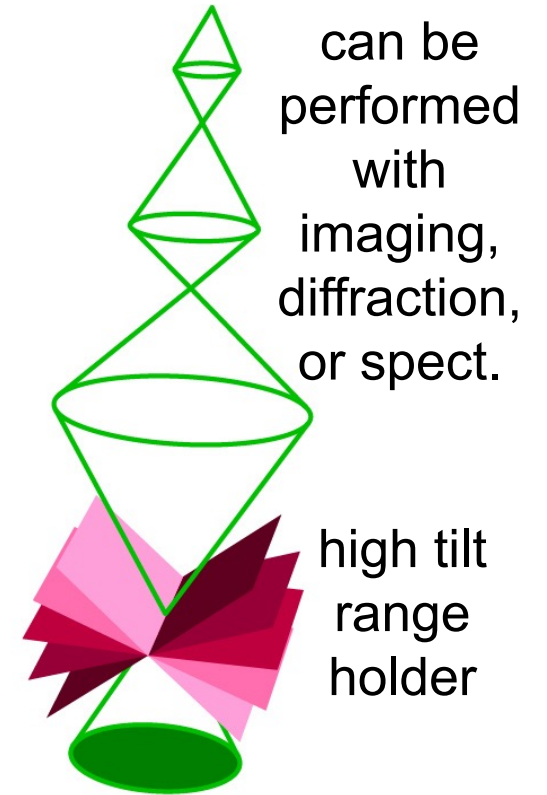
Diffraction



Spectroscopy

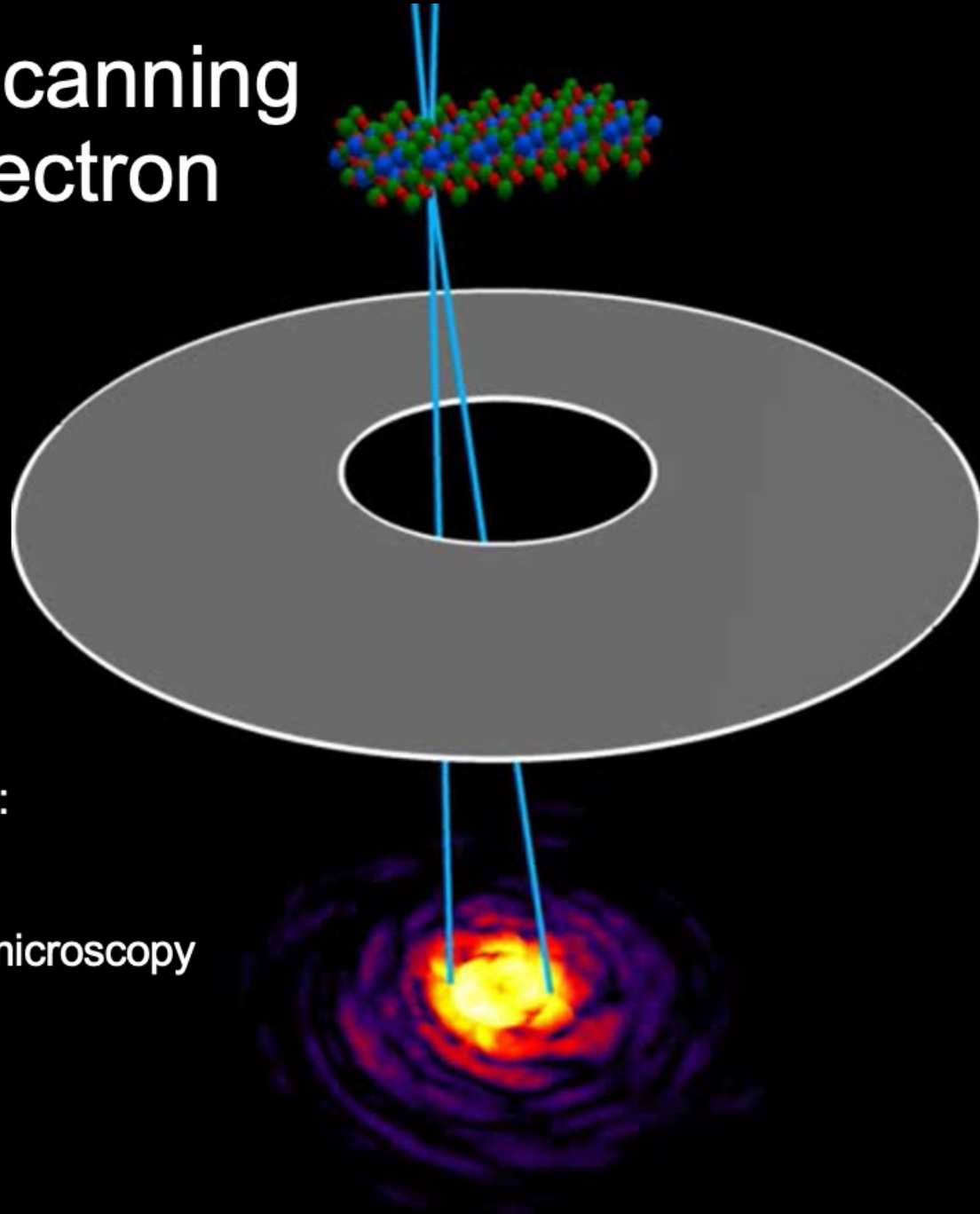


Tomography



“A Synchrotron in a Microscope” – Mick Brown

Introduction to Scanning Transmission Electron Microscopy



converged electron probe

sample

annular dark field
(ADF) detector

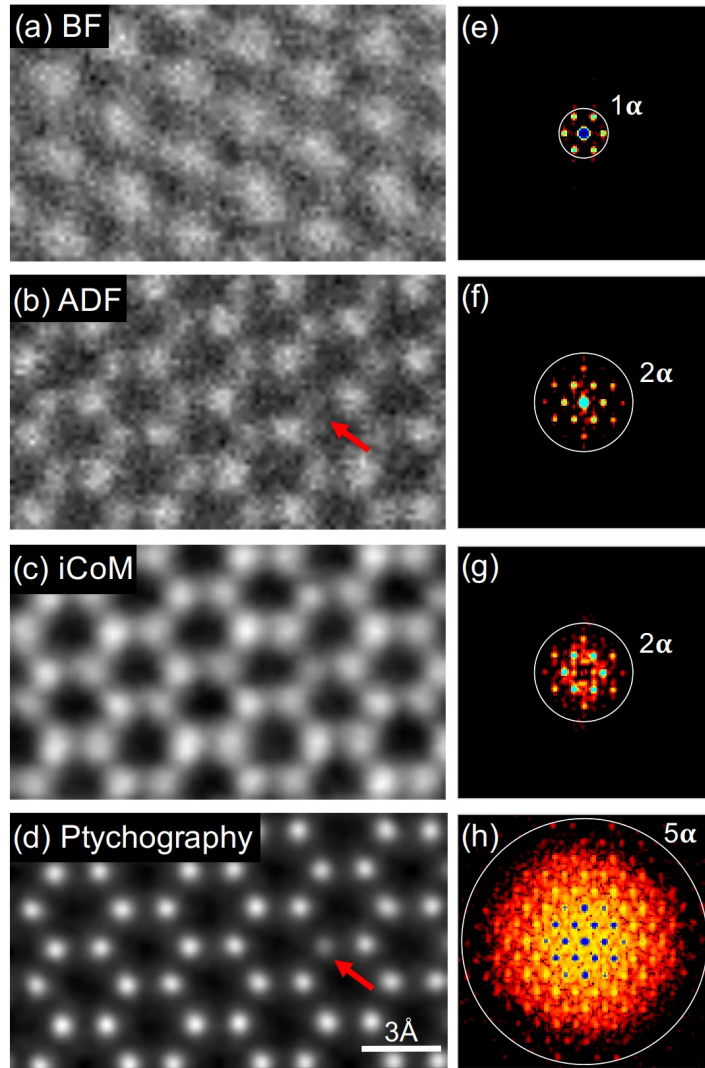
2D images recorded
over a 2D grid of probe positions:

Four dimensional
scanning transmission electron microscopy
(4D-STEM)

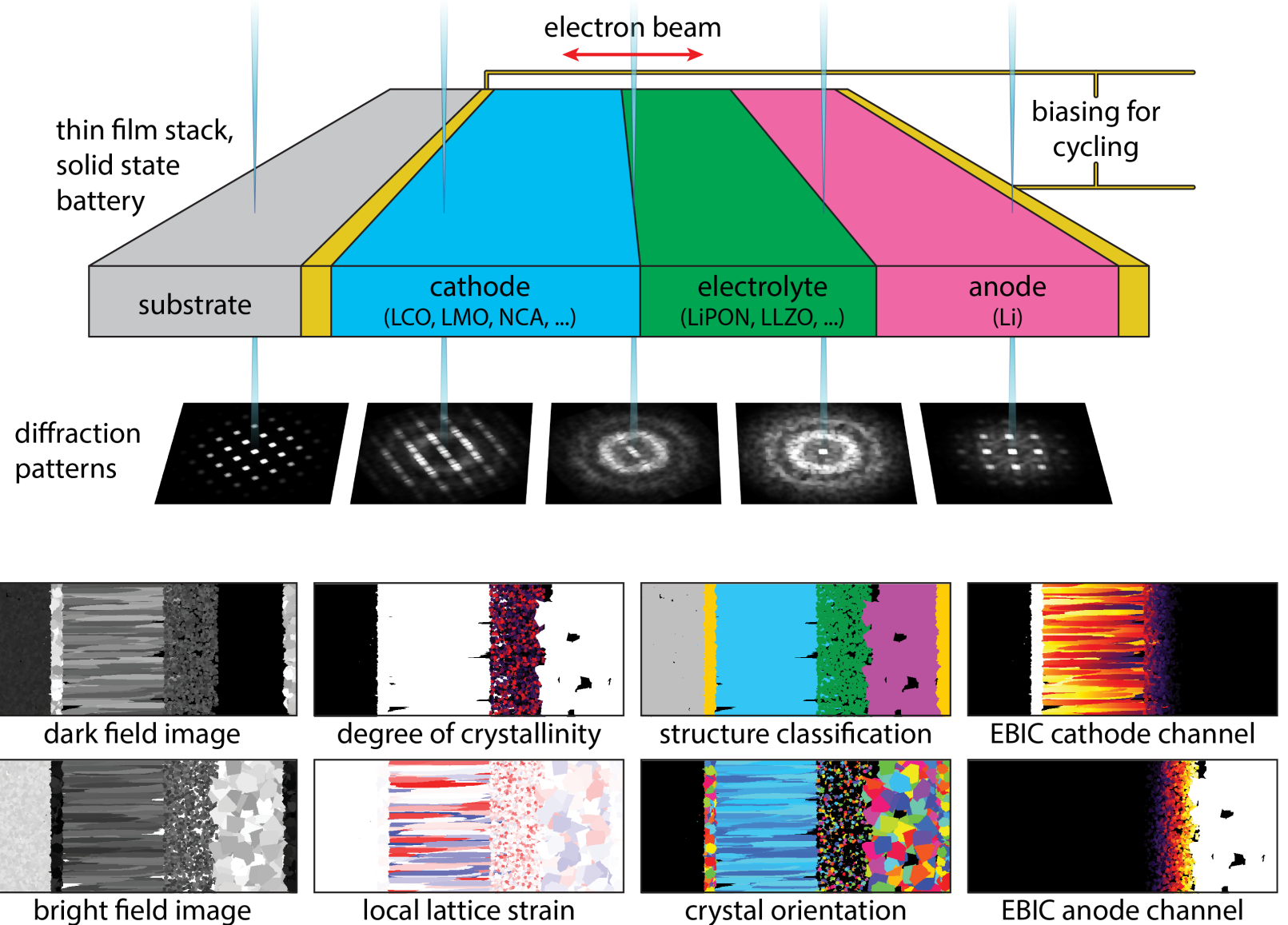
diffraction pattern

pixelated detector

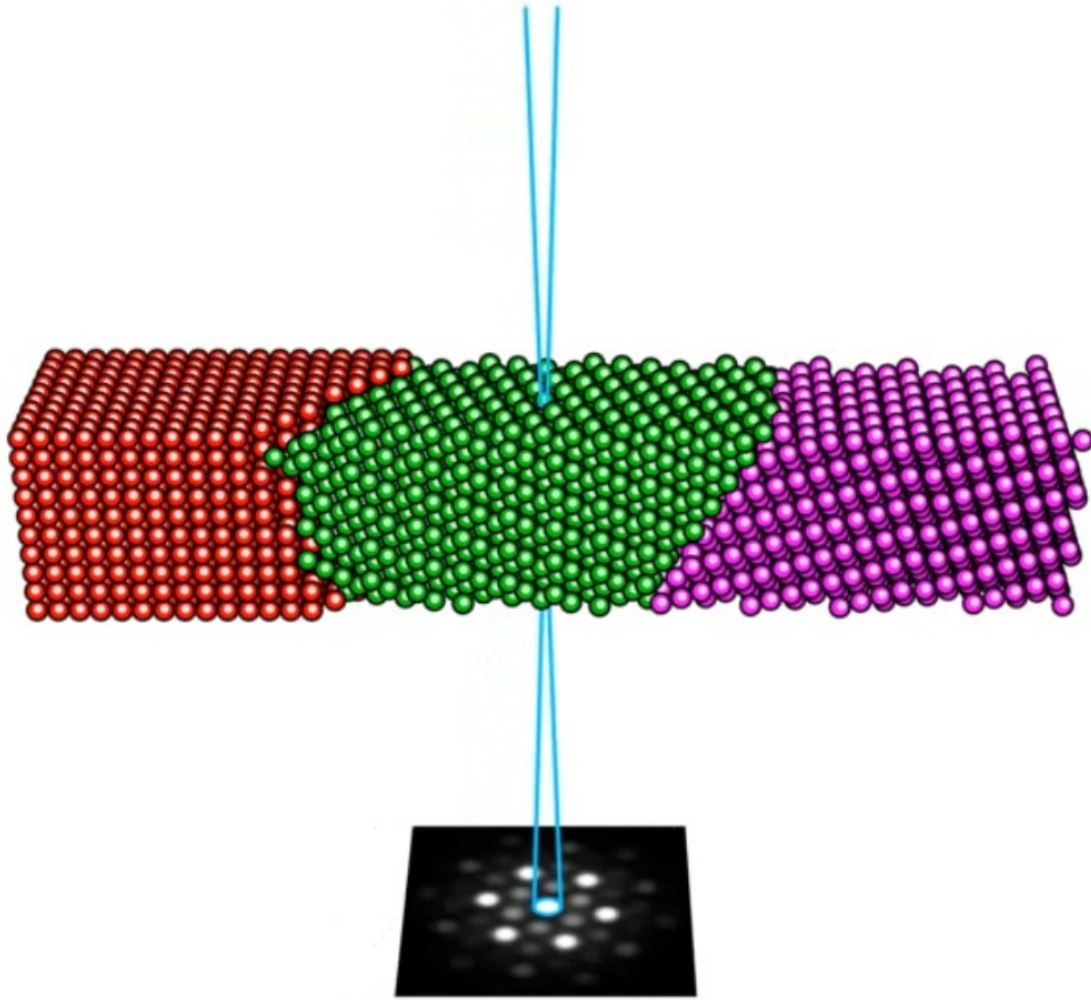
Motivation – Why do 4D-STEM?



Jiang et al., Nature 559, 343 (2018)

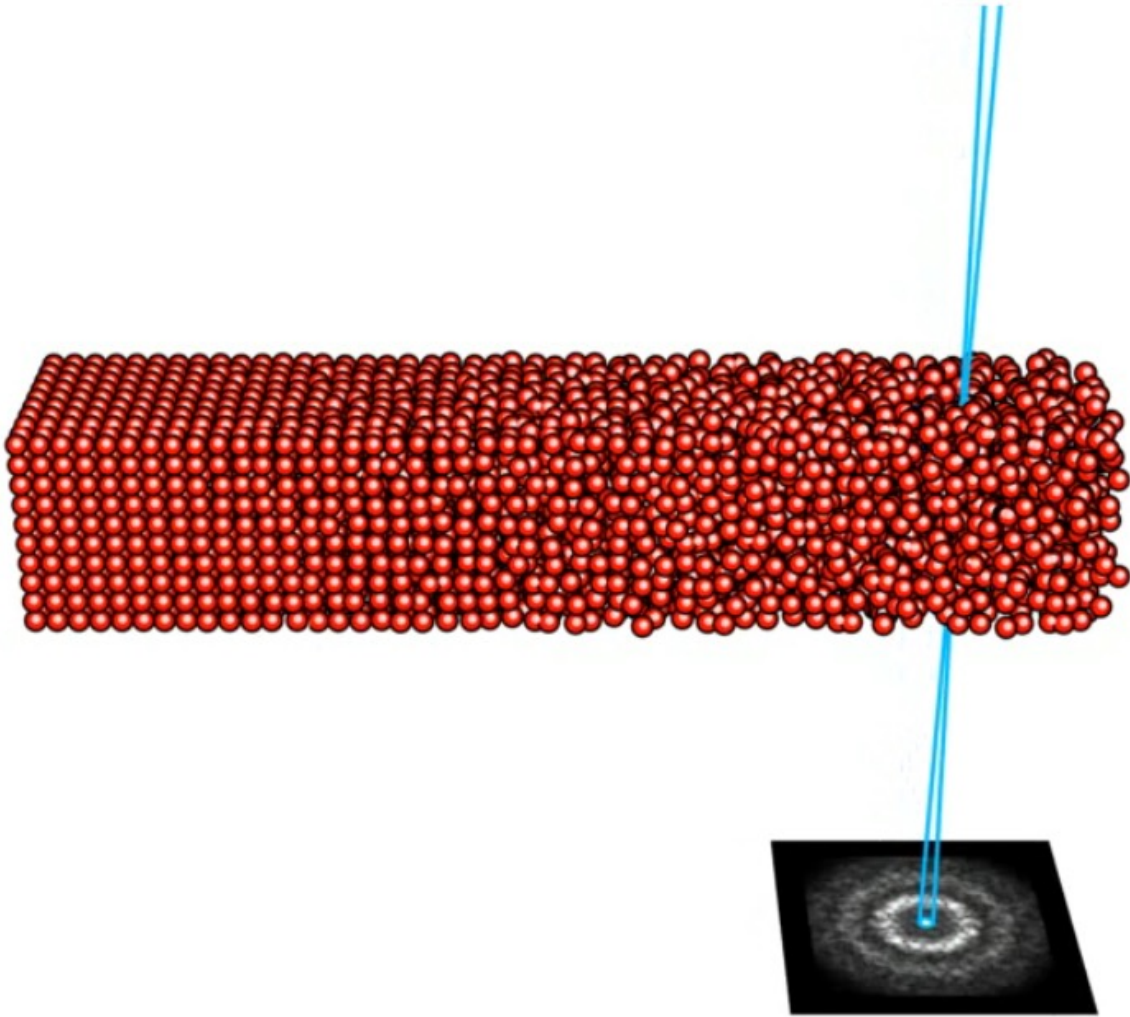


STEM Diffraction from Crystalline Samples



- Ideally, the diffracted signal is simply a 2D **Fourier transform** of the projected potential, multiplied by the probe intensity.
- Thus the position and intensity of **Bragg disks** of each diffraction pattern acts as a **fingerprint** for the local structure and orientation of the (crystal) sample.
- Interpretation is complicated by multiple / dynamical scattering (thickness effects), overlapping grains, background signals.

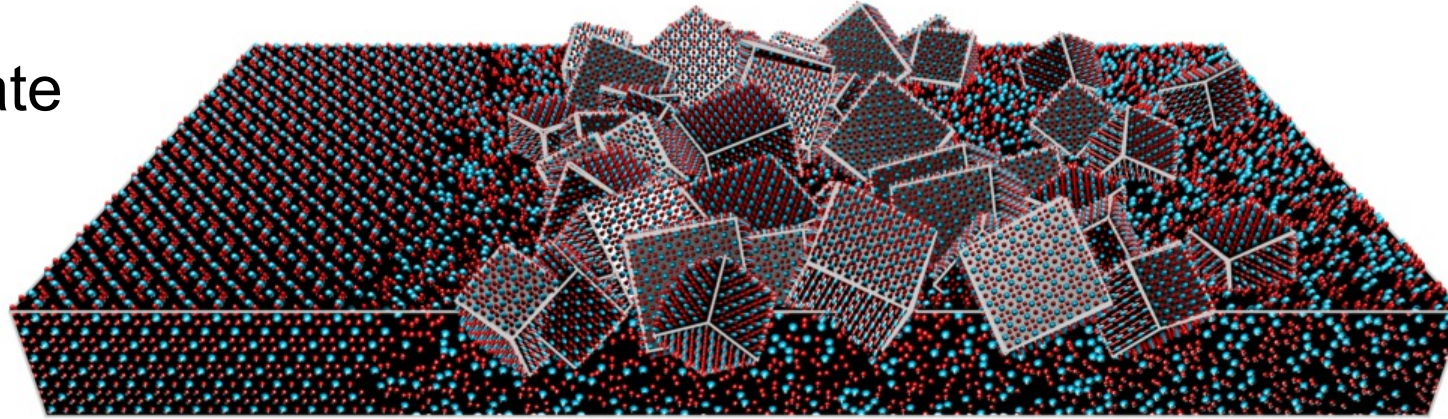
4D-STEM Diffraction from Amorphous Samples



- Ideally, the diffracted signal is simply a 2D **Fourier transform** of the projected potential, multiplied by the probe intensity.
- The position and shape of **amorphous halos** of each diffraction pattern acts as a **fingerprint** for the local structure factor, given by the mean atomic arrangement.
- Interpretation is **complicated** by multiple / dynamical scattering (thickness effects), background, **more** than crystal diffraction!

Complex Sample Analysis with 4D-STEM

Gadolinium Titanate

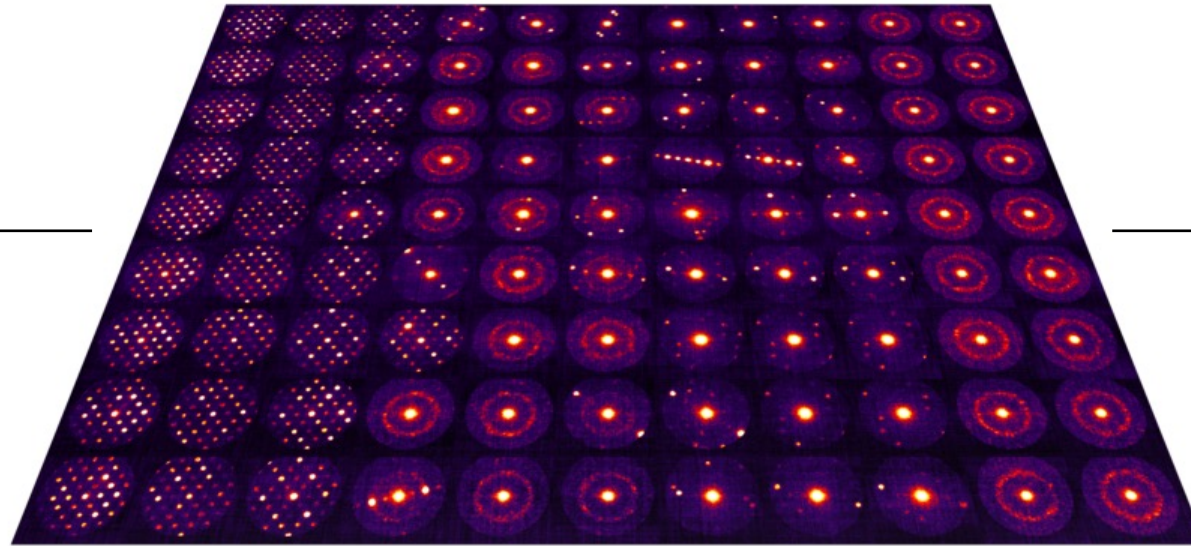


4D-STEM
experiment

single crystal
pyrochlore



amorphous



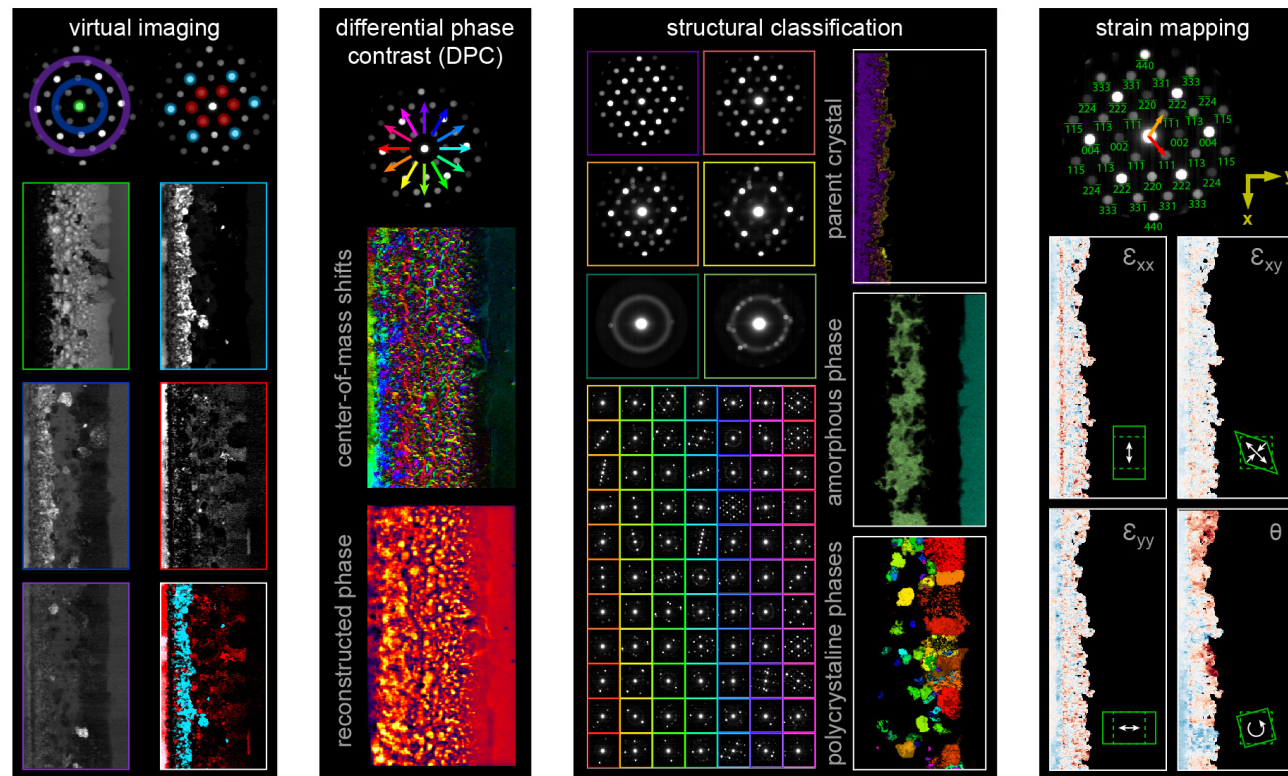
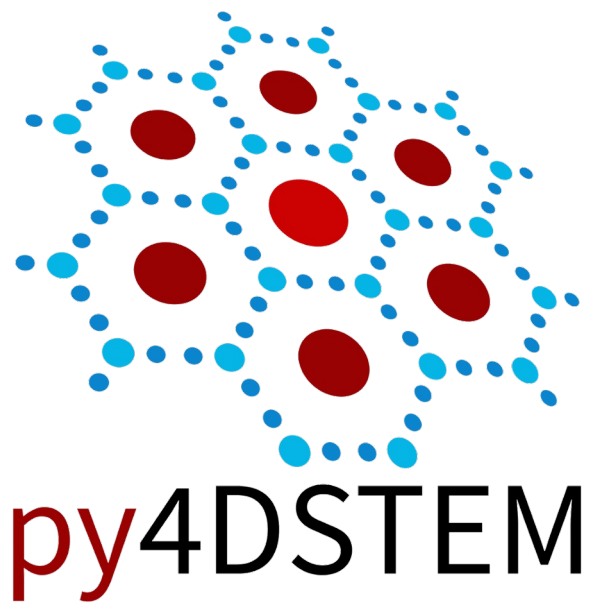
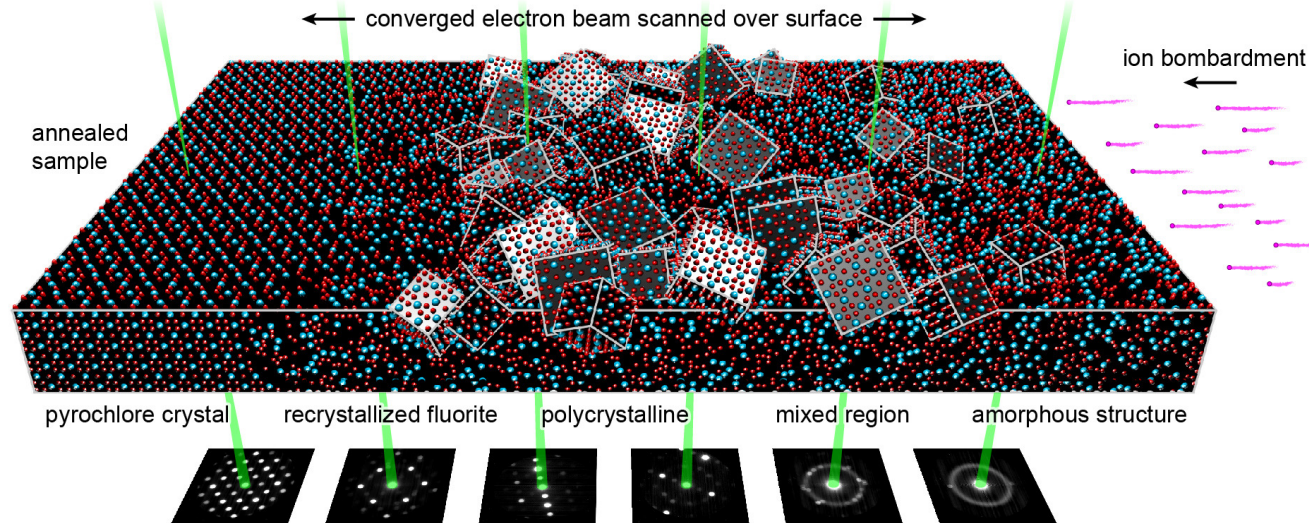
recrystallized fluorite

mixed

polycrystalline fluorite

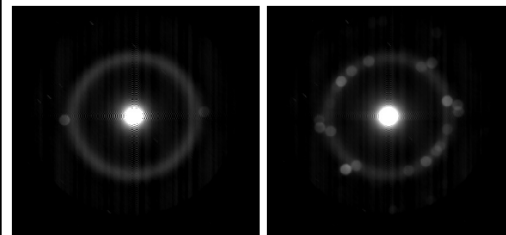
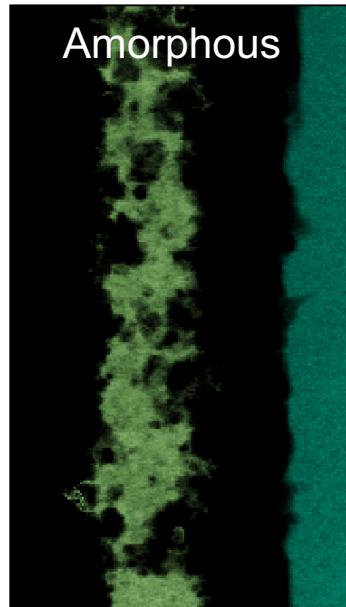
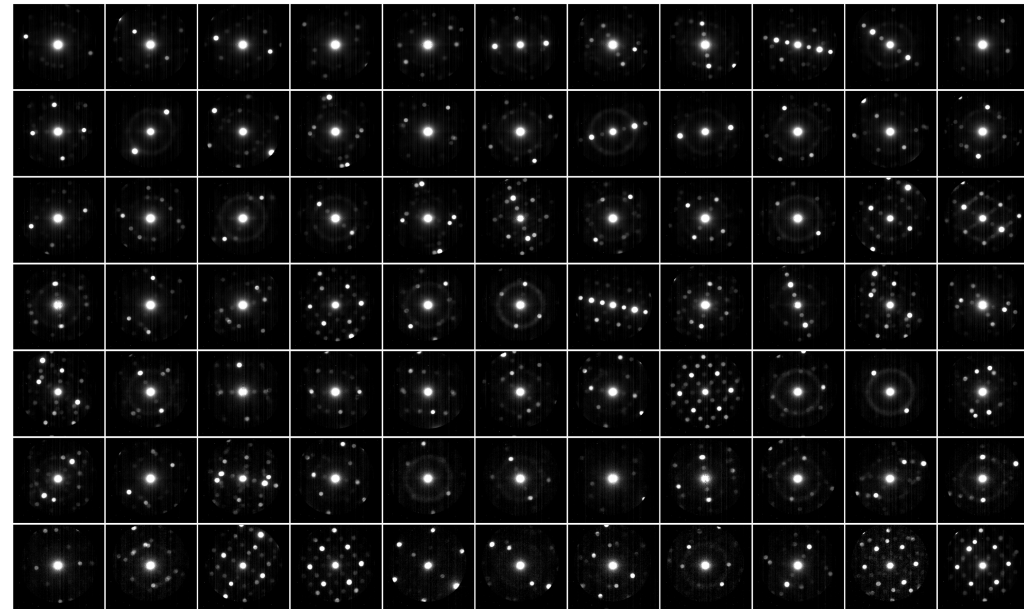
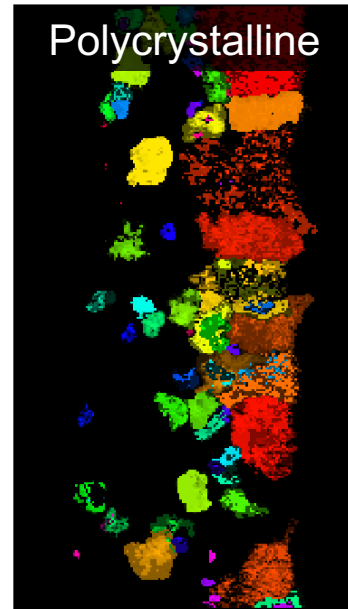
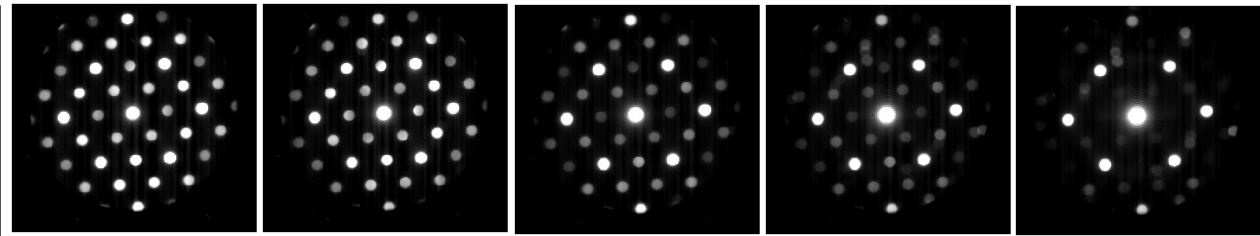
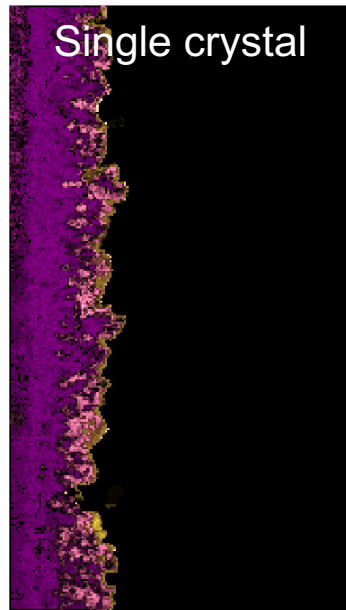
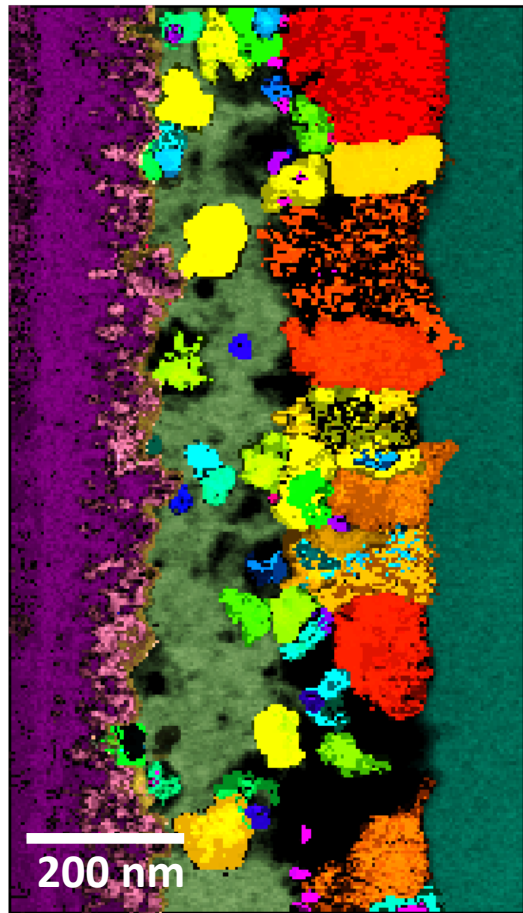
mixed

4D-STEM



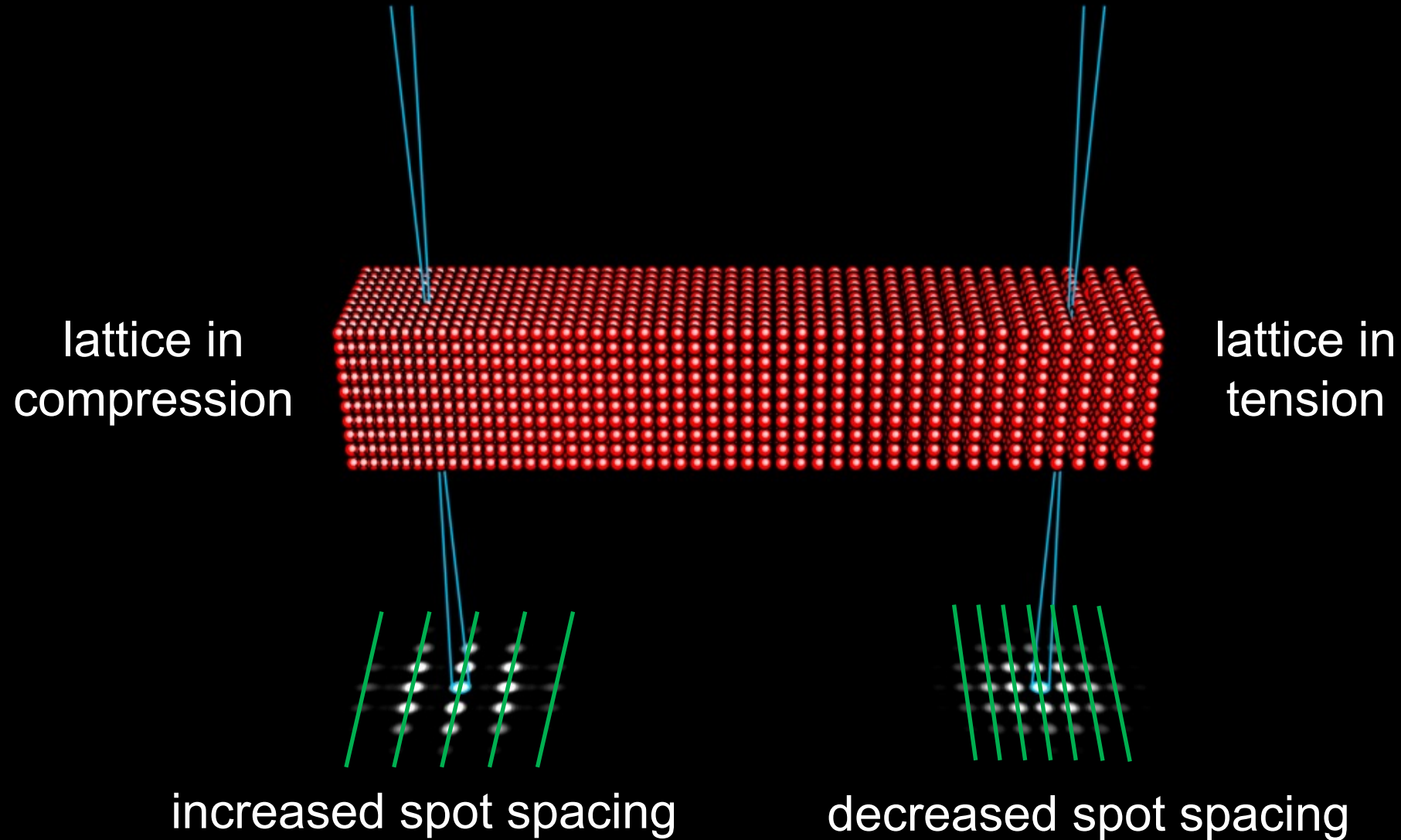
4D-STEM – Classification and Segmentation

Unsupervised
classification of the
GTO sample:



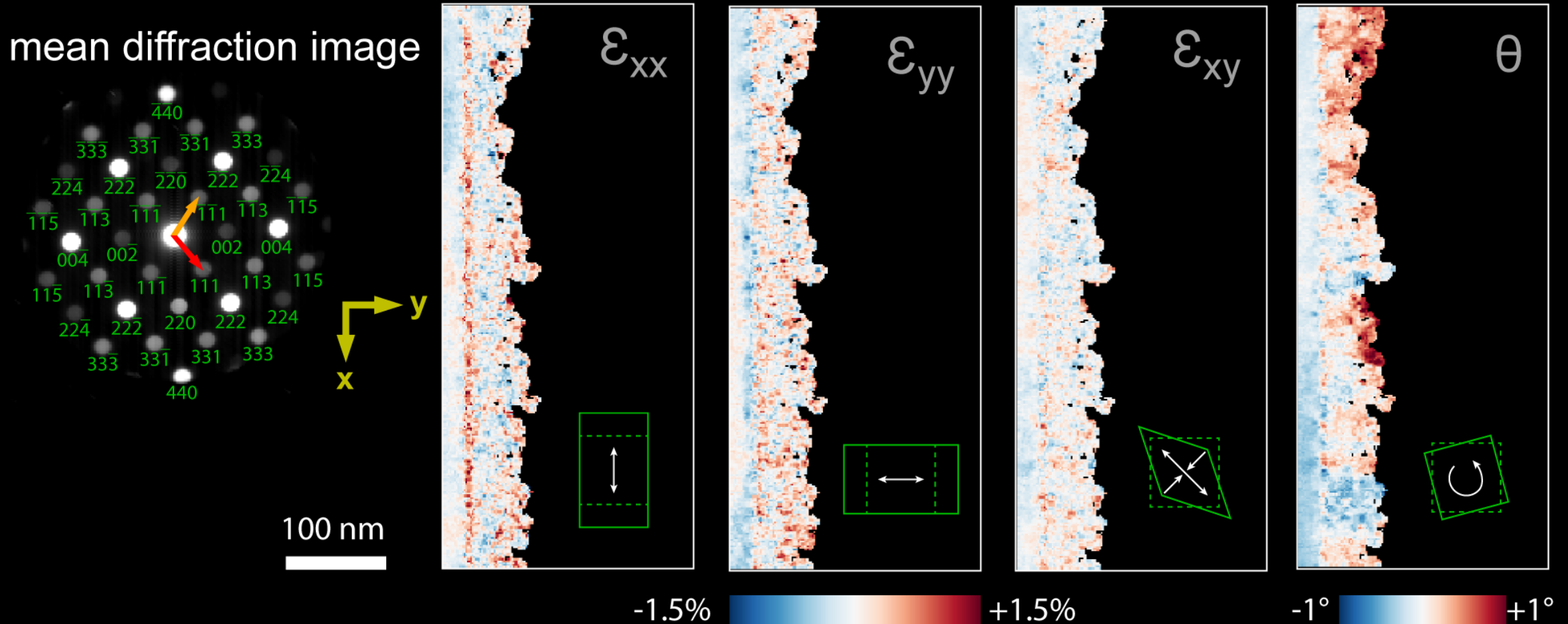
General classification is performed by using **NNMF** on **feature vectors**, constructed from Bragg vector maps, amorphous signals, virtual images, etc.

4D-STEM – Crystalline Strain Mapping



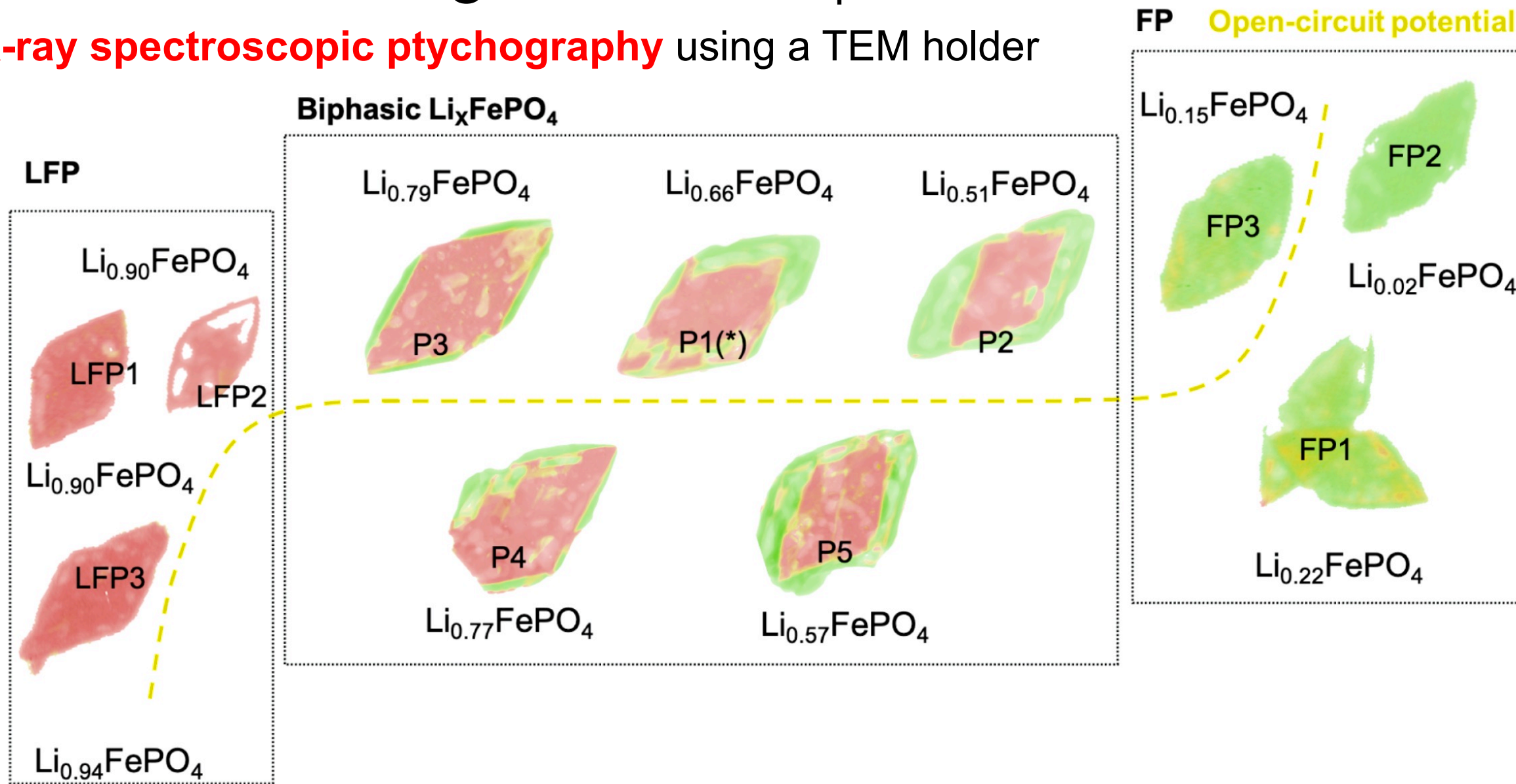
4D-STEM – Crystalline Strain Mapping

Strain measured in single-crystal GTO pyrochlore / recrystallized fluorite



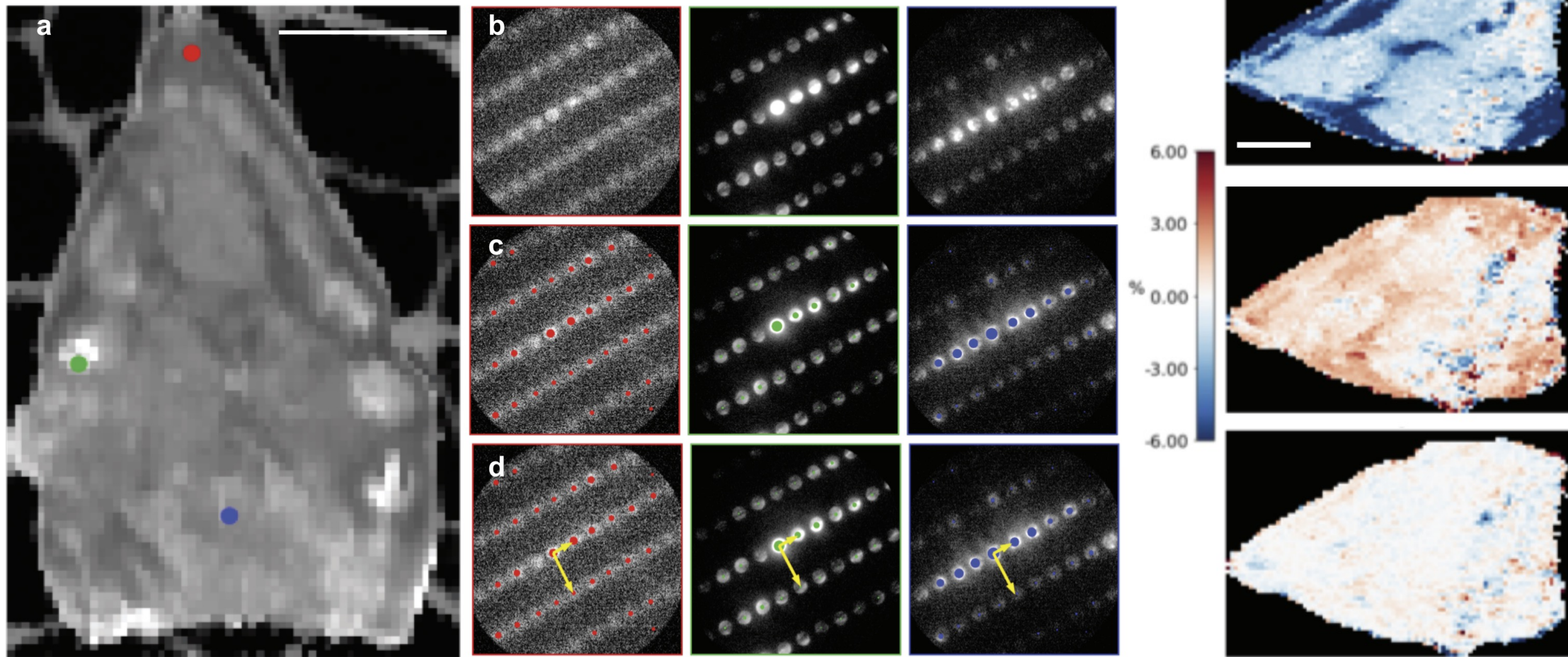
Inverse Learning of LiFePO₄ Chemo-Mechanics

X-ray spectroscopic ptychography using a TEM holder



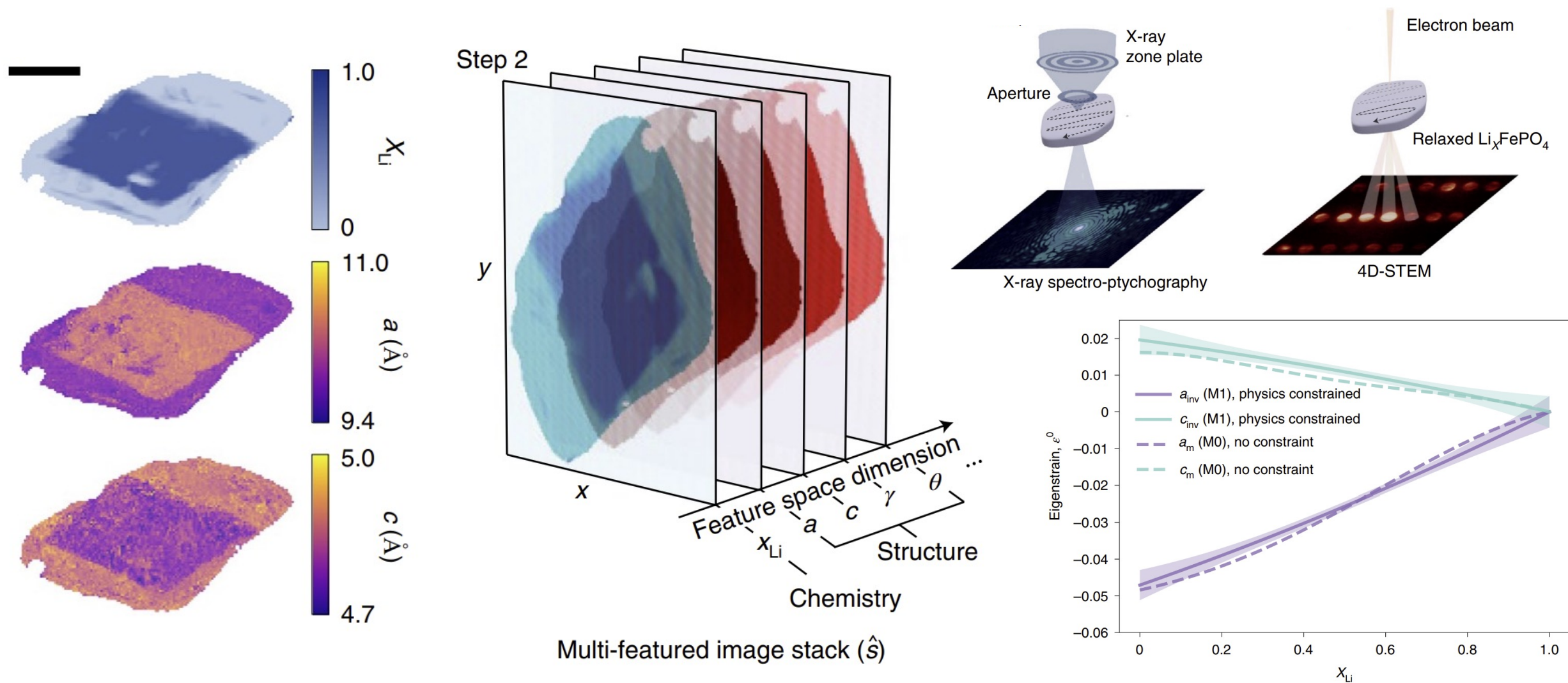
Inverse Learning of LiFePO_4 Chemo-Mechanics

4D-STEM strain mapping of the same particles from x-ray study.

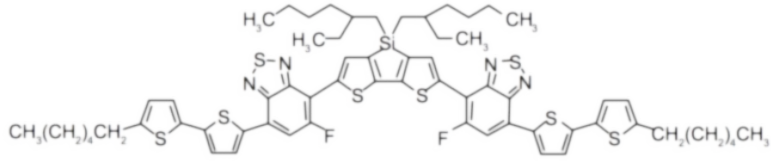


Inverse Learning of LiFePO₄ Chemo-Mechanics

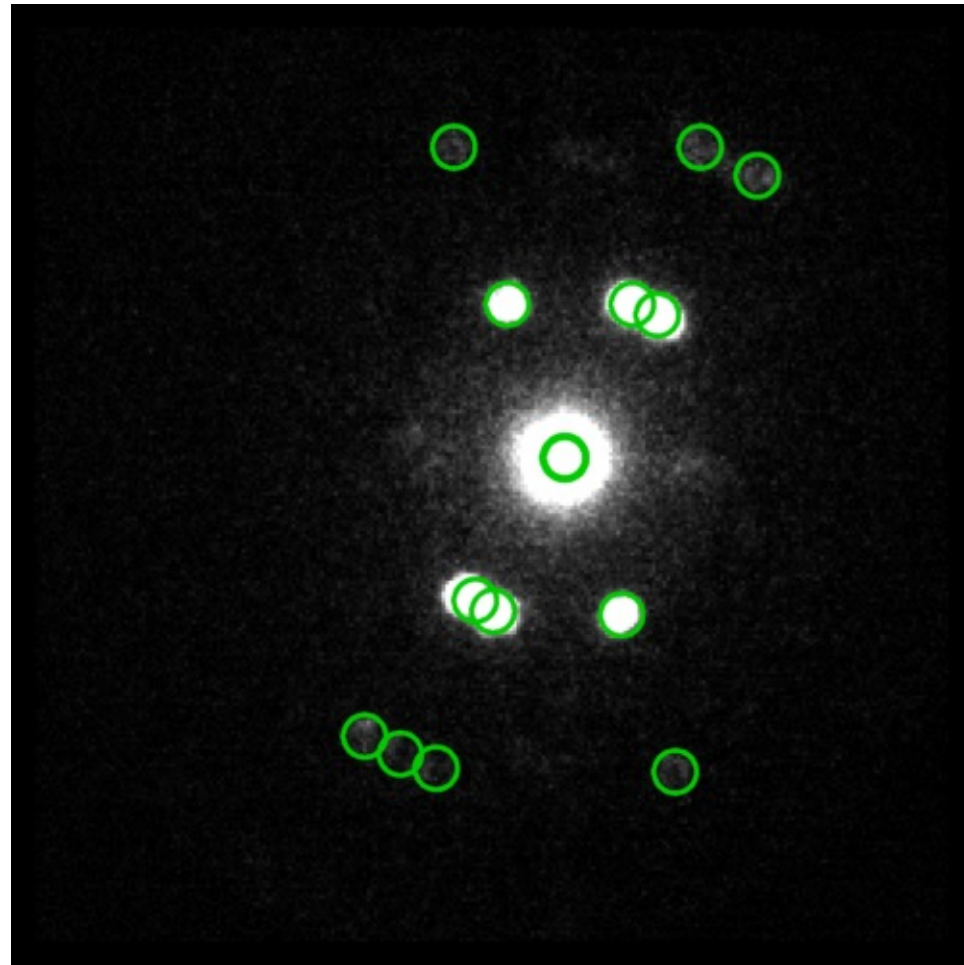
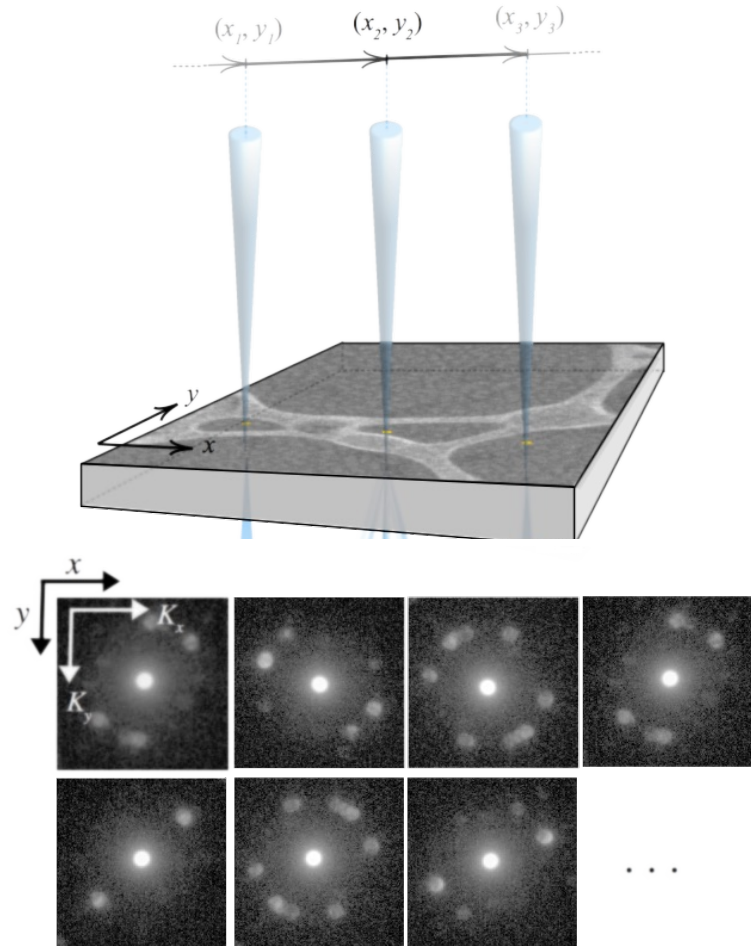
Alignment and correlation of all channels → **inverse learning of constitutive law**



4D-STEM – Orientation Mapping of Soft Matter



Bragg peaks detected in each diffraction pattern:



- Image template from vacuum reference probe or synthetic disk.
- Use template matching / image correlation to identify peaks.
- Record data, move onto next image.

4D-STEM – Orientation Mapping of Soft Matter

Visualization of the two morphologies:

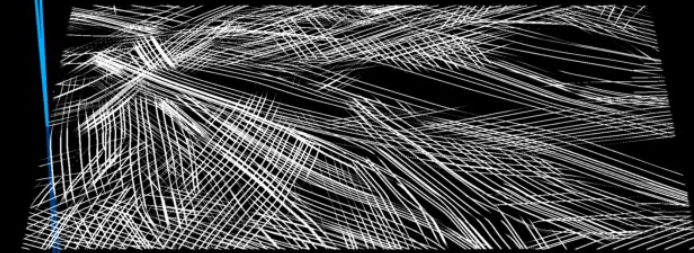
No additive to T1:

Single orientation through thickness,
large continuously-turning domains.

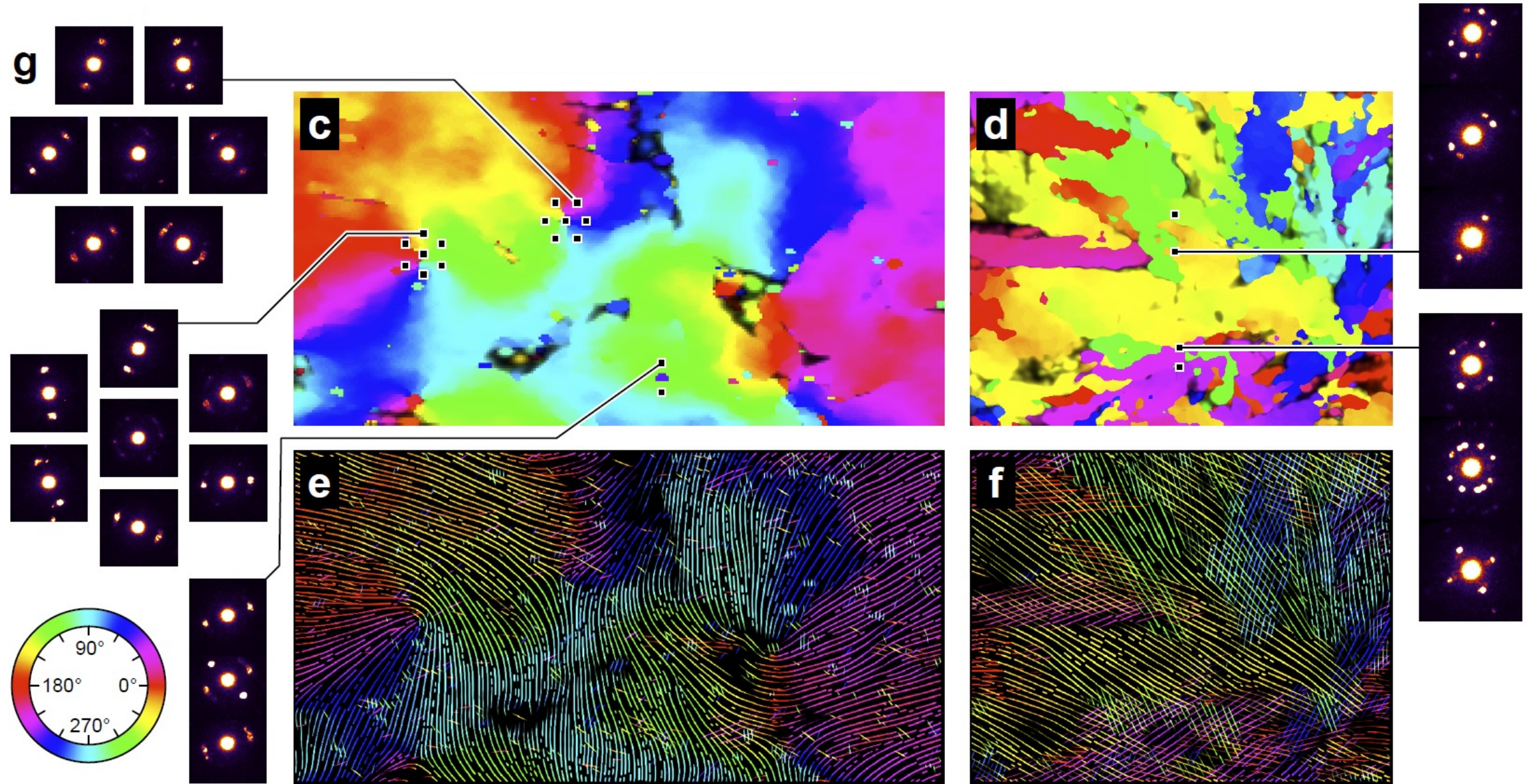


DIO additive to T1:

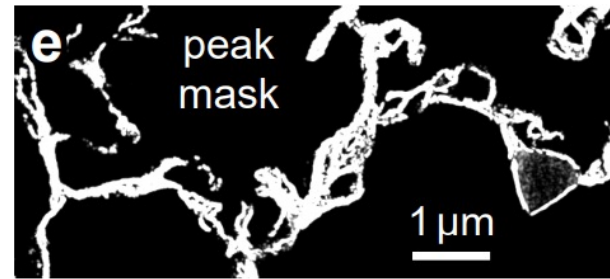
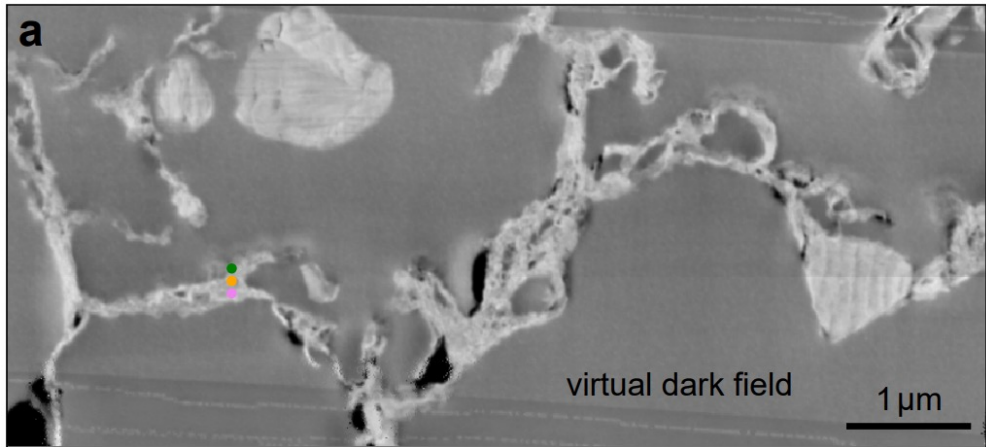
Multiple orientations through thickness,
small single-orientation domains.



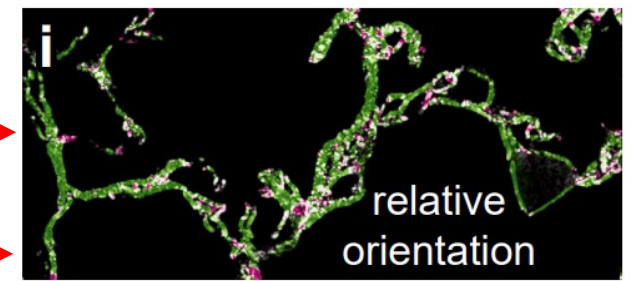
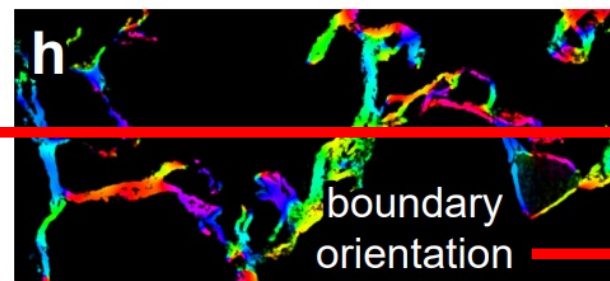
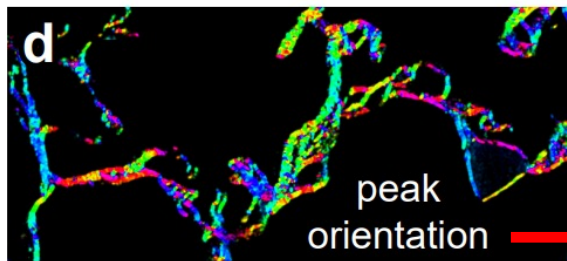
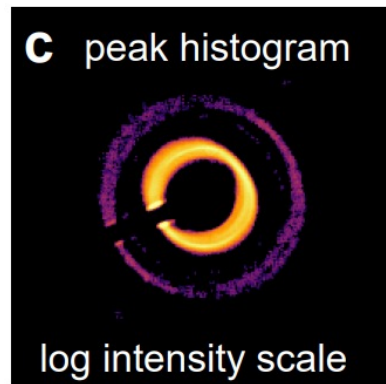
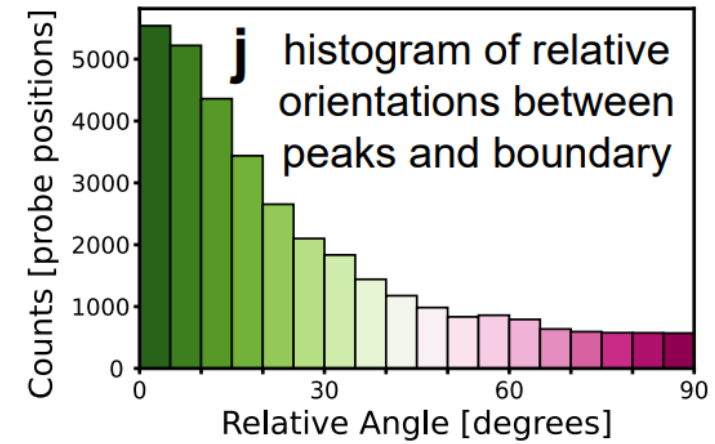
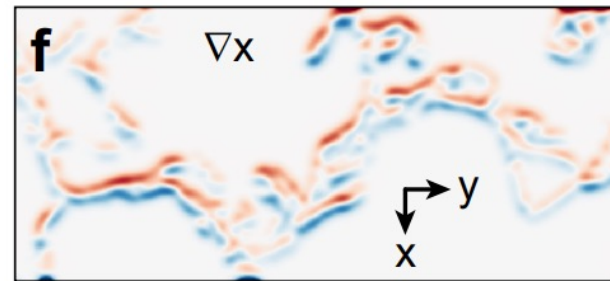
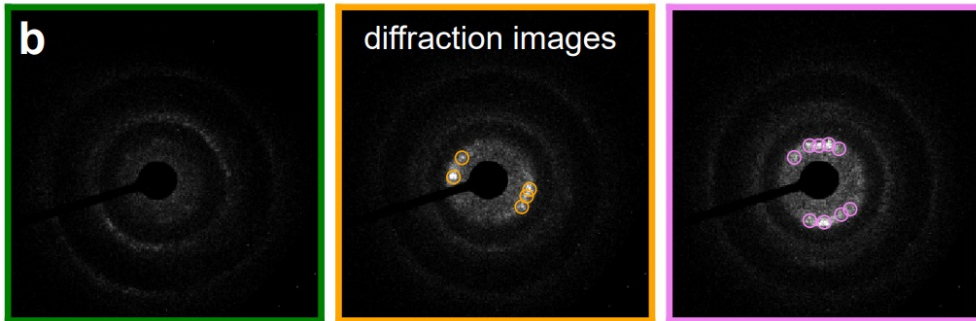
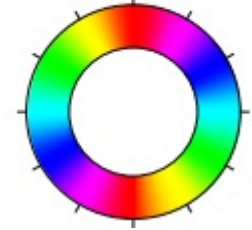
4D-STEM – Orientation Mapping of Soft Matter



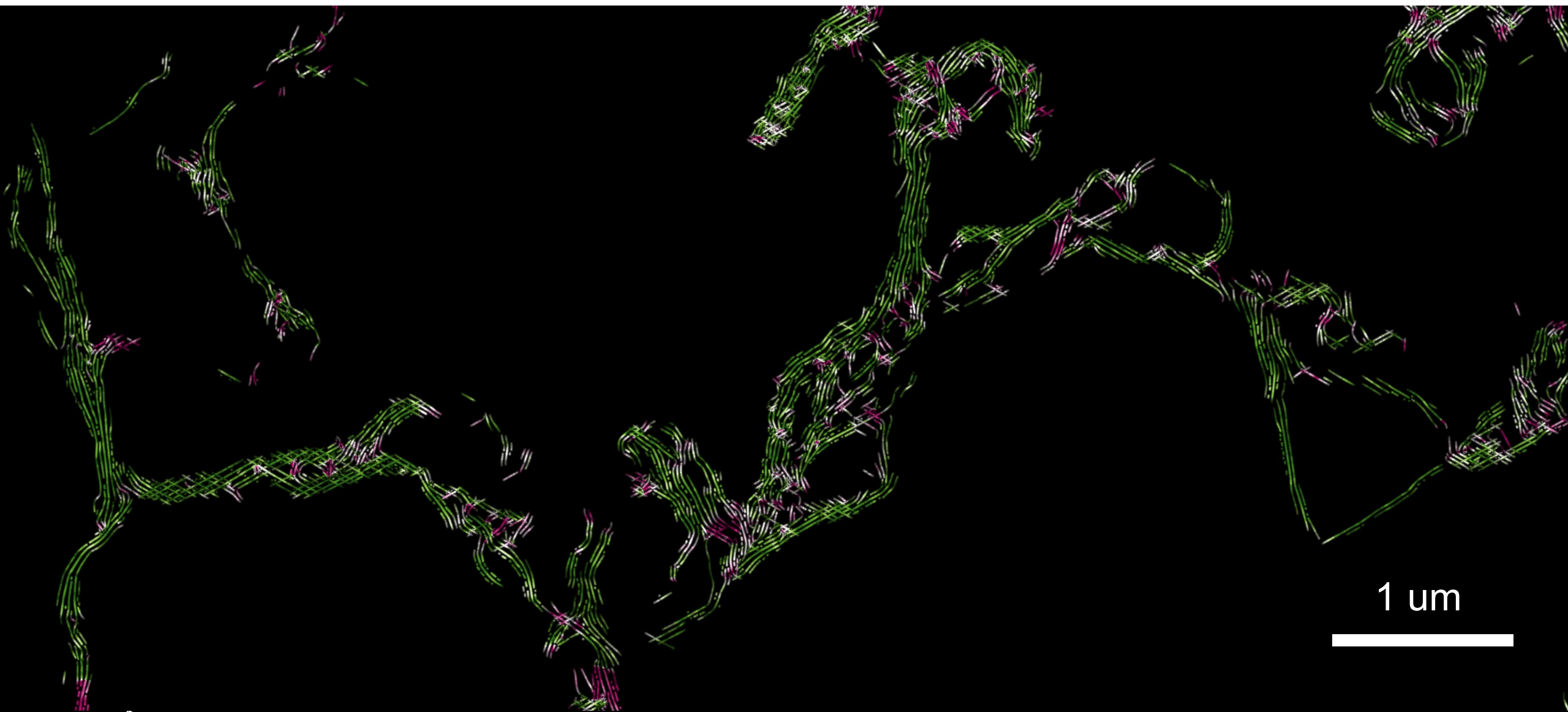
Carbon Basal Plane Orientations, Color Relative to Pores



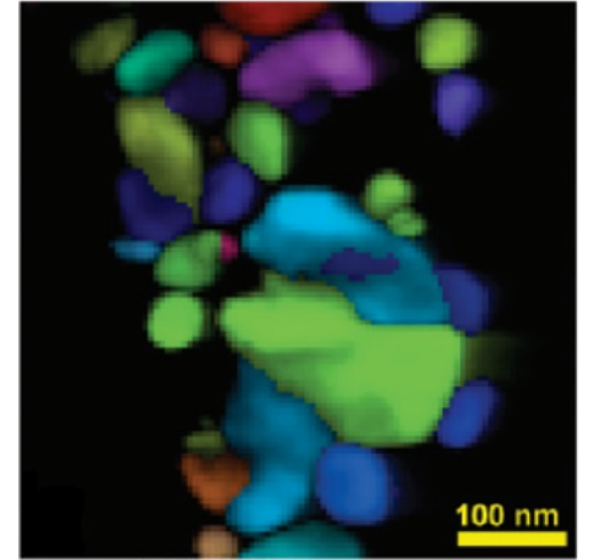
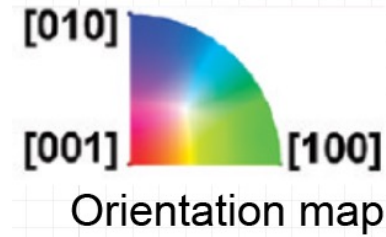
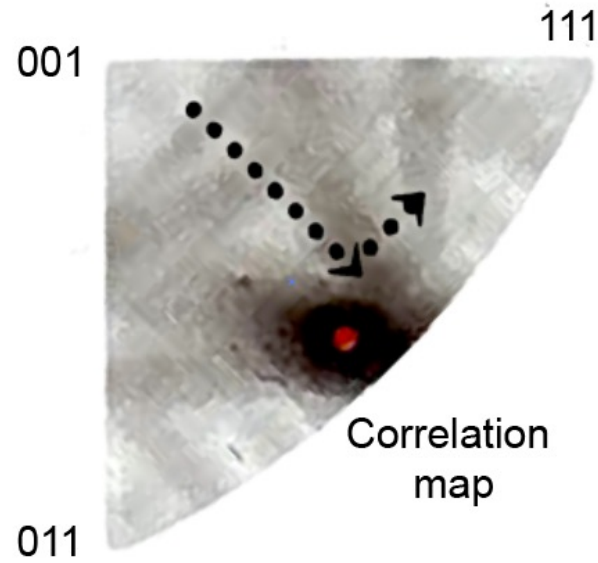
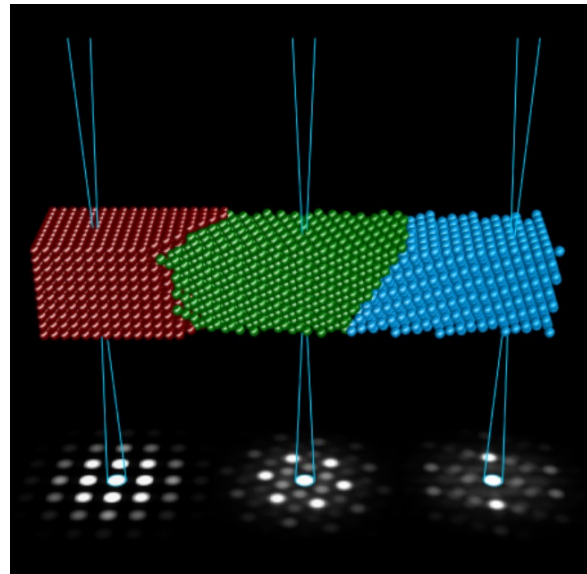
orientation



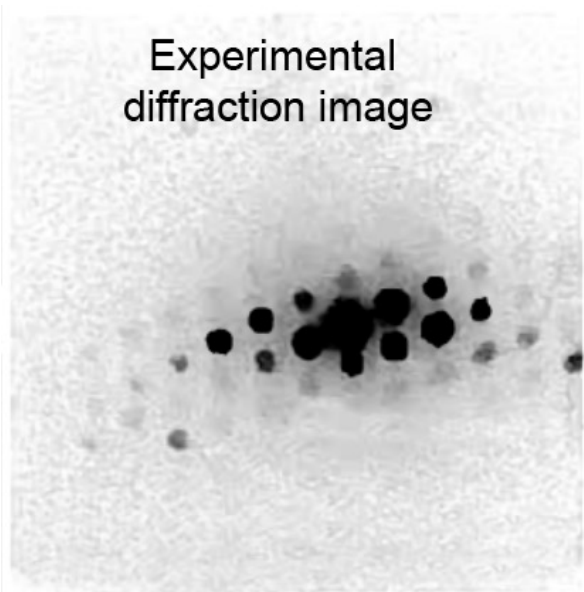
Carbon Basal Plane Orientations, Color Relative to Pores



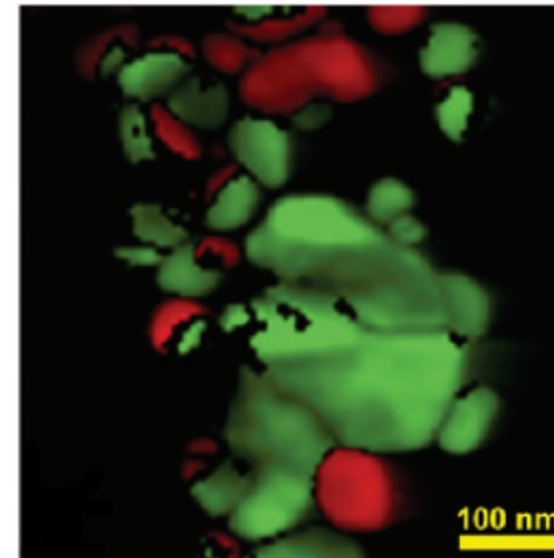
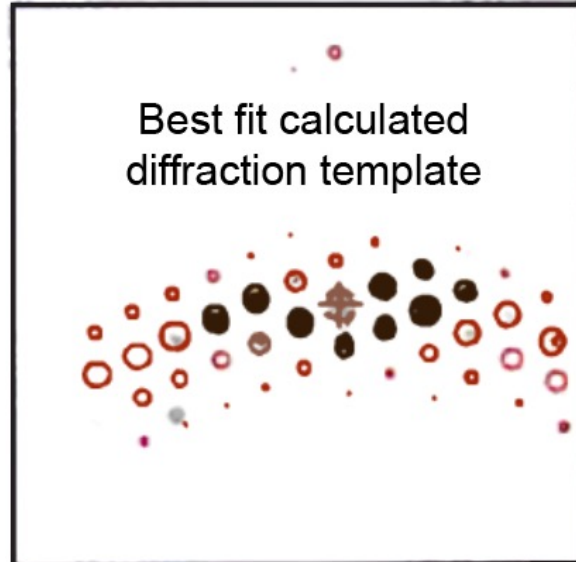
Orientation / Phase from a Diffraction Pattern Library



Experimental diffraction image



Best fit calculated diffraction template

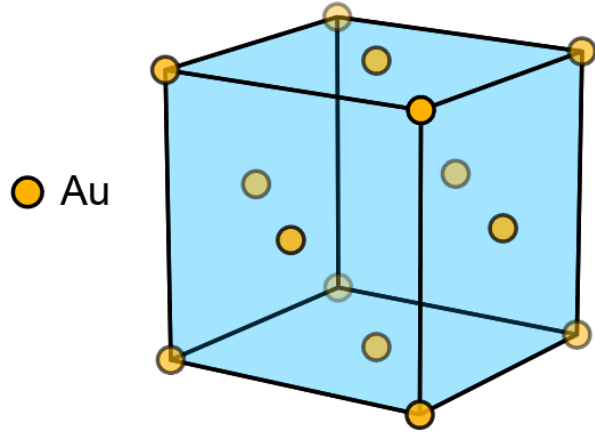


Phase map

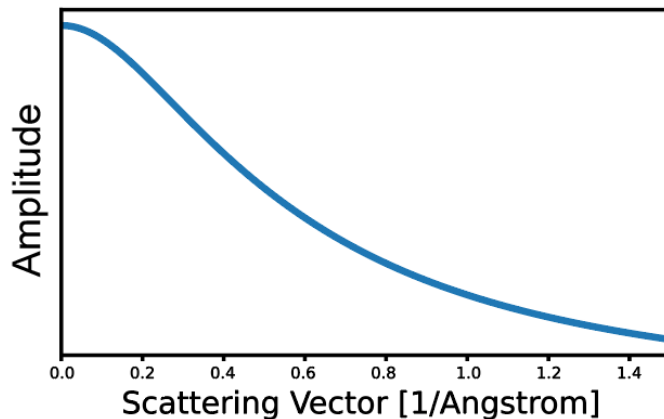
- LiFePO₄
- FePO₄

Kinematical / Dynamical Diffraction Patterns

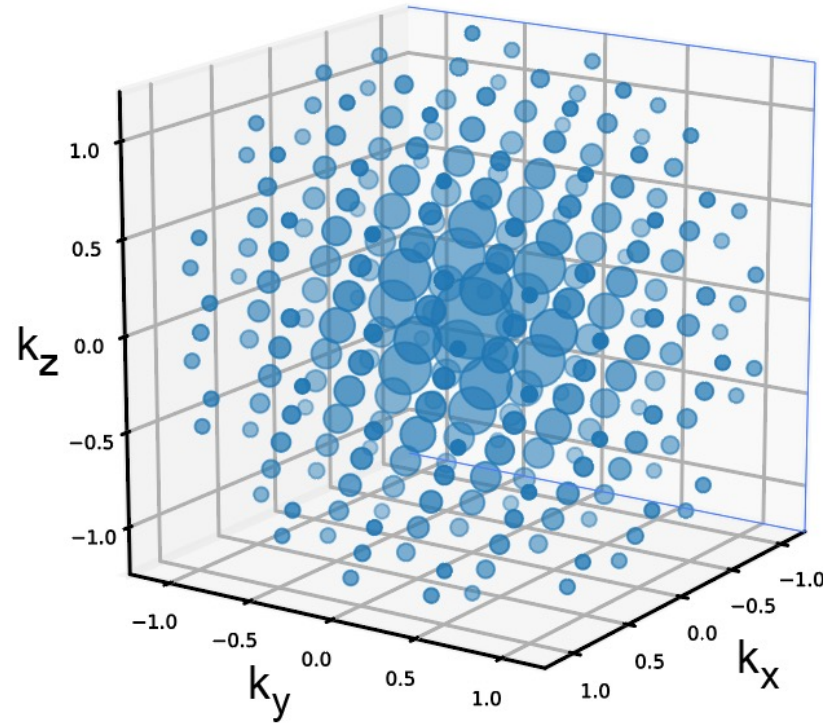
Unit Cell Structure



Single Atom Scattering

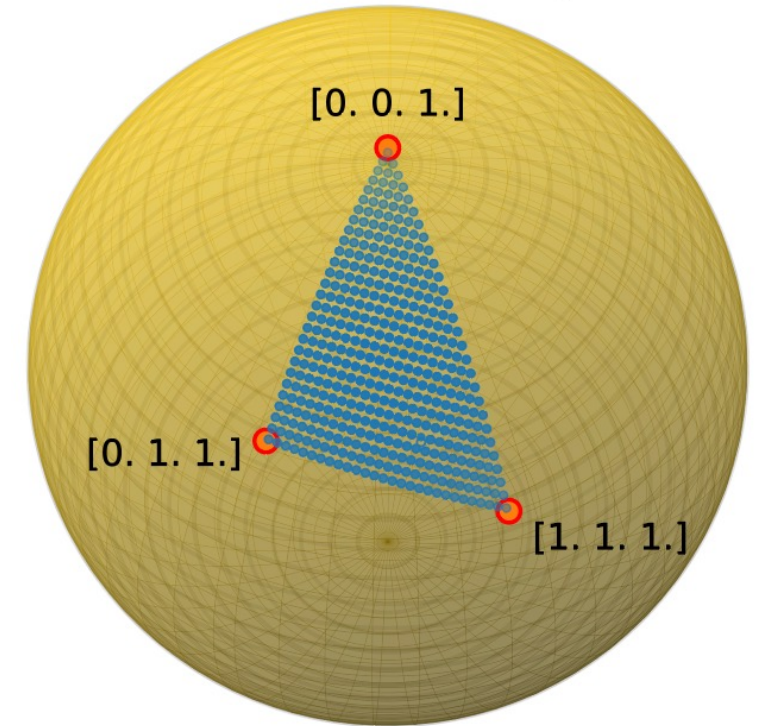


Structure Factors



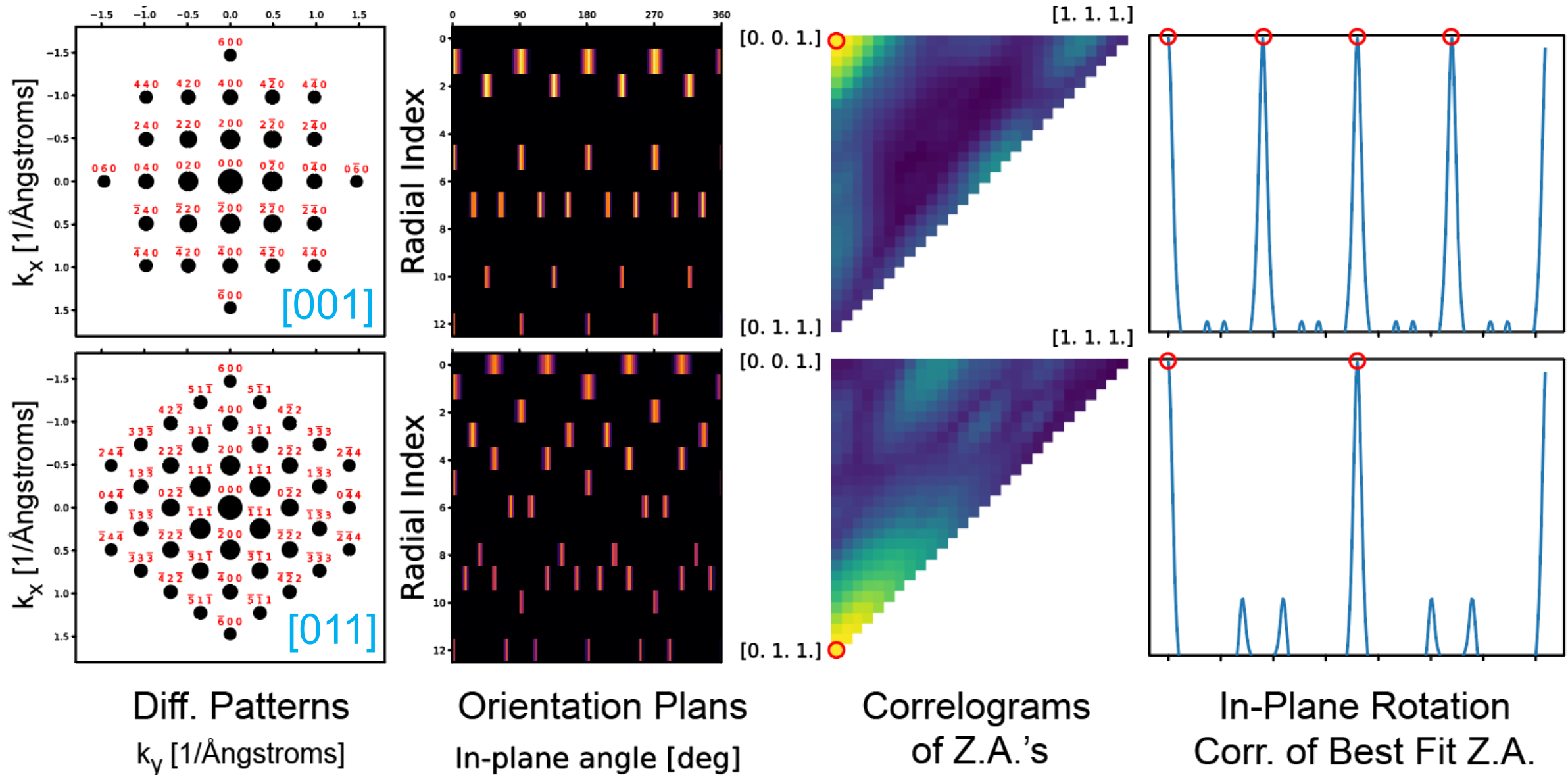
$$F_{hkl} = \sum_{n=1}^N f_n(\|\mathbf{q}\|) \exp[-2\pi i(h, k, l) \cdot \mathbf{p}_n]$$

Zone Axis Range

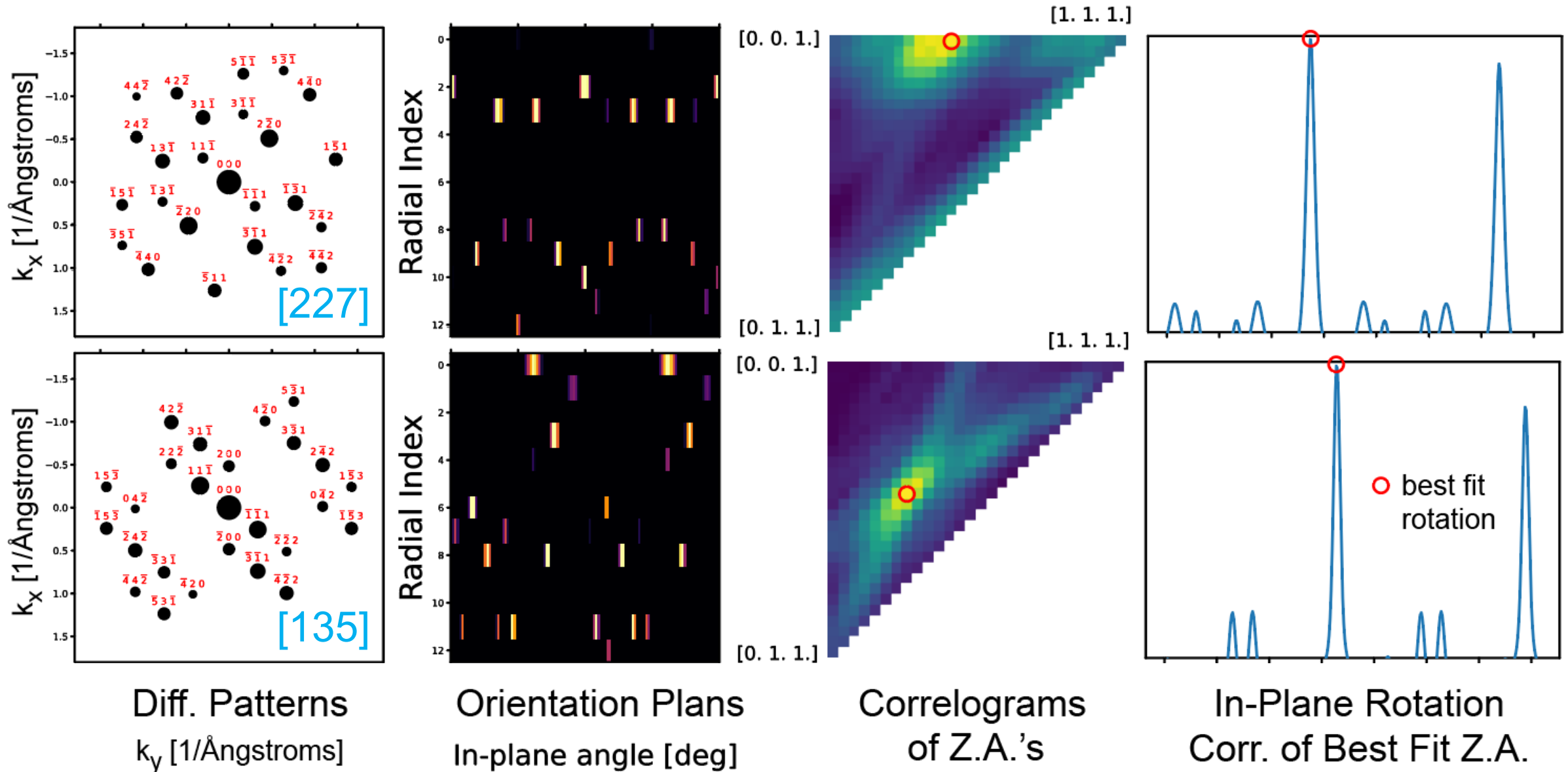


$$\text{Slerp}(p_0, p_1; t) = \frac{\sin[(1-t)\Omega]}{\sin \Omega} p_0 + \frac{\sin[t\Omega]}{\sin \Omega} p_1$$

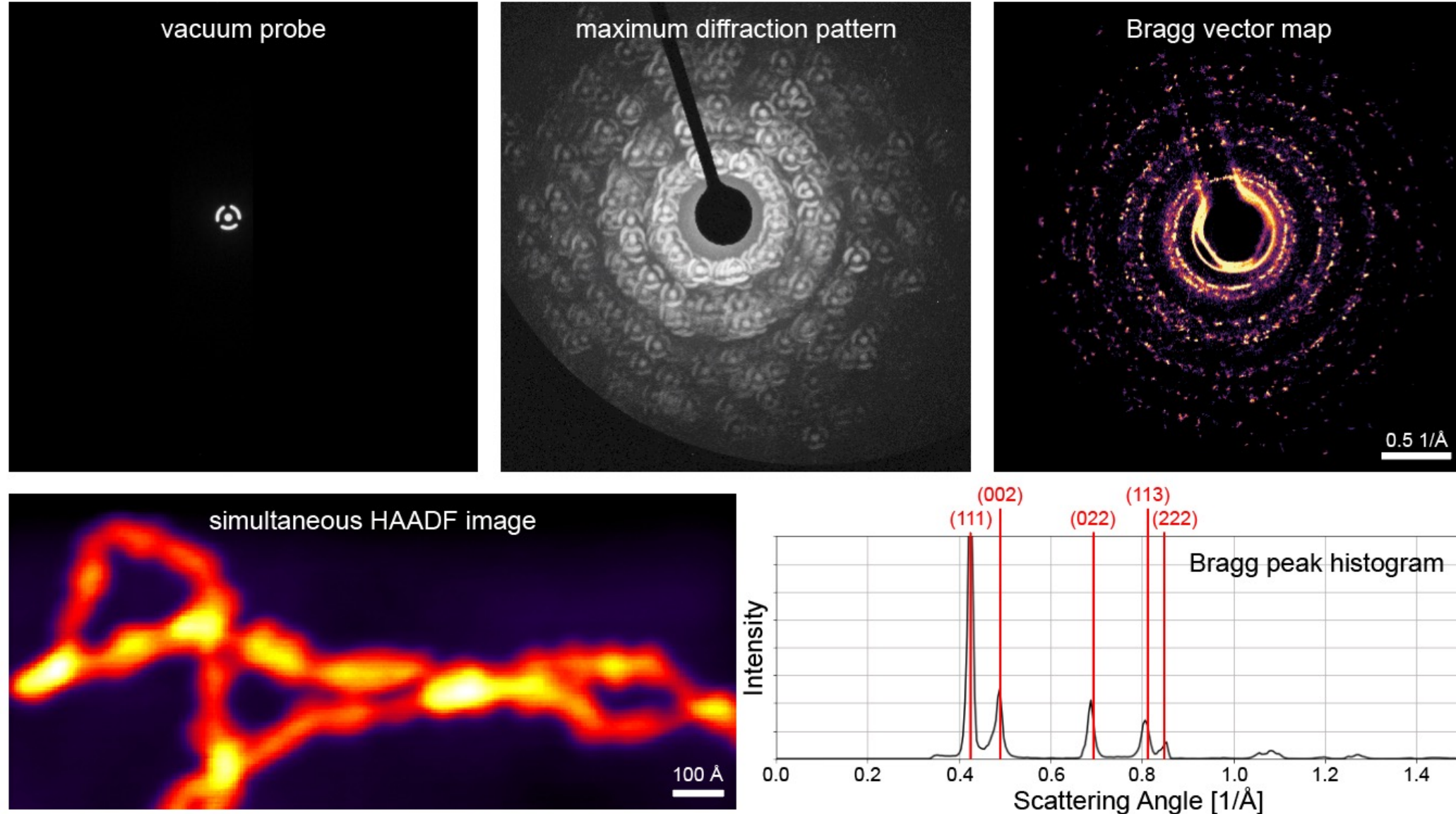
Orientation Mapping via Sparse Correlation



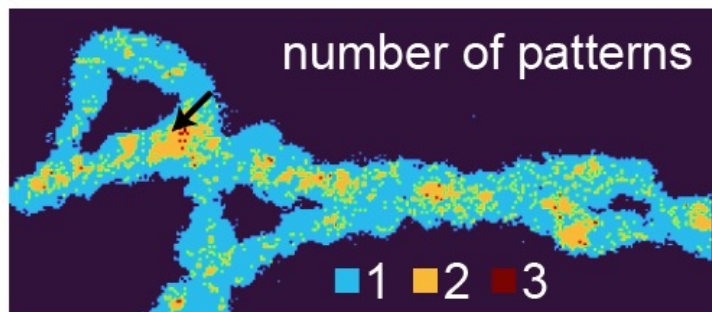
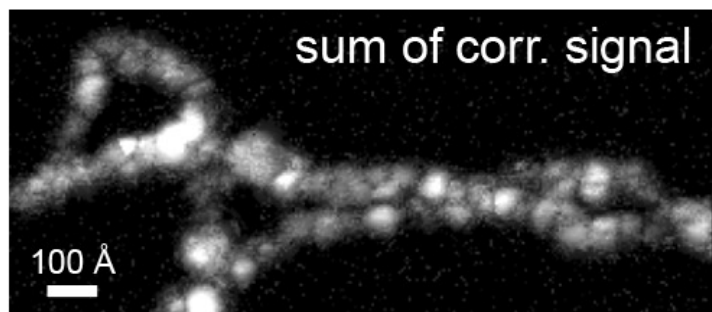
Orientation Mapping via Sparse Correlation



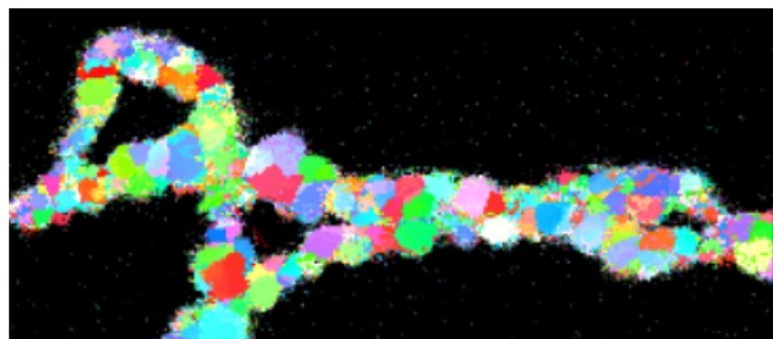
4D-STEM of Twisted AuAgPd Nanowires



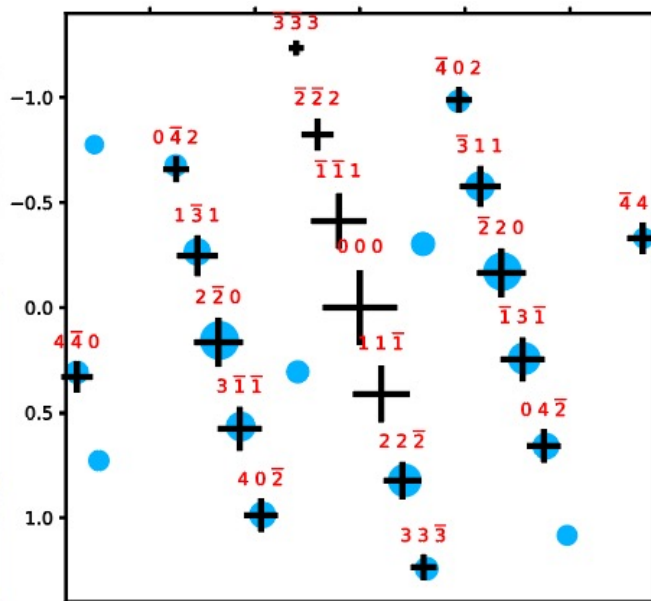
Orientation Mapping of AuAgPd Nanowires



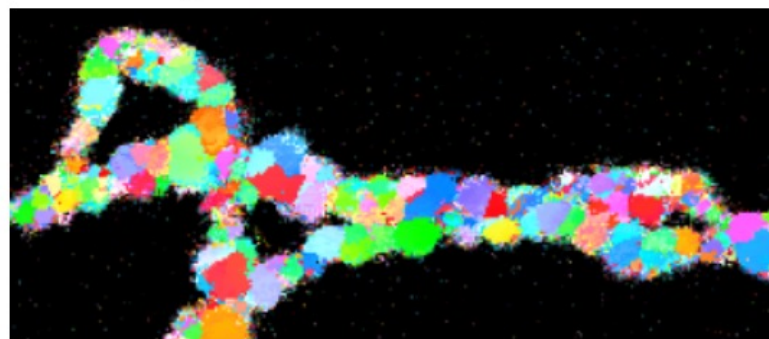
x-axis Orientation



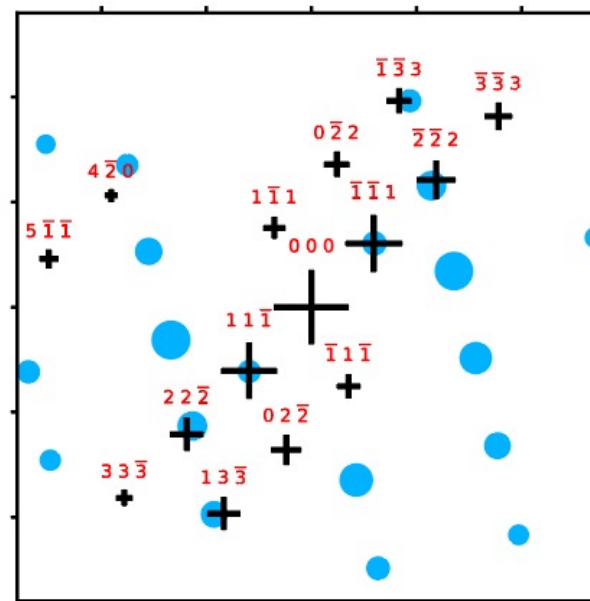
First Match



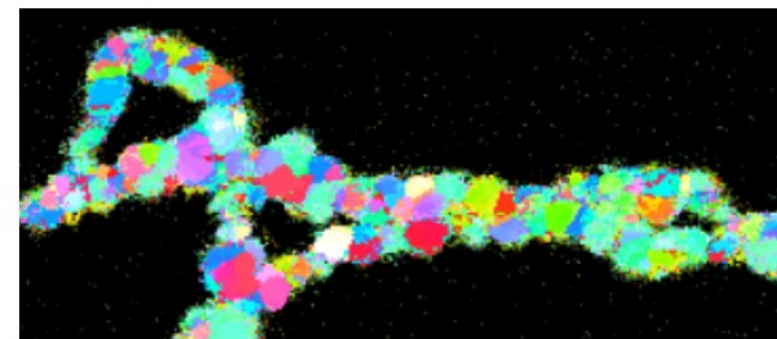
y-axis Orientation



Second Match

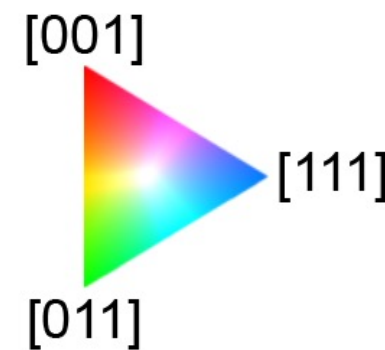


Zone Axis (z-axis Orientation)



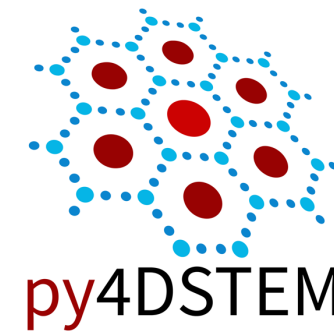
● experiment

hkl
+ simulation



py4DSTEM Tutorials

Tutorial repository – https://github.com/py4dstem/py4DSTEM_tutorials

A screenshot of the GitHub repository page for py4dstem/py4DSTEM_tutorials. The page shows the repository name, navigation tabs for Code, Issues, Pull requests, Actions, Projects, Wiki, Security, Insights, and Settings. Below the navigation, there are buttons for "main" (selected), "3 branches", and "0 tags". On the right, there are buttons for "Go to file", "Add file", and "Code". The main content area shows a commit history table with columns for the commit author, description, commit hash, date, and number of commits.

Author	Description	Commit Hash	Date	Commits
alex-rakowski	updating index notebook path	d7b0d1e	yesterday	63
	binder		5 days ago	
	data		10 days ago	
	images		11 days ago	
	notebooks		yesterday	
	strain_crystalline		5 days ago	

Crystalline Orientation Mapping in py4DSTEM

The screenshot shows a JupyterLab environment. On the left is a file browser with a search bar and a list of files and folders. The current directory is `/python/2022_tutorials/`. The file `05_AuAgPd_wire_disks...` is selected. On the right is a notebook titled "ACOM of AuAgPd nanowires - disk detection". The notebook content includes a title, a paragraph about disk detection, a goal statement, a link to a tutorial, a "Data" section with two links, and an "Acknowledgements" section with a list of names and email addresses.

File browser contents:

Name	Last Modified
archive	4 months ago
Ben_Steve_Jenn_lectures	4 months ago
Germany	6 hours ago
snapshot02	3 days ago
snapshot03	6 hours ago
00_jupyter_notebooks....	3 days ago
01_py4DSTEM_basics.i...	a day ago
02_DPC_nanotube.ipynb	a day ago
03_Si_SiGe_disks_strain...	a day ago
04_kinematical_diffra...	34 minutes ago
05_AuAgPd_wire_disks...	34 minutes ago
py4DSTEM_polycrystal...	32 minutes ago

ACOM of AuAgPd nanowires - disk detection

This notebook performs disk detection for the AuAgPd nanowire 4D-STEM bullseye experiment. The data has been downsampled for the purposes of the tutorial.

Our goal is to perform automated crystal orientation mapping (ACOM), as described in: [Automated Crystal Orientation Mapping in py4DSTEM using Sparse Correlation Matching](#)

Data

[small_AuAgPd_wire_dataset_04.h5](#) (2.0 GB)

[downsampled_AuAgPd_wire_probe.h5](#)

Acknowledgements

This tutorial was created by the py4DSTEM instructor team:

- Alex Rakowski (arakowski@lbl.gov)
- Stephanie Ribet (sribet@u.northwestern.edu)
- Ben Savitzky (bhsavitzky@lbl.gov)

Crystalline Orientation Mapping in py4DSTEM

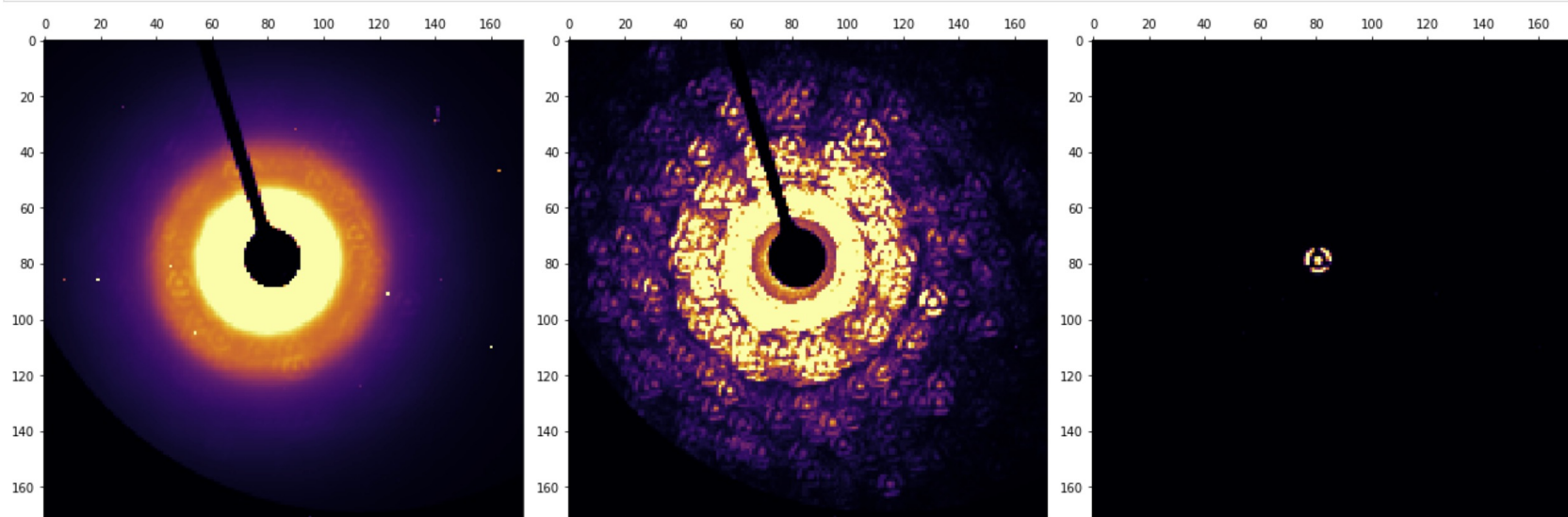
File Edit View Run Kernel Tabs Settings Help

Filter files by name

/ ... / python / 2022_tutorials /

Name	Last Modified
archive	4 months ago
Ben_Steve_Jenn_lectures	4 months ago
Germany	6 hours ago
snapshot02	3 days ago
snapshot03	6 hours ago
00_jupyter_notebooks....	3 days ago
01_py4DSTEM_basics.i...	a day ago
02_DPC_nanotube.ipynb	a day ago
03_Si_SiGe_disks_strain...	a day ago
04_kinematical_diffract...	36 minutes ago
05_AuAgPd_wire_disks...	36 minutes ago
py4DSTEM_polycrystal...	35 minutes ago

```
[7]: py4DSTEM.visualize.show_image_grid(  
      lambda i:[  
        # dataset.tree['dp_mean'],  
        dataset.tree['dp_mean'].data * 10,  
        dataset.tree['dp_max'],  
        dataset_probe.tree['dp_mean'],  
      ][i],  
      H=1,  
      W=3,  
      cmap='inferno',  
      clipvals='manual',  
      vmin=0,  
      vmax=1500,  
    )
```



Crystalline Orientation Mapping in py4DSTEM

File Edit View Run Kernel Tabs Settings Help

Filter files by name

/ ... / python / 2022_tutorials /

Name	Last Modified
archive	4 months ago
Ben_Steve_Jenn_lectures	4 months ago
Germany	6 hours ago
snapshot02	3 days ago
snapshot03	6 hours ago
00_jupyter_notebooks...	3 days ago
01_py4DSTEM_basics.i...	a day ago
02_DPC_nanotube.ipynb	a day ago
03_Si_SiGe_disks_strain...	a day ago
04_kinematical_diffra...	38 minutes ago
05_AuAgPd_wire_disks...	38 minutes ago
py4DSTEM_polycrystal...	37 minutes ago

```
[12]: # Construct a probe template to use as a kernel for correlation disk detection

probe_kernel = py4DSTEM.process.probe.get_probe_kernel_edge_sigmoid(
    probe_align,
    (probe_semiangle * 0.0, probe_semiangle * 3.0),
    #   bilinear=True,
)

# Plot the probe kernel
py4DSTEM.visualize.show_kernel(
    probe_kernel,
    R=20,
    L=20,
    W=1)
```

0 5 10 15 20 25 30 35

0 5 10 15 20 25 30 35

0.030
0.025
0.020
0.015
0.010
0.005
0.000
-0.005

Crystalline Orientation Mapping in py4DSTEM

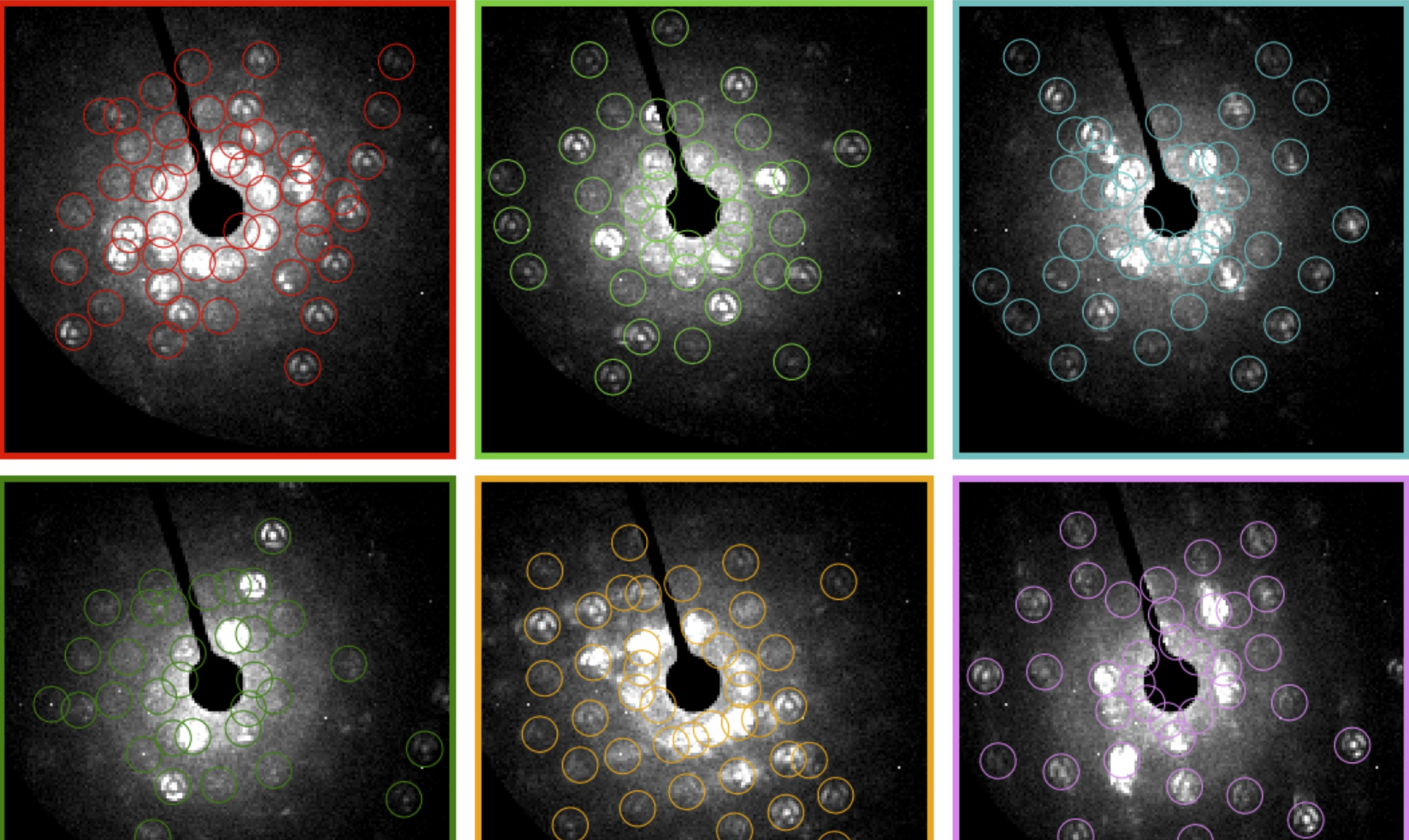
File Edit View Run Kernel Tabs Settings Help

Filter files by name

/ ... / python / 2022_tutorials /

Name	Last Modified
archive	4 months ago
Ben_Steve_Jenn_lectures	4 months ago
Germany	6 hours ago
snapshot02	3 days ago
snapshot03	6 hours ago
00_jupyter_notebooks...	3 days ago
01_py4DSTEM_basics.i...	a day ago
02_DPC_nanotube.ipynb	a day ago
03_Si_SiGe_disks_strain...	a day ago
04_kinematical_diffract...	40 minutes ago
05_AuAgPd_wire_disks...	40 minutes ago
py4DSTEM_polycrystal...	38 minutes ago

Code Python 3 (ipykernel)



Crystalline Orientation Mapping in py4DSTEM

File Edit View Run Kernel Tabs Settings Help

strains_c × 00_jupyter × 01_py4I × 02_DPC × orientat × 04_kine × 05_AuA × py4DST × ACOM / × paper_fi × polycrys ×

Code Python 3 (ipykernel)

```
Best fit lattice directions: z axis = ([0.301 0.486 0.82 ]), x axis = ([0.558 0.566 0.607]), with corr value = 5.397
Best fit lattice directions: z axis = ([0.159 0.564 0.81 ]), x axis = ([0.107 0.12 0.987]), with corr value = 3.951
Best fit lattice directions: z axis = ([0.492 0.61 0.621]), x axis = ([0.405 0.471 0.783]), with corr value = 3.375
```

q_x [\AA^{-1}]

q_y [\AA^{-1}]

Name	Last Modified
archive	4 months ago
Ben_Steve_Jenn_lectures	4 months ago
Germany	6 hours ago
snapshot02	3 days ago
snapshot03	6 hours ago
00_jupyter_notebooks...	3 days ago
01_py4DSTEM_basics.i...	a day ago
02_DPC_nanotube.ipynb	a day ago
03_Si_SiGe_disks_strain...	a day ago
04_kinematical_diffract...	42 minutes ago
05_AuAgPd_wire_disks...	42 minutes ago
py4DSTEM_polycrystal...	40 minutes ago

Crystalline Orientation Mapping in py4DSTEM

File Edit View Run Kernel Tabs Settings Help

Filter files by name


/ ... / python / 2022_tutorials /

Name	Last Modified
archive	4 months ago
Ben_Steve_Jenn_lectures	4 months ago
Germany	6 hours ago
snapshot02	3 days ago
snapshot03	6 hours ago
00_jupyter_notebooks...	3 days ago
01_py4DSTEM_basics.i...	a day ago
02_DPC_nanotube.ipynb	a day ago
03_Si_SiGe_disks_strain...	a day ago
04_kinematical_diffra...	43 minutes ago
05_AuAgPd_wire_disks...	43 minutes ago
py4DSTEM_polycrystal...	41 minutes ago

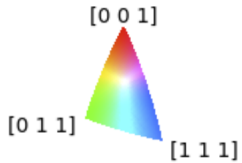
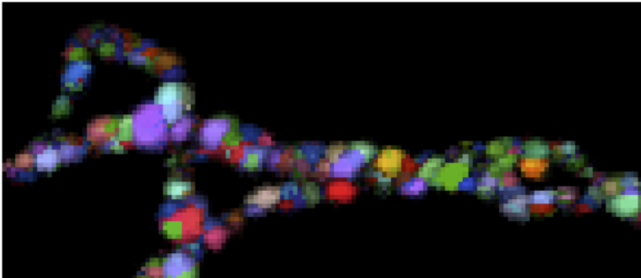
Plot the resulting orientation maps

```
[52]: # plot orientation map
images_orientation = crystal.plot_orientation_maps(
    orientation_map,
    corr_range = np.array([1,4]),
    camera_dist = 12,
    show_axes = False,
)
```

In-Plane Orientation



Out-of-Plane Orientation



```
[ ]:
[ ]:
[ ]:
```

Deploying py4DSTEM into the Materials Project

Home / Apps / Crystal Toolkit



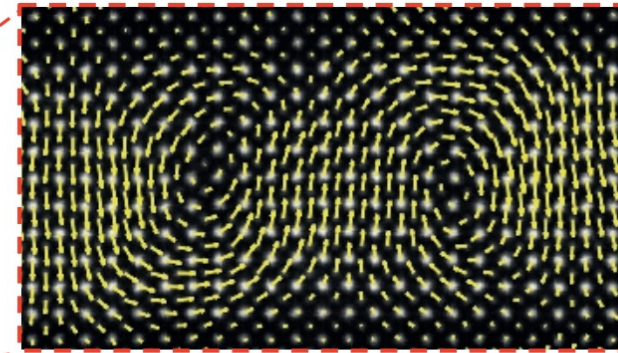
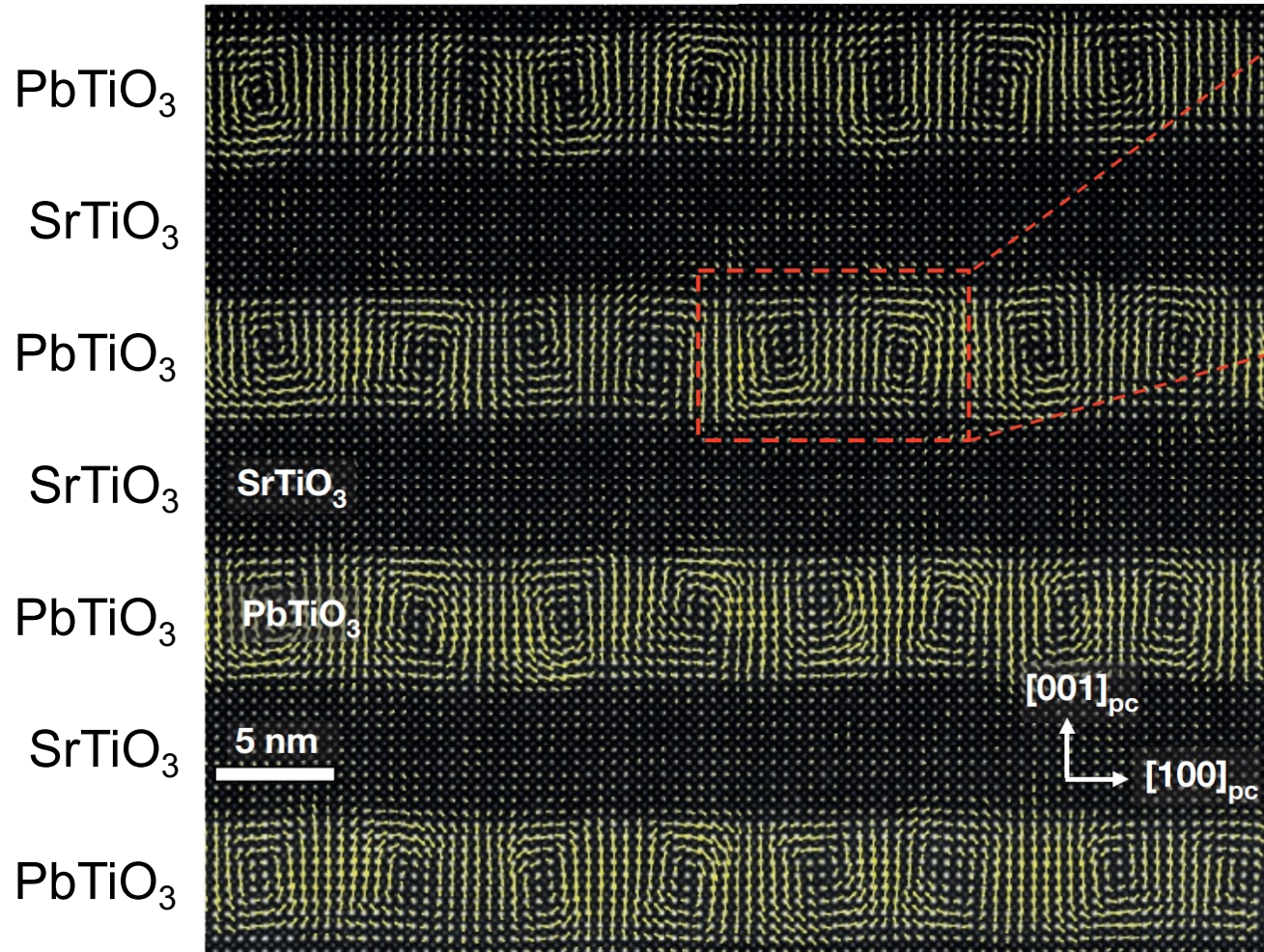
■ PR contribution accepted into crystal Toolkit repo, live “soon”

The screenshot displays the Crystal Toolkit web application interface. On the left, a 3D model of the Au crystal structure is shown as a yellow lattice of spheres. A vertical toolbar on the far left contains various icons for navigation and tool manipulation. In the center, the 'Au' section is active, showing search results for 'Au' from the Materials Project. The search results indicate 'Au (Fm $\bar{3}$ m) predicted stable phase'. Below this, there is a 'Load from your computer' section with an upload icon and the text 'Choose a file to upload or drag and drop'. On the right, a 2D Diffraction Pattern is displayed, titled '2D Diffraction Pattern Beam Direction: (001)'. The plot shows a grid of diffraction spots in the q_x vs q_y plane, with axes ranging from -1.5 to 1.5 \AA^{-1} . The central spot is the largest and darkest. To the right of the plot, there are control panels for 'Voltage / kV' (set to 200), 'Beam Direction' (set to 0, 0, 1), 'Maximum Scattering Angle [\AA^{-1}]' (set to 1.5), 'Use Bloch Wave Dynamical Calculator' (set to Off), and 'Thickness [\AA]' (set to 500). An 'Advanced Options' section is partially visible at the bottom right.

Vortex Structures in STO/PTO Superlattices

High angle annular dark field (HAADF) image

vortex-antivortex pair

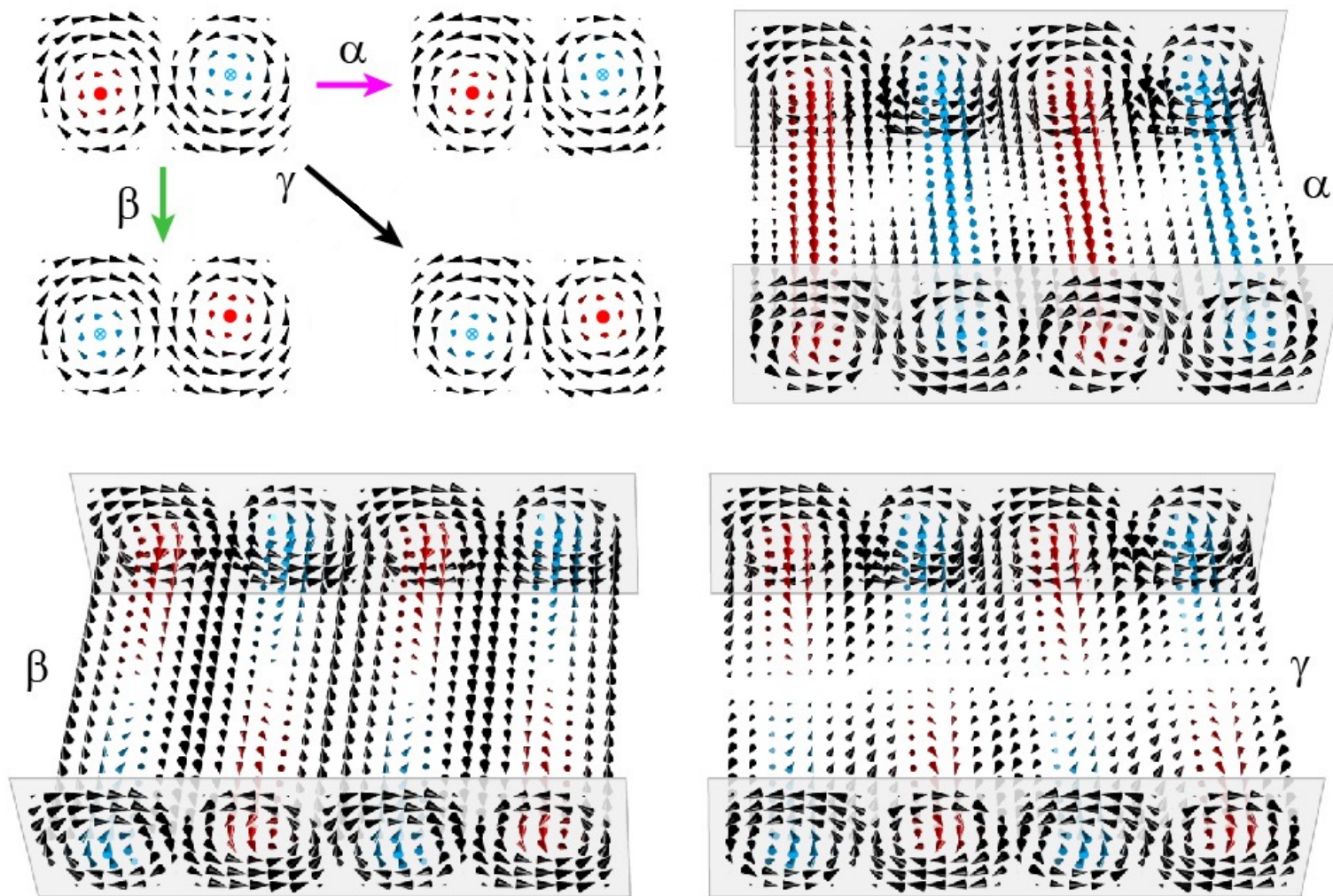
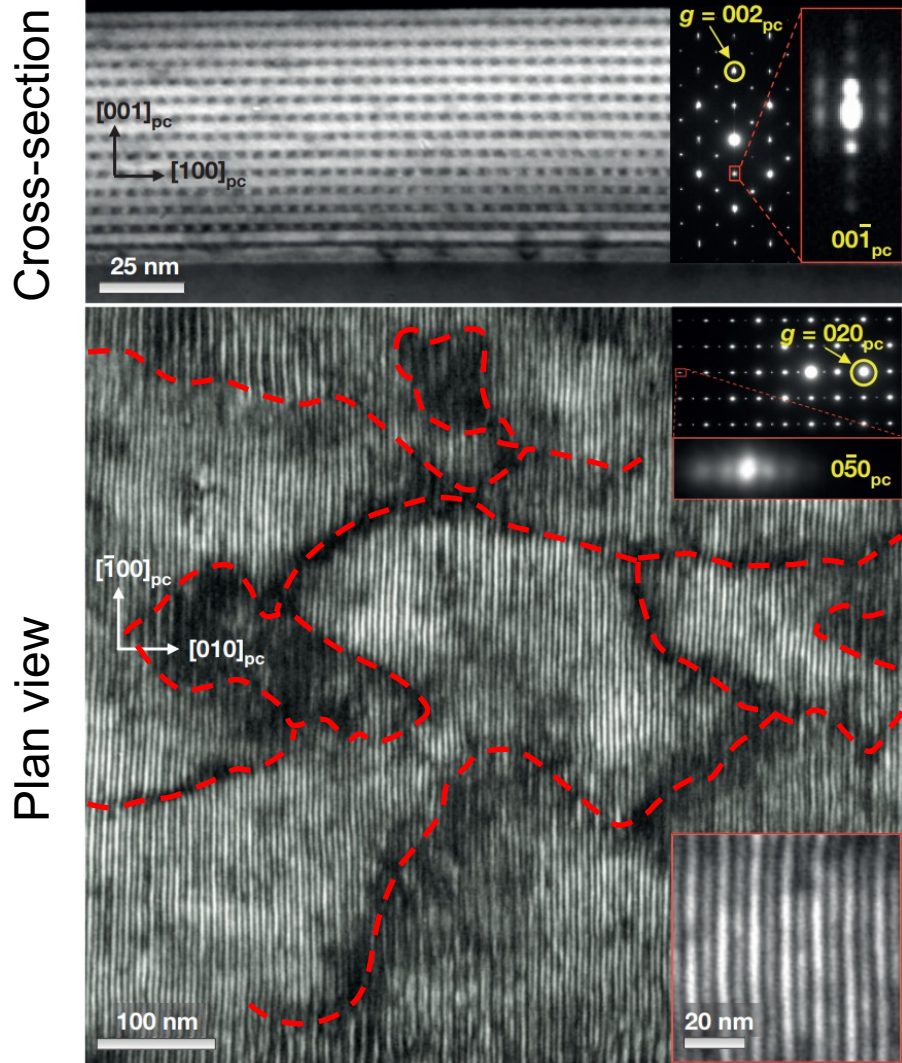


Polar displacements overlaid on HAADF image, from A sites.

Multilayers grown on SrRuO₃/DyScO₃ substrate

Domain Wall Configuration of STO/PTO Layers

Dark field TEM



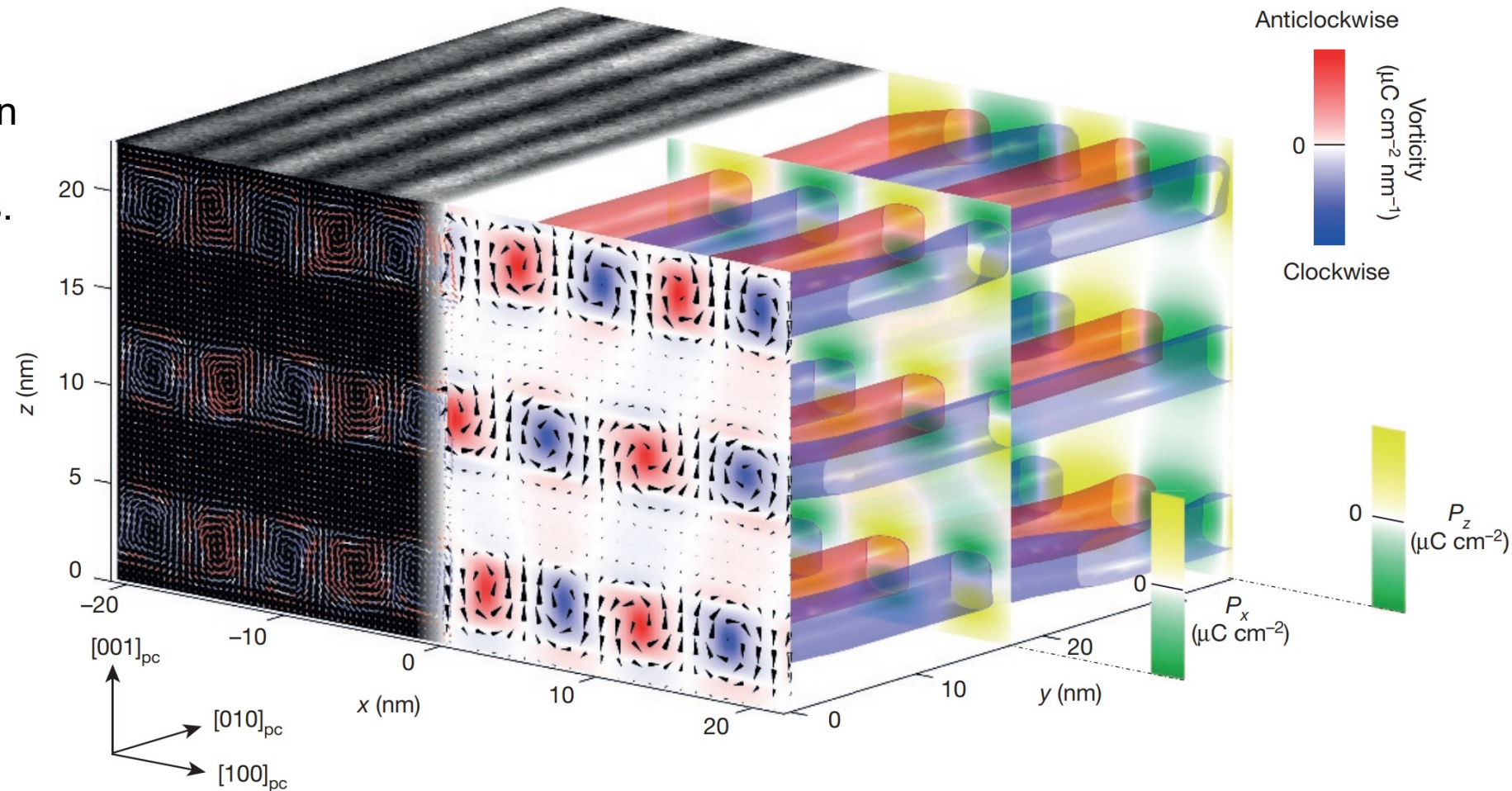
3D Vortex Structures in STO/PTO Superlattices

Large gradient energy of vortices is balanced by:

- Electrostatic energy reduction by removing polar **discontinuities** at interfaces.
- Elastic energy from with **epitaxial** constraints.

Open questions about vortex structure in 3D:

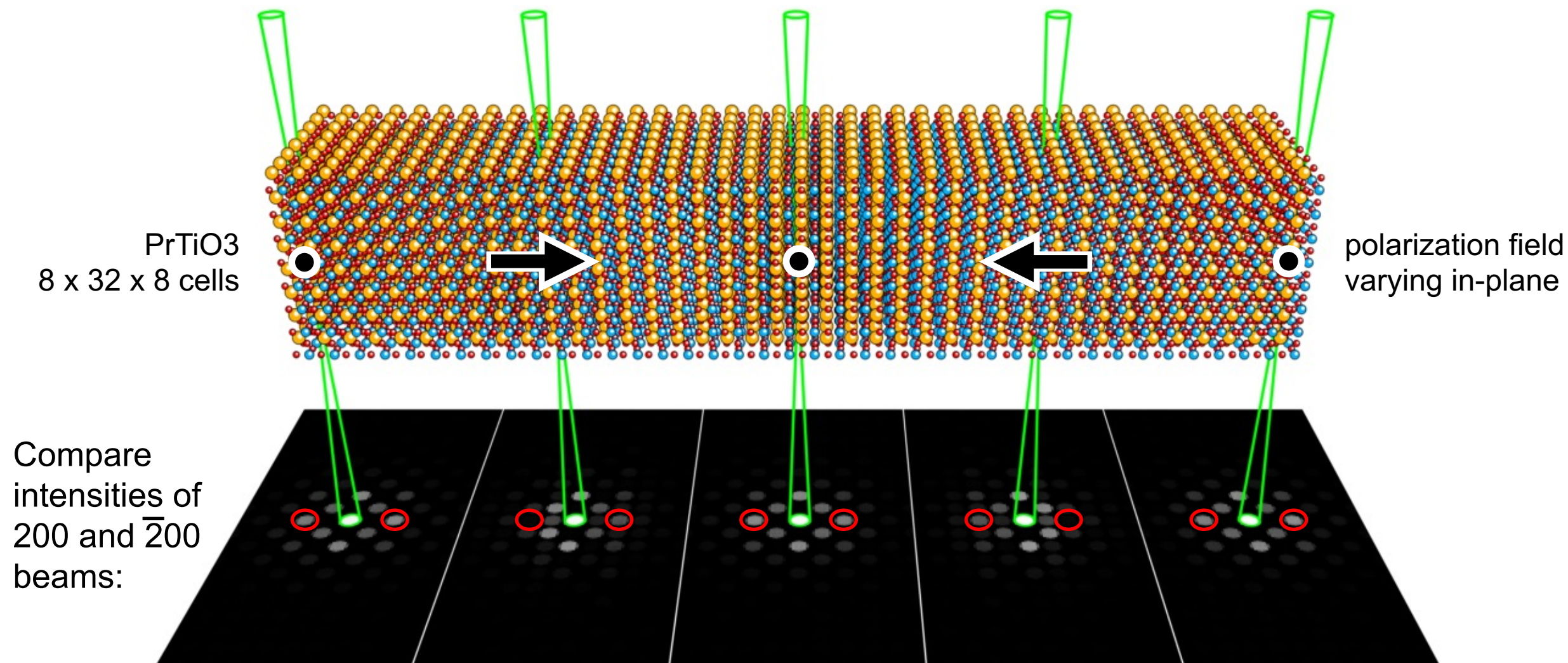
- Vertical [001] **asymmetry in position** of vortex cores?
- Non-zero **polarization** vectors along **vortex cores**?



Atomic-resolution imaging uses 2D projections – difficult if structure varies along beam direction.

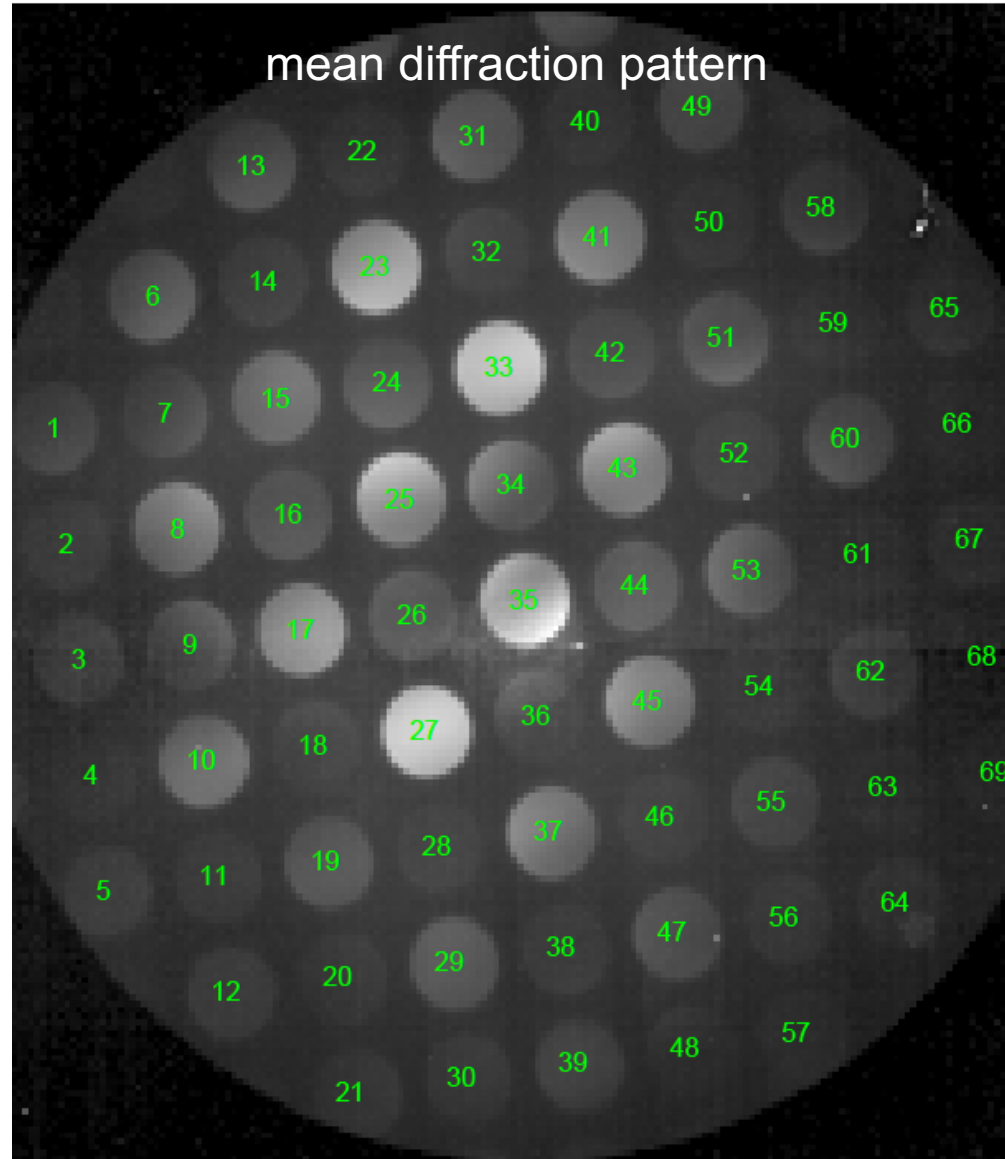
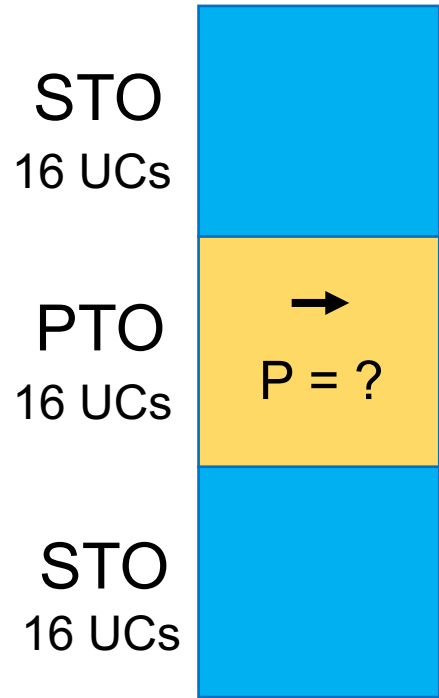
Alternatives?

Measuring PbTiO_3 Polarization using 4D-STEM

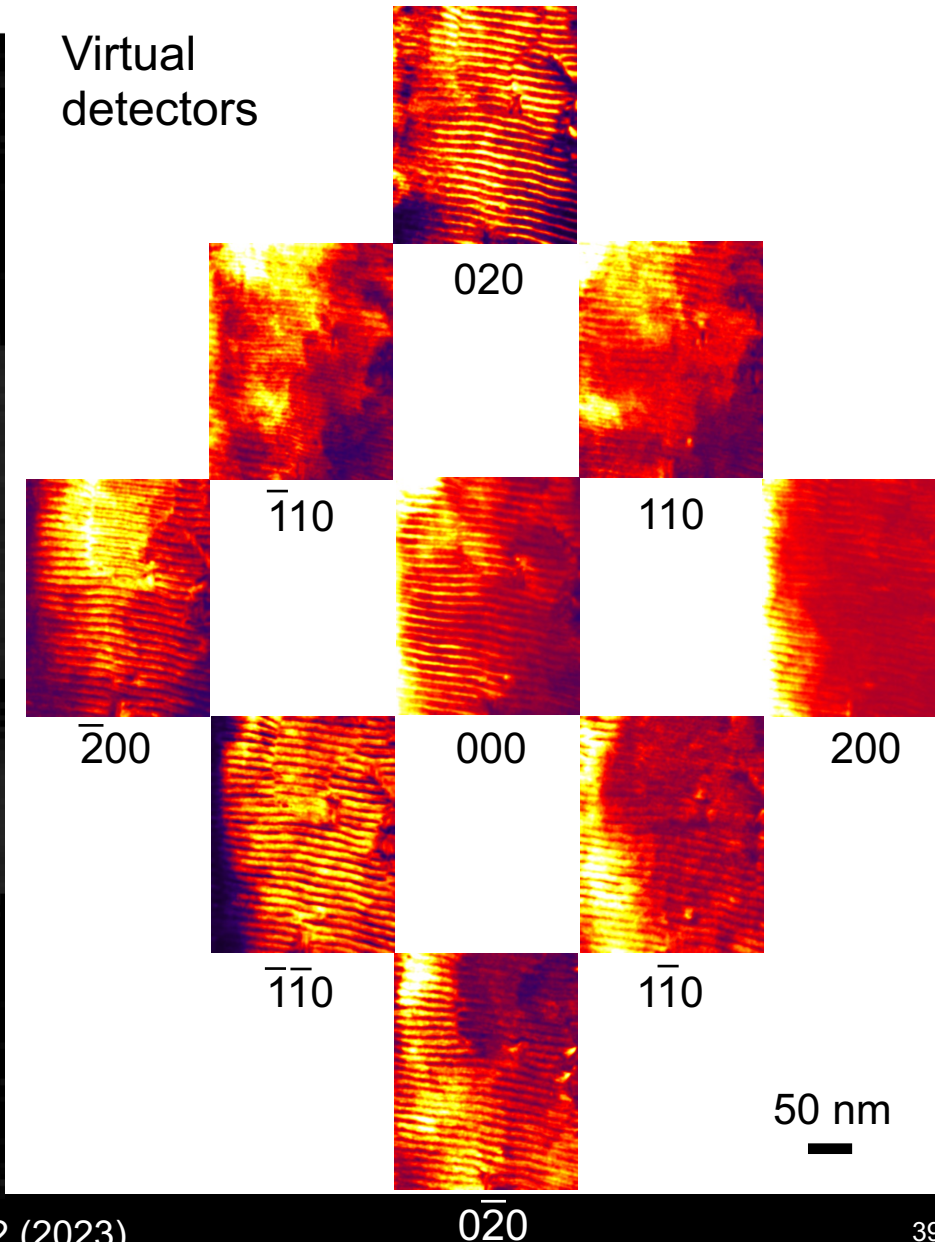


STO/PTO/STO Multilayer – 4D-STEM Experiments

converged
electron beam ↓



Virtual
detectors



PbTiO₃ Polarization with Dynamical Diffraction

4D-STEM measurements of intensities differences in **Friedel pairs** of Bragg disks works for **kinematical diffraction** (thin samples).

But what about **dynamical diffraction** (thick samples)?

Investigate with **Bloch wave** simulations:

$$\bar{A}\mathcal{C} = 2k_n\gamma\mathcal{C}$$

|

Bloch wave coefficients

|

normal comp. wavevectors

structure matrix:

$$\bar{A} = \begin{bmatrix} 0 & U_{-g} & \cdots & U_{-h} \\ U_g & 2k_0s_g & \cdots & U_{g-h} \\ \vdots & \vdots & \ddots & \vdots \\ U_h & U_{h-g} & \cdots & 2k_0s_h \end{bmatrix}$$

electron wave at depth z in sample:

$$\Psi(z) = \mathcal{C}\mathcal{E}(z)\mathcal{C}^{-1}\Psi(0)$$

where:

$$\mathcal{E}(z) = e^{2\pi i\gamma^{(j)}z}\delta_{ij}$$

|

Scattering matrix
(**S-matrix**)

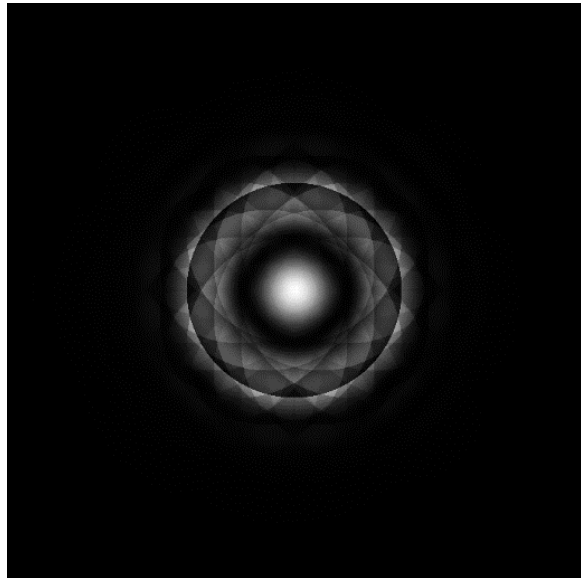
Simulating multilayers with an **S-matrix** is straightforward: $\mathcal{S} = \mathcal{S}_{\text{STO}} \mathcal{S}_{\text{PTO}} \mathcal{S}_{\text{STO}}$

What is a Scattering Matrix?

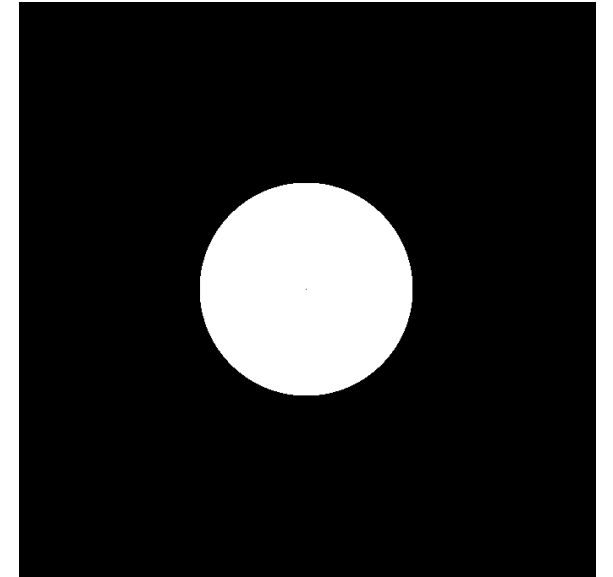
Probe at exit surface

Initial probe

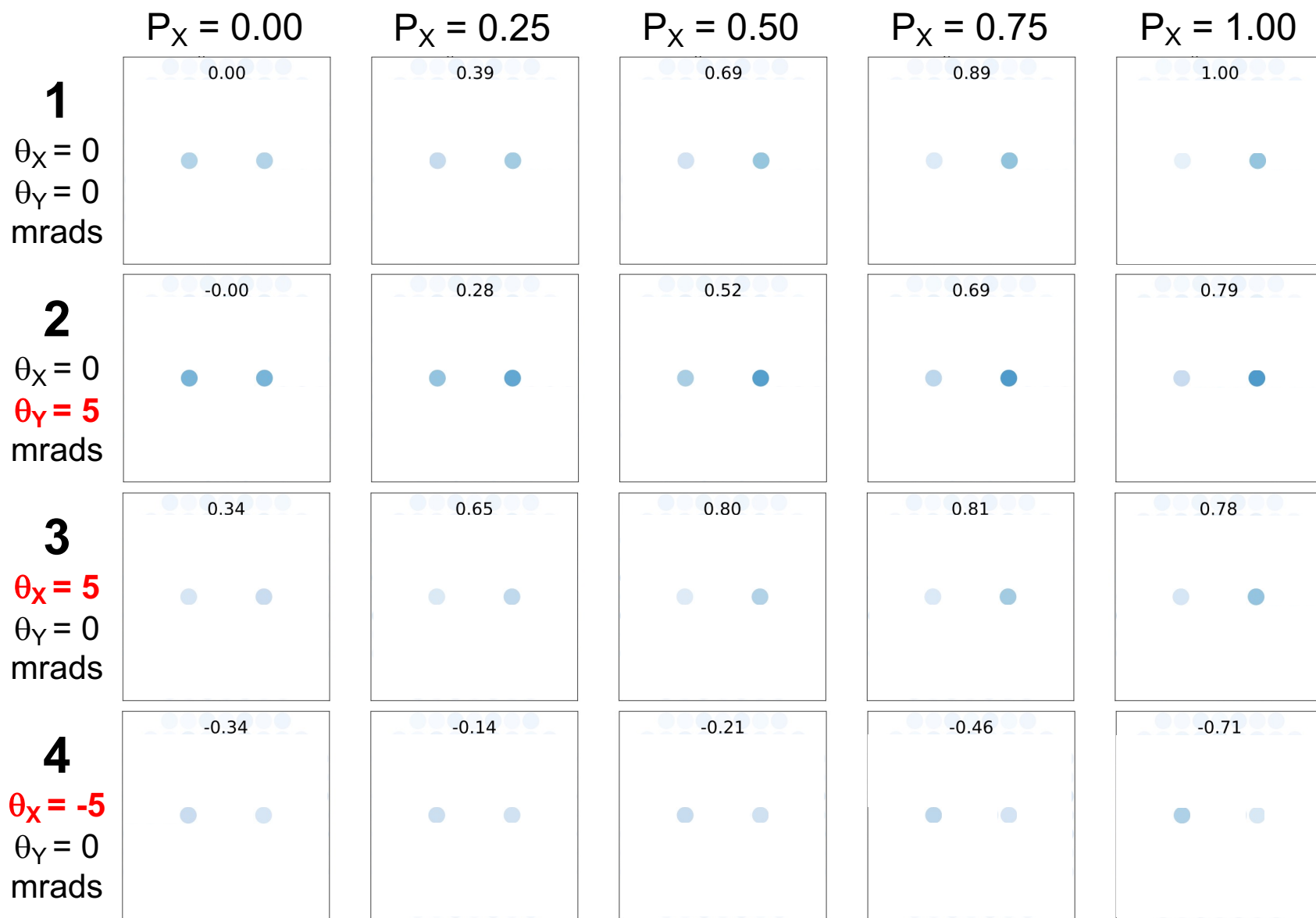
$$\Psi(x, y, z) = \exp \left\{ \int_0^z \left[i\sigma V(x, y, z) + \frac{i\lambda}{4\pi} \nabla_{x,y}^2 \right] \right\} \Psi(x, y, 0)$$



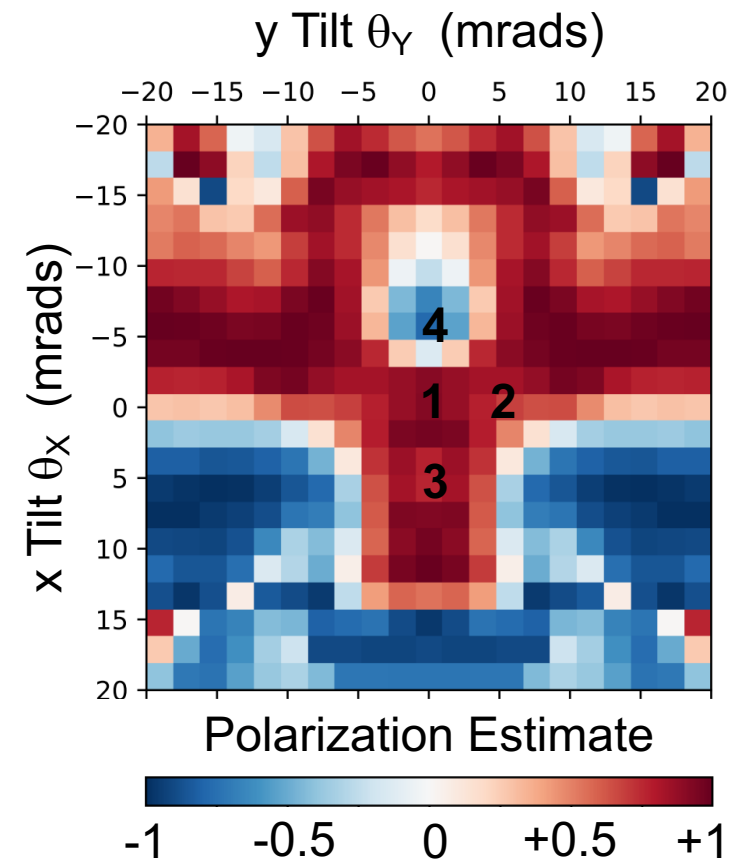
$$= \begin{bmatrix} S_{g_1, g_1} & S_{g_1, g_2} & \cdots & S_{g_1, g_n} \\ S_{g_2, g_1} & S_{g_2, g_2} & \cdots & S_{g_2, g_n} \\ \vdots & \vdots & \ddots & \vdots \\ S_{g_n, g_1} & S_{g_n, g_2} & \cdots & S_{g_n, g_n} \end{bmatrix}$$



PTO Polarization in 16/16/16 STO/PTO/STO



$$P_X = \frac{I_{200} - I_{\bar{2}00}}{I_{200} + I_{\bar{2}00}} \text{ polarization estimate (inset, normalized to } P_X=1)$$

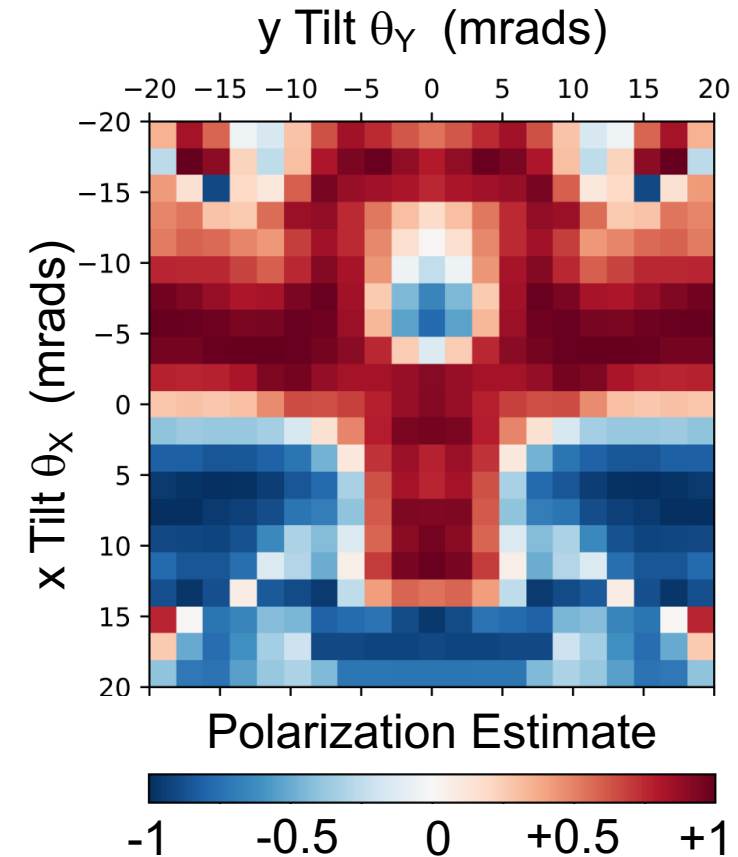


PTO Polarization in 16/16/16 STO/PTO/STO

Under dynamical diffraction conditions, **tilt** and **polarization** are **not orthogonal**.

Multiple scattering leads to complex nonlinear intensity response, contrast decrease, even **contrast reversals**.

How can we measure **polarization** in complex structures, locally tilted, **thick samples**?



Flexible Inversion of Dynamical Scattering Data



Advances in Applied
Mathematics

ELSEVIER Volume 16, Issue 3, September 1995, Pages 321-375



$$D_V(t, \mathbf{A}) \equiv \lim_{h \rightarrow 0} \frac{1}{h} (e^{t(\mathbf{A}+h\mathbf{V})} - e^{t\mathbf{A}})$$

Directional **derivative**
of matrix exponential.

$$D_V(t, \mathbf{A}) = \mathbf{U} ((\mathbf{U}^{-1}\mathbf{V}\mathbf{U}) \odot \Phi(t)) \mathbf{U}^{-1}$$

Derivative of matrix after
spectral decomposition.

where $\Phi_{ij}(t) = \begin{cases} (e^{t\lambda_i} - e^{t\lambda_j})/(\lambda_i - \lambda_j) & \text{if } \lambda_i \neq \lambda_j \\ te^{t\lambda_i} & \text{if } \lambda_i = \lambda_j \end{cases}$

Regular Article

Derivatives of the Matrix Exponential and Their Computation

Najfeld, I., Havel, T.F.

$$\frac{d\mathcal{S}}{d\theta} = \sum_i^N \left[\prod_{j=0}^{i-1} \mathcal{S}^{(j)} \cdot \frac{d\mathcal{S}^{(i)}}{d\theta} \cdot \prod_{k=i+1}^{k=N} \mathcal{S}^{(k)} \right]$$

Product rule for
multiple S-matrices

Sample **tilt** derivatives

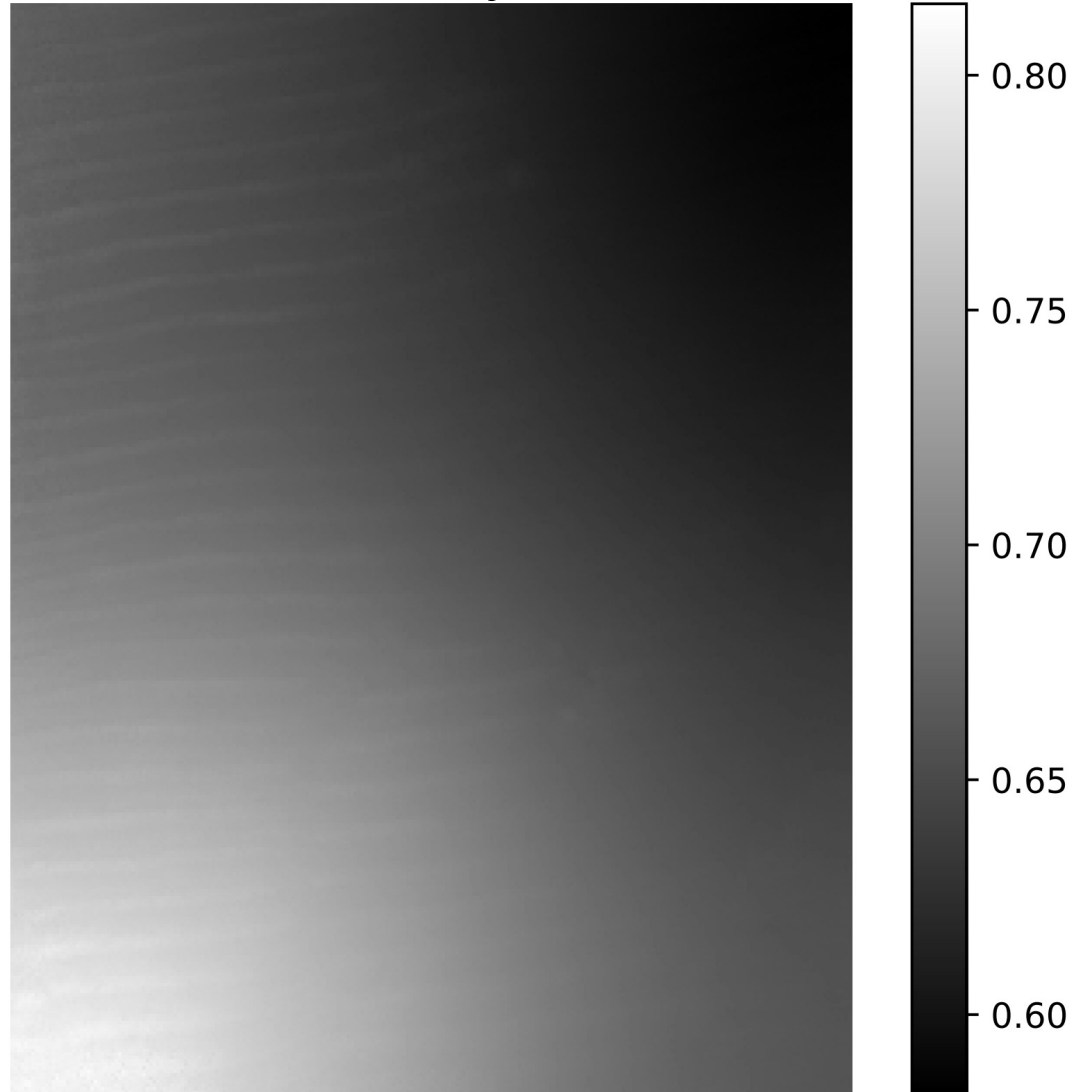
$$\frac{ds_g}{dk_{\{x,y\}}} = -\frac{g_{\{x,y\}}}{|\mathbf{g} + \mathbf{k}_0|} + \frac{(g_{\{x,y\}} + k_{\{x,y\}})(\mathbf{g} \cdot (2\mathbf{k} + \mathbf{g}))}{2|\mathbf{g} + \mathbf{k}|^3}$$

Sample **polarization** derivatives

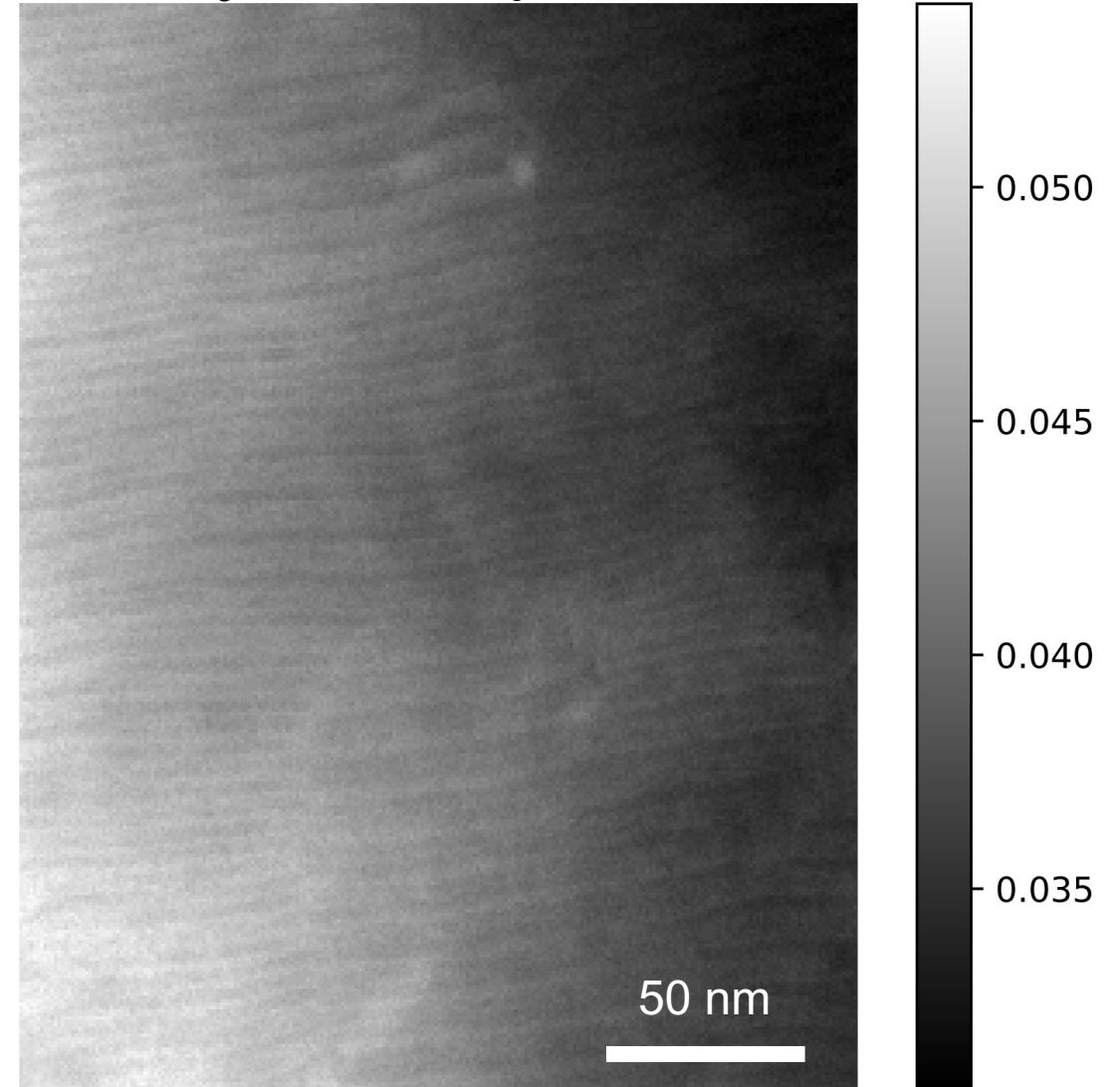
$$\frac{dU_g}{d\rho_a} = \frac{1}{\Omega} \sum_j 2\pi i f_e^{(j)}(\mathbf{g} \cdot \delta\mathbf{r}_a) e^{2\pi i((\mathbf{r}^{(j)} + \rho_a \delta\mathbf{r}_a^{(j)} + \rho_b \delta\mathbf{r}_b^{(j)}) \cdot \mathbf{g})}$$

Preliminary 16/16/16 STO/PTO/SRO Inversion

ΔI – intensity scale



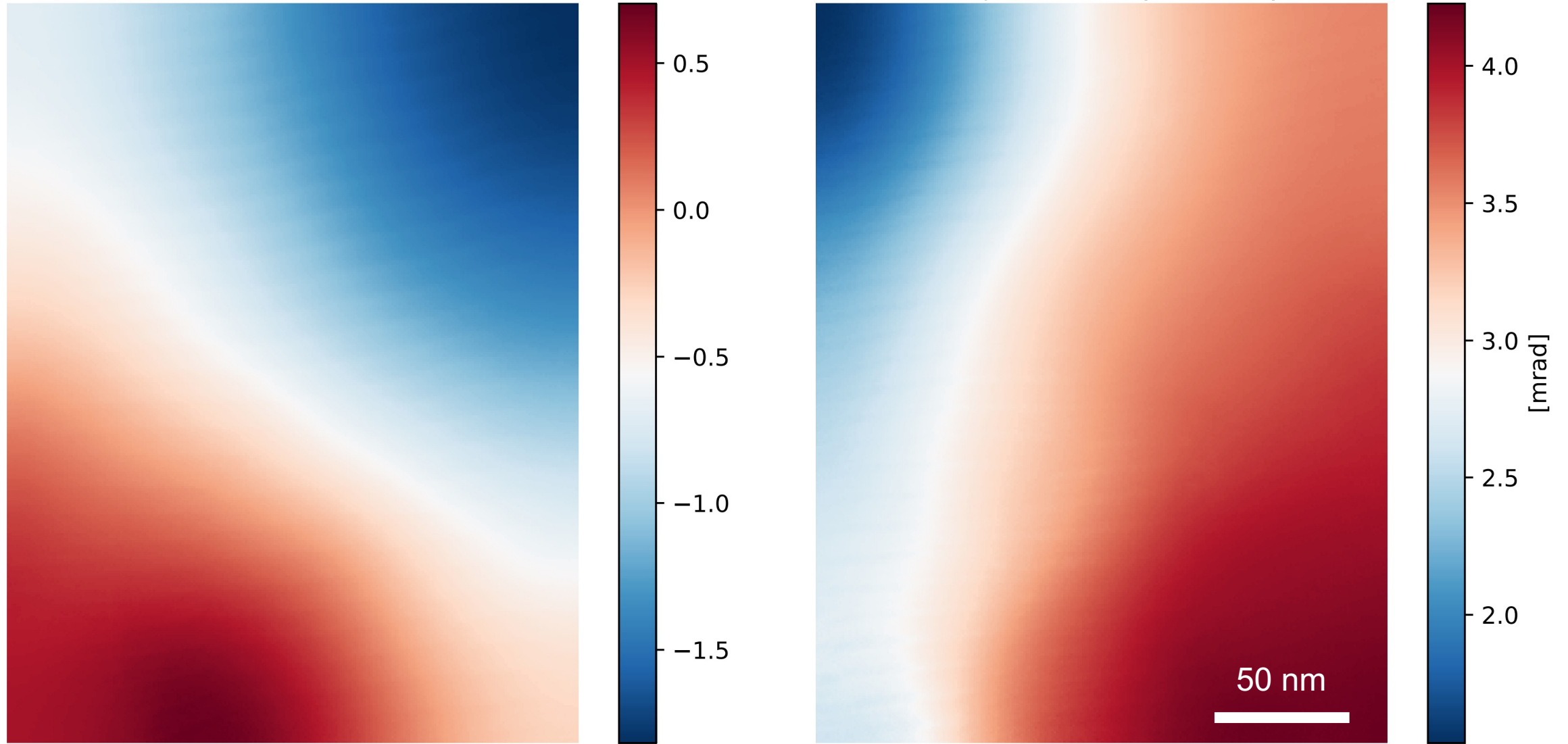
I_0 – intensity offset



Preliminary 16/16/16 STO/PTO/SRO Inversion

x Tilt θ_x (mrads)

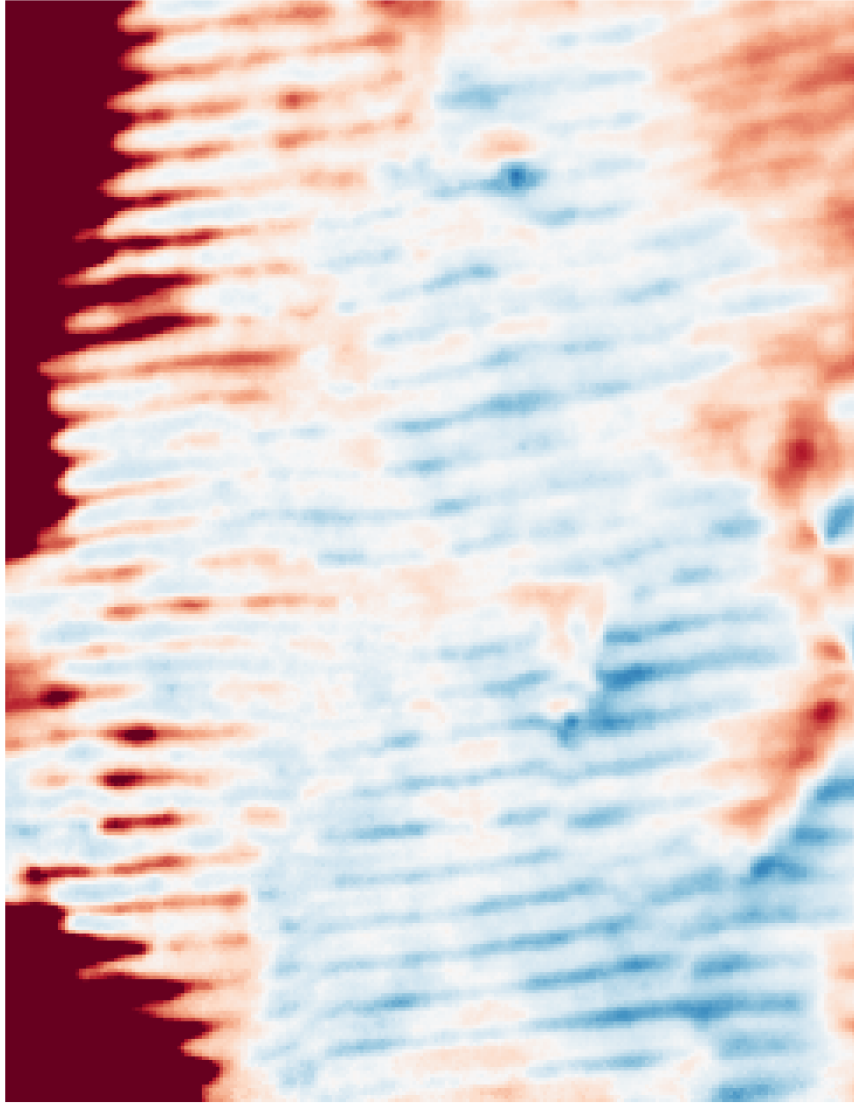
y Tilt θ_y (mrads)



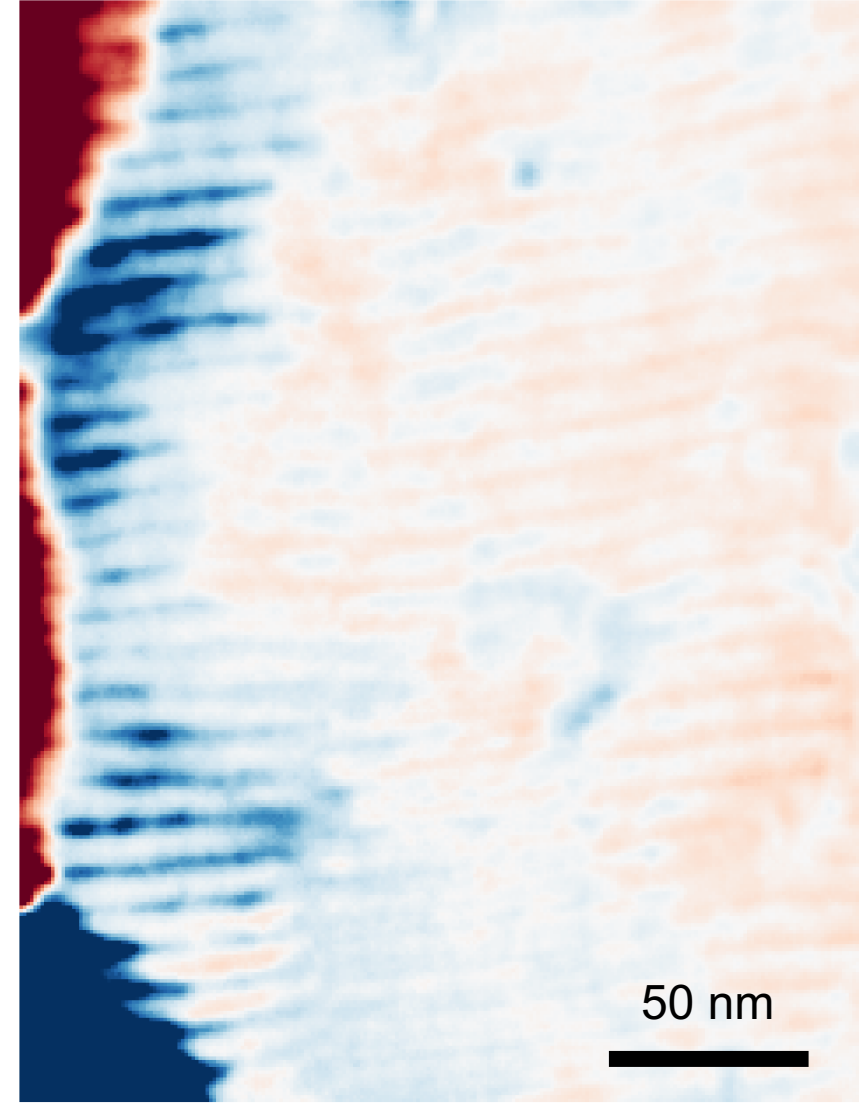
Preliminary 16/16/16 STO/PTO/SRO Inversion



Axial Polarization P_x

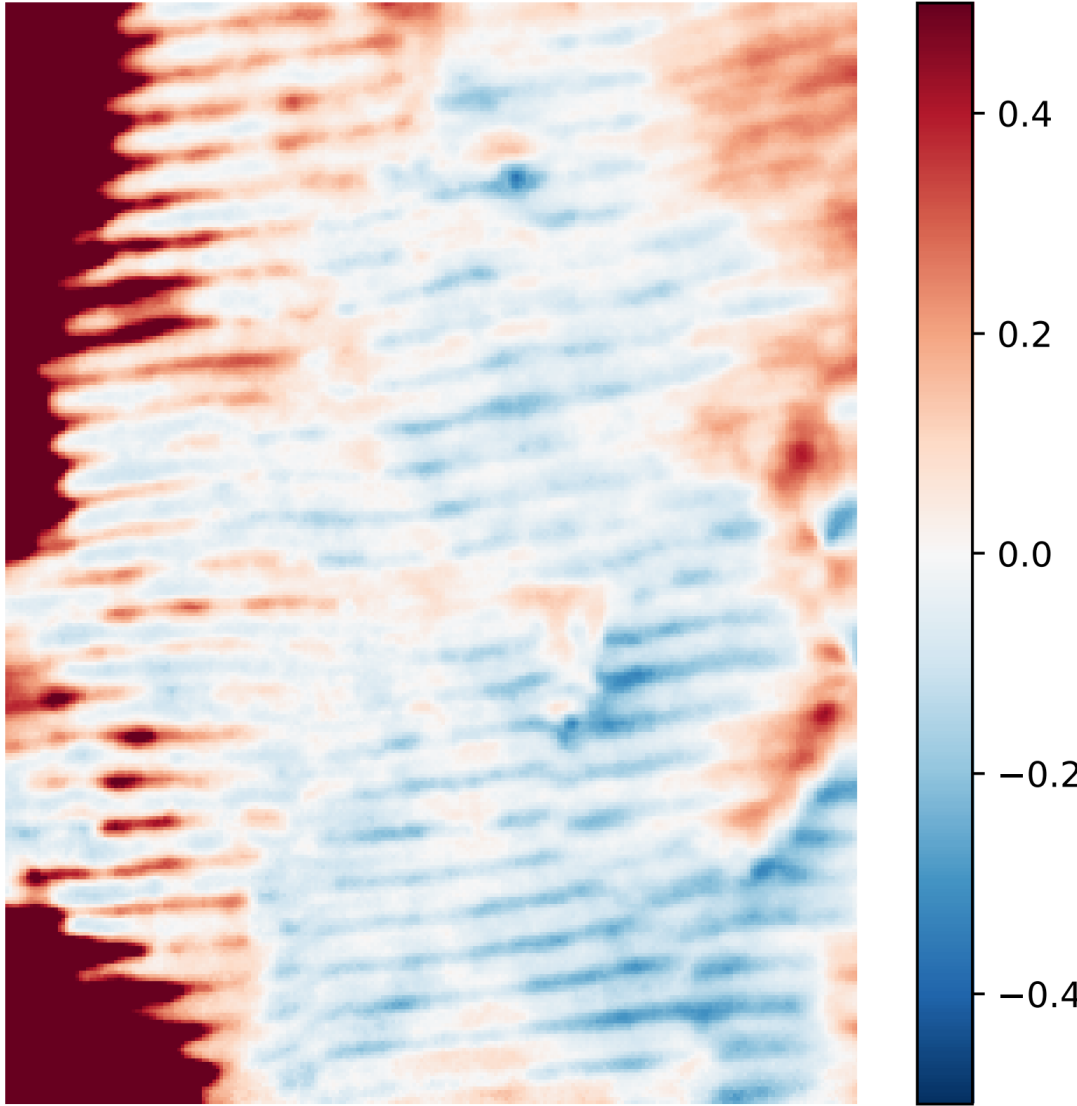


Lateral Polarization P_y

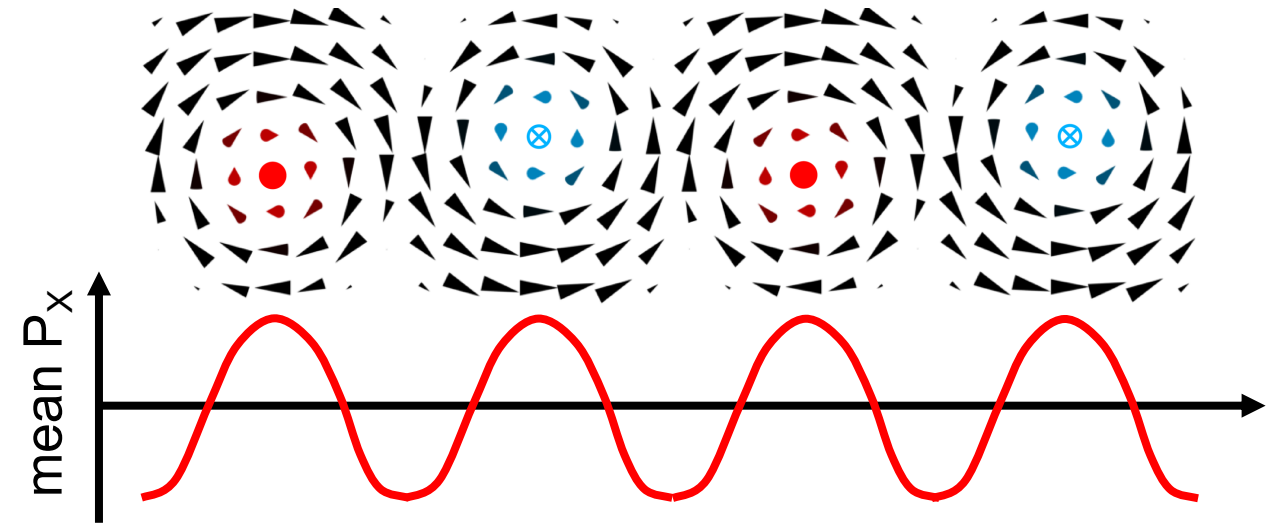


Preliminary 16/16/16 STO/PTO/SRO Inversion

↔ Axial Polarization P_x

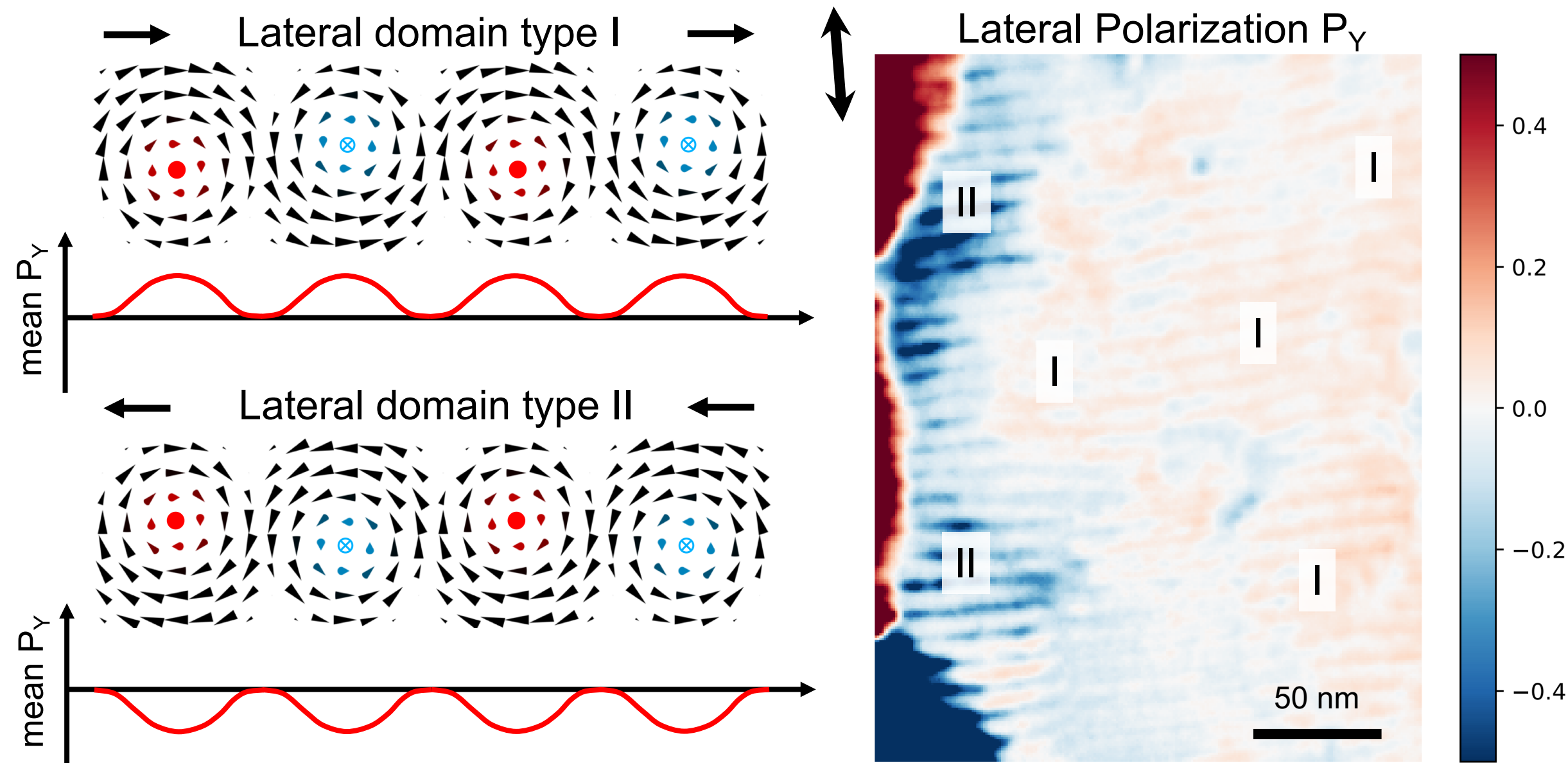


Axial Polarization – expected to alternate



- Oscillating behavior observed everywhere.
- However, many domains show net polarization in one direction.
- Need a more complex 3D model of P ?

Preliminary 16/16/16 STO/PTO/SRO Inversion



4DCamera Distillery

From Massive Transmission Electron
Microscopy Scattering Data

To Useful Information with AI/ML

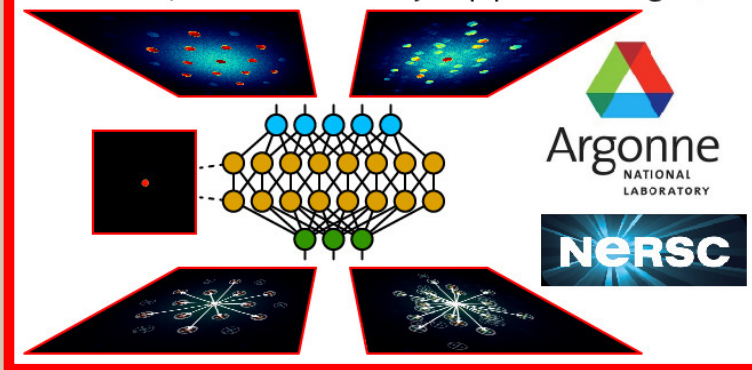


BERKELEY LAB

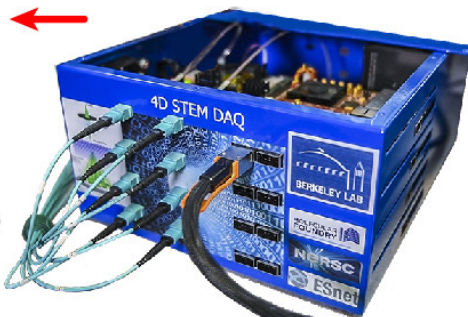
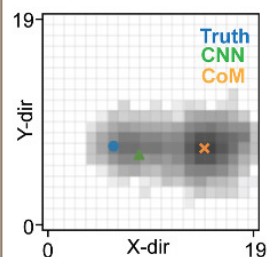
MOLECULAR
FOUNDRY

TEAM
scanning/transmission
electron microscope

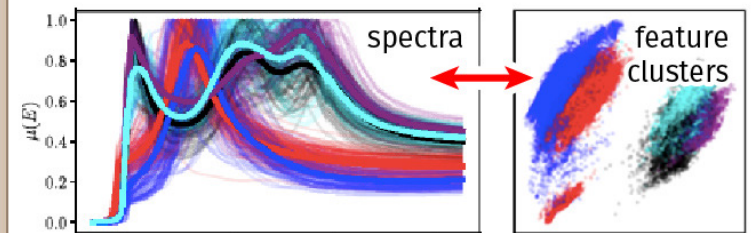
T3 - Robust, fast 4D-STEM analysis pipelines using AI/ML



T1 - Electron strike localization with FPGA neural networks

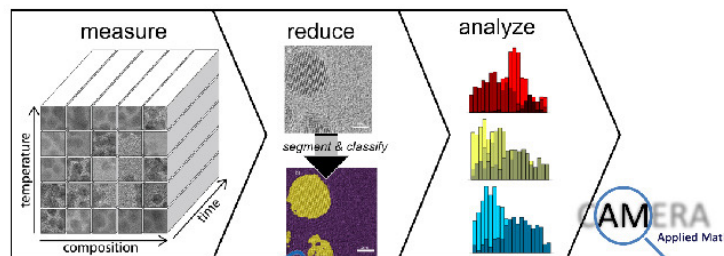


T4 - AI/ML interpretation of e⁻ energy loss spectroscopy



BROOKHAVEN NATIONAL LABORATORY OAK RIDGE National Laboratory

T2 - Computer vision for quantitative structural analysis

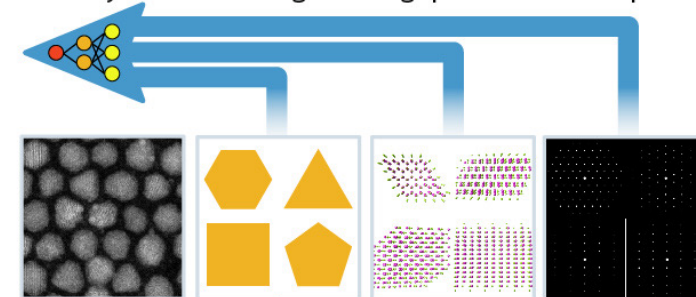


Sandia National Laboratories Los Alamos NATIONAL LABORATORY BROOKHAVEN NATIONAL LABORATORY CAMERA Applied Math



4D Camera - 400 gigabits / second

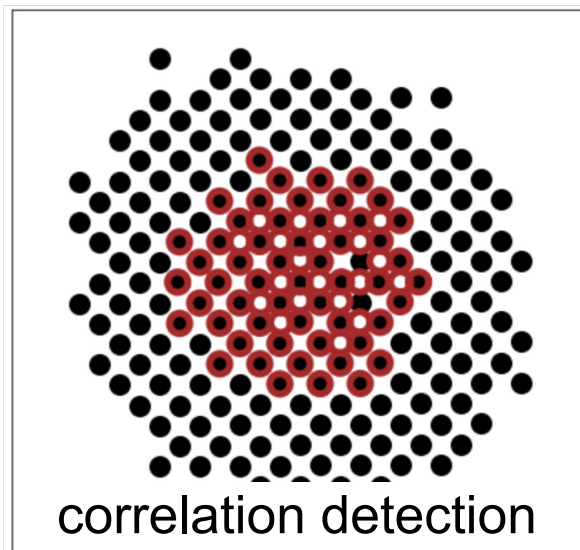
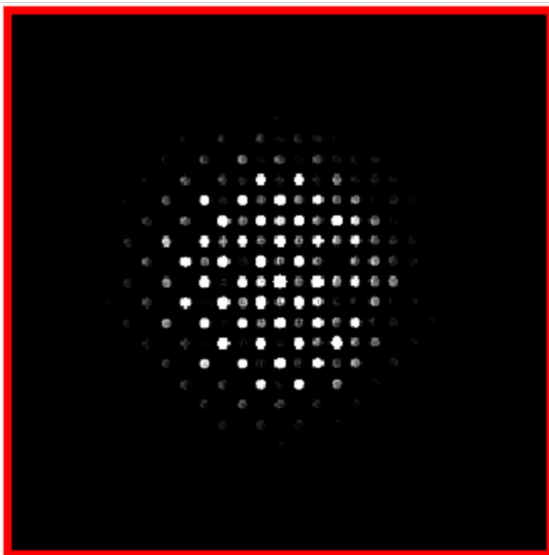
T5 - Fully automated high-throughput 4D-STEM acquisition



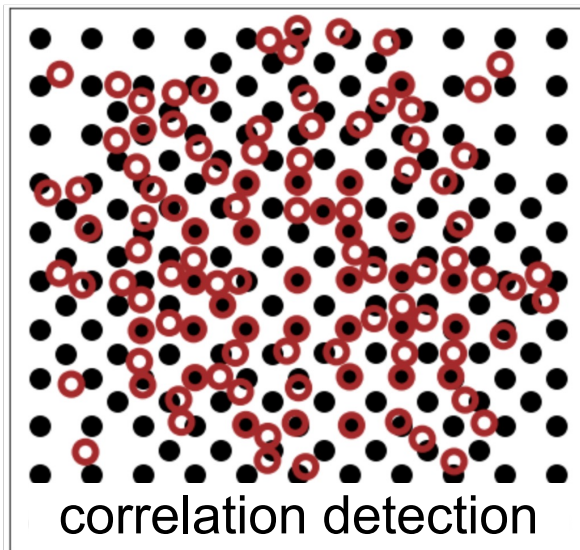
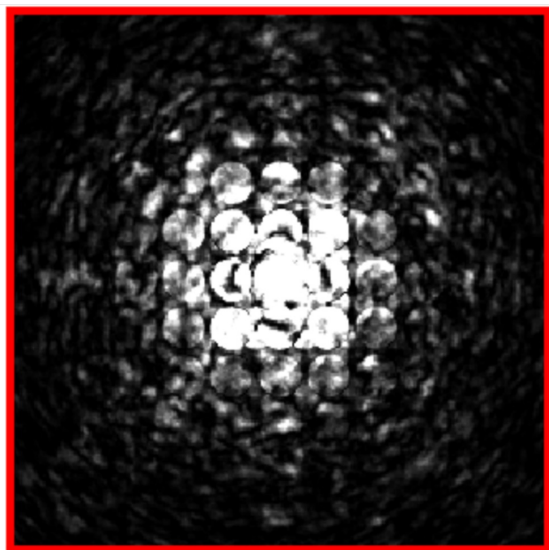
Kitware

Dynamical Diffraction Complicates Disk Detection

Diffraction pattern from using small convergence angle, thin sample



Diffraction pattern from using large convergence angle, thick sample



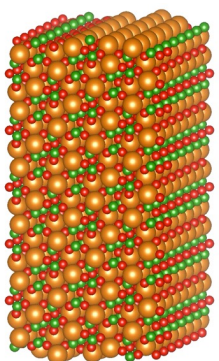
Can machine learning methods help us when our conventional image analysis pipelines fail?

Simulation Pipeline Infrastructure

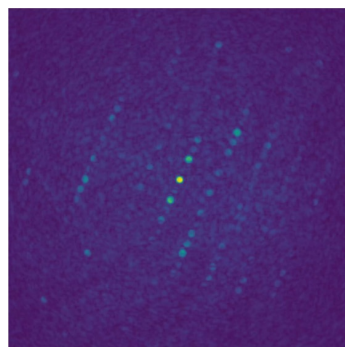
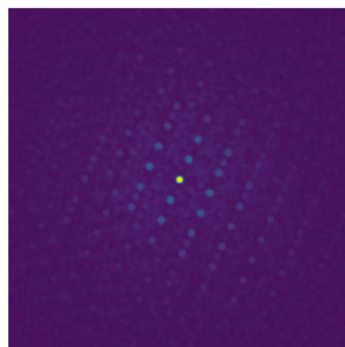
4D-SCRAPE & Manipulatt



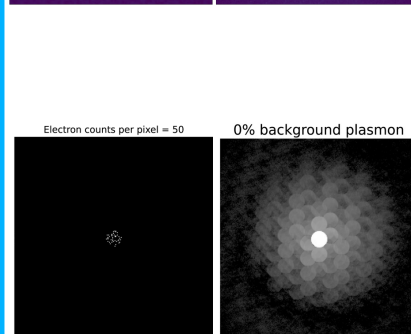
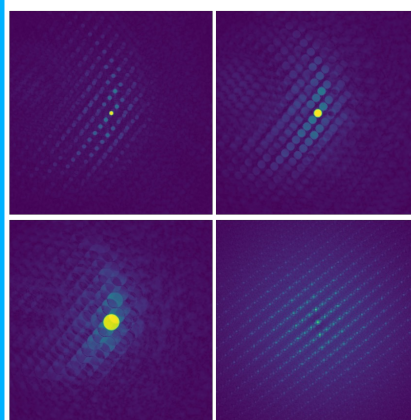
AFLOW
Automatic - FLOW for Materials Discovery



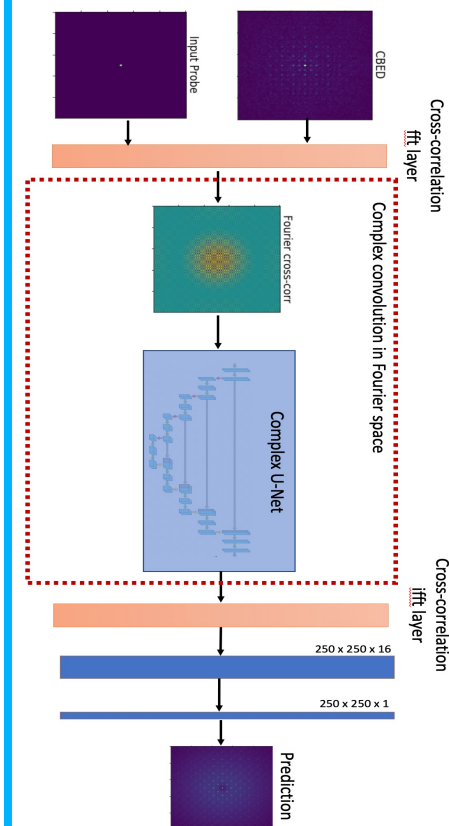
4D-MAKE



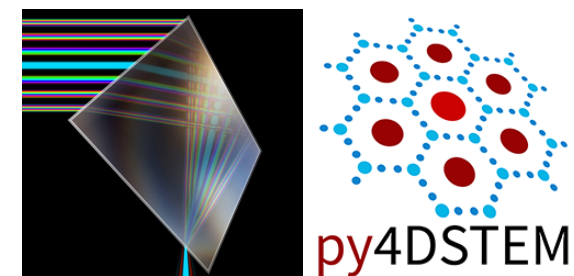
4D-PREP



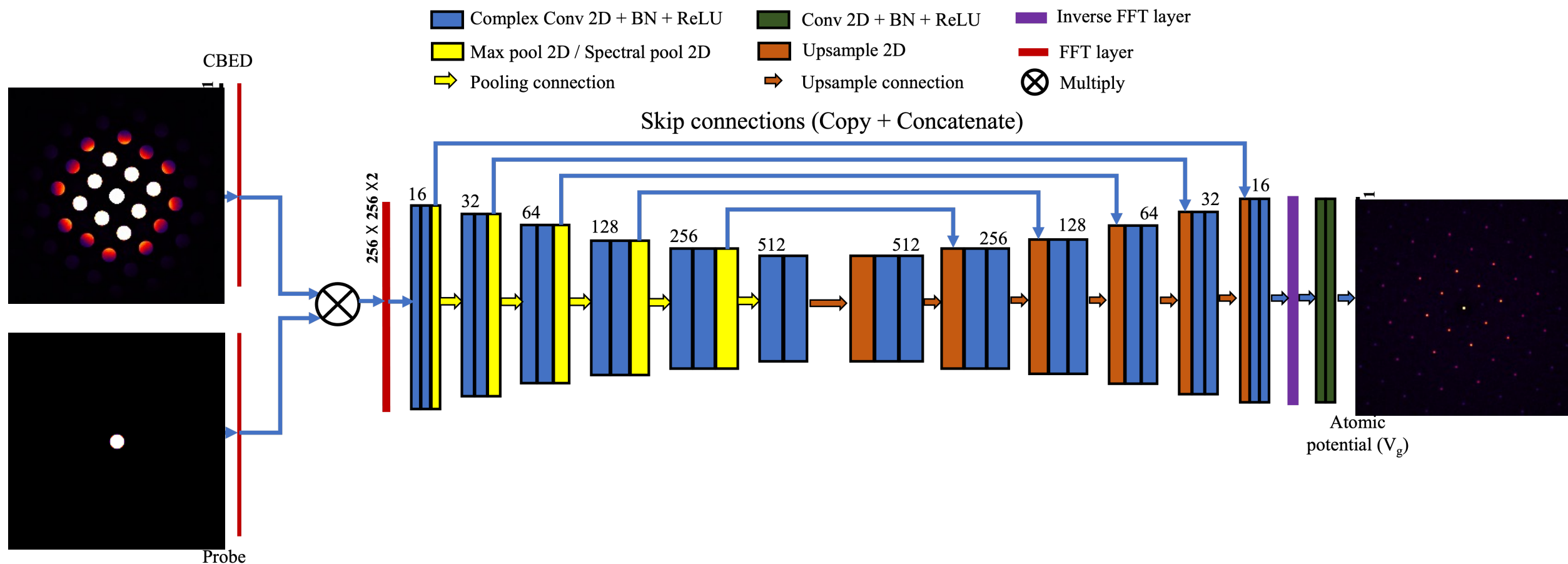
4D-OPTIMIZE



Many open source software tools used:

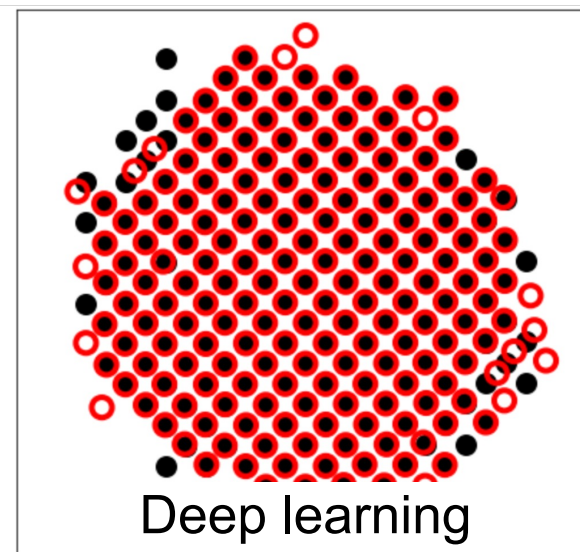
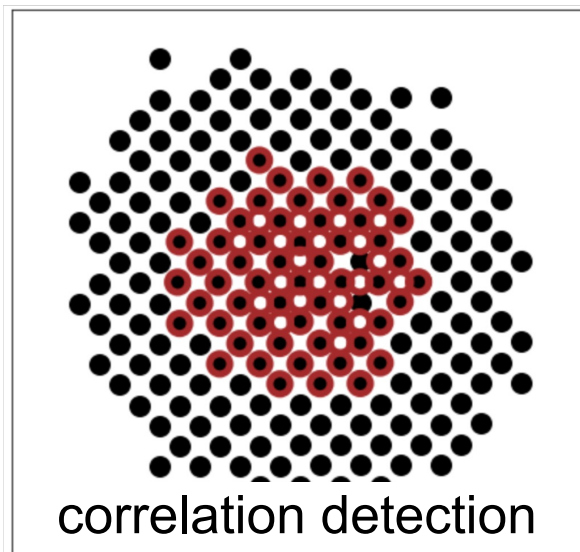
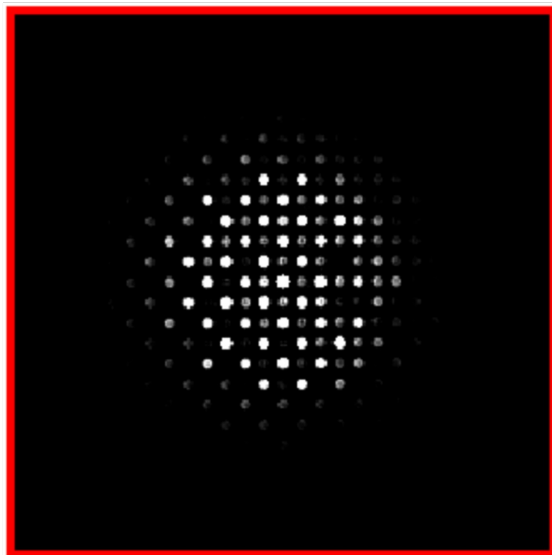


Solving Diffraction with Deep Learning

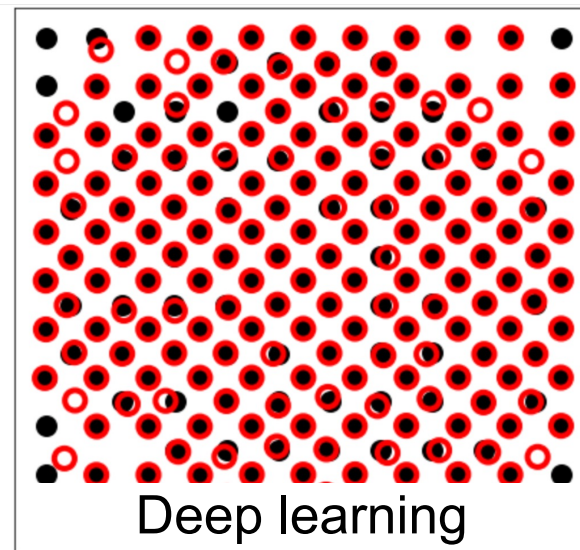
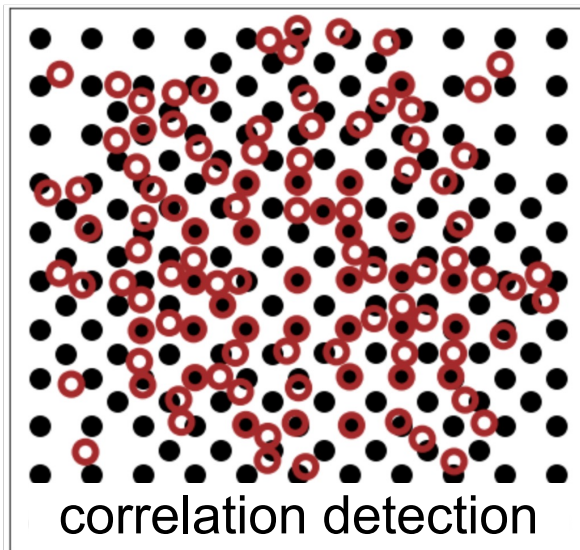
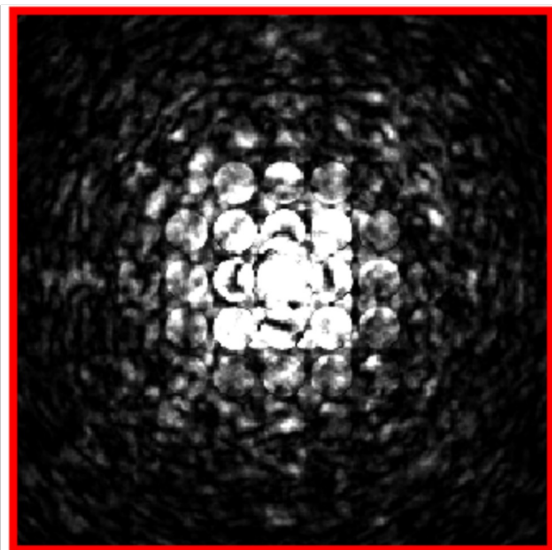


Dynamical Diffraction **Defeated** by Deep Learning

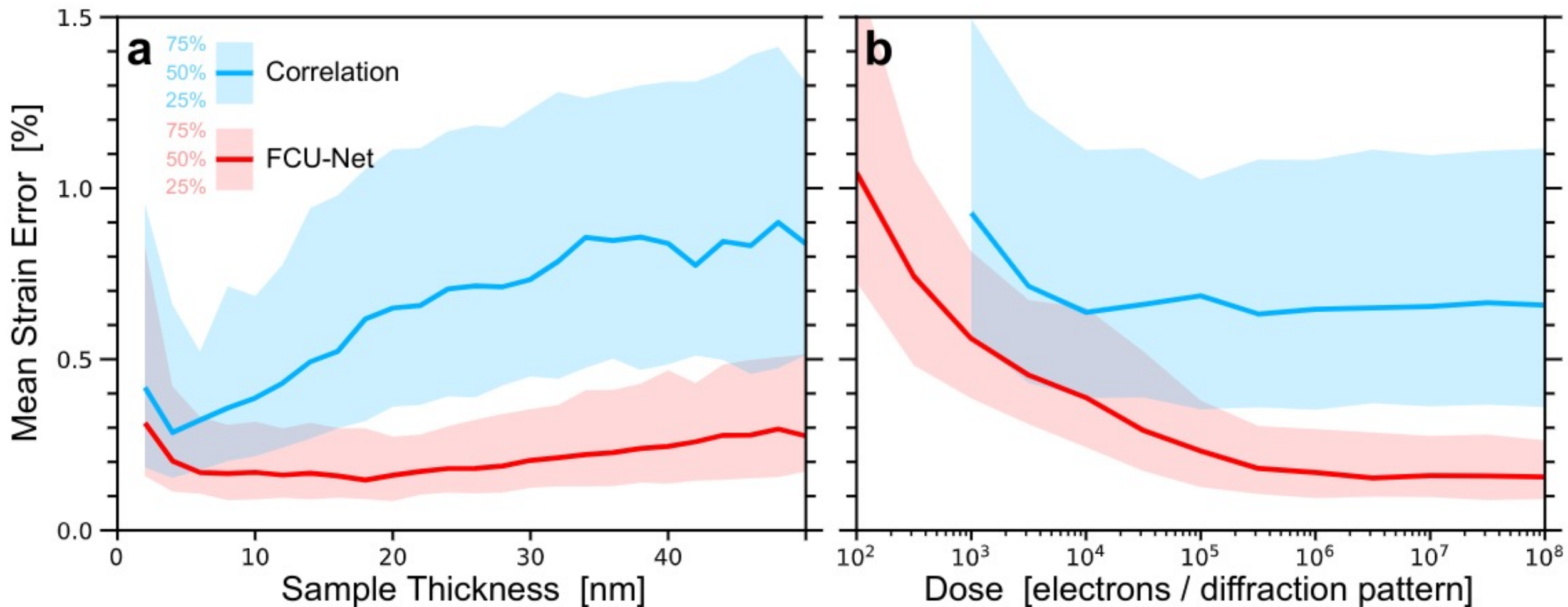
Diffraction pattern from using small convergence angle, thin sample



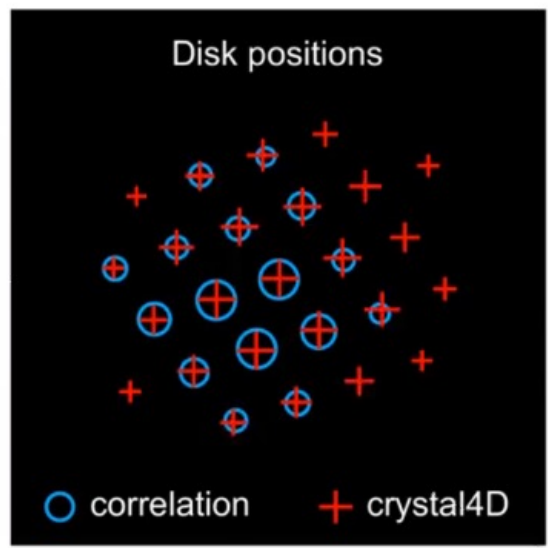
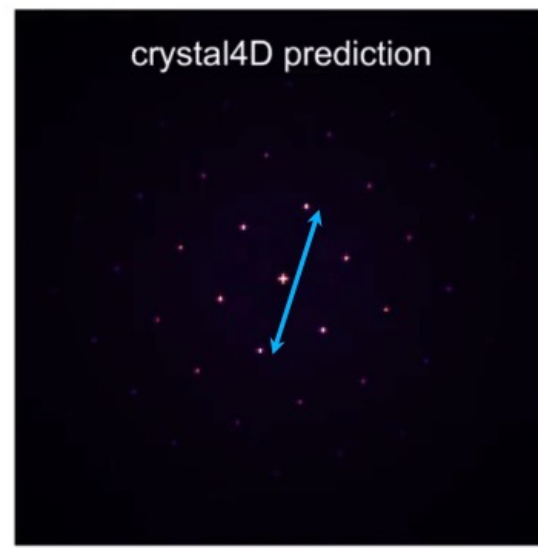
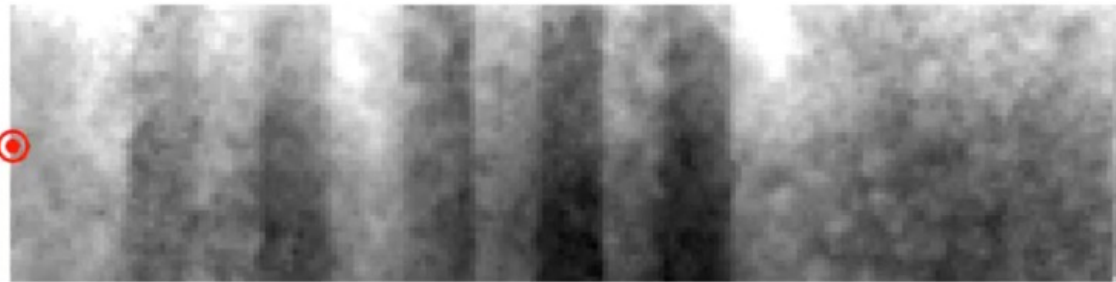
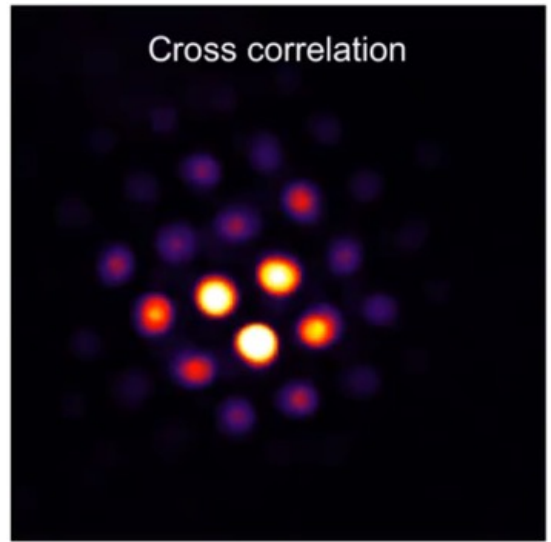
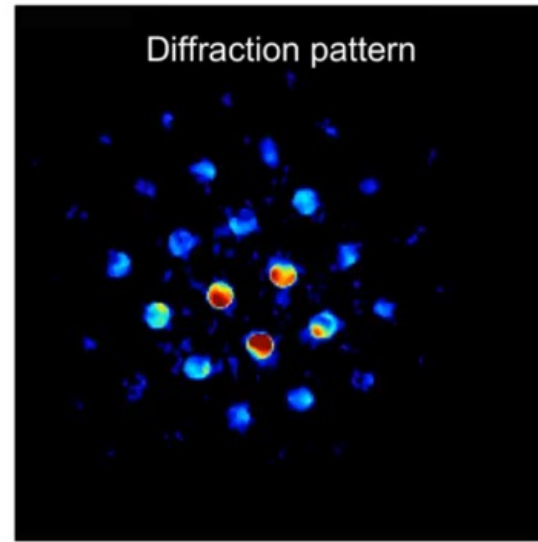
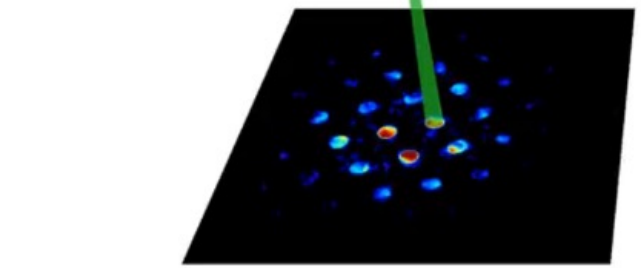
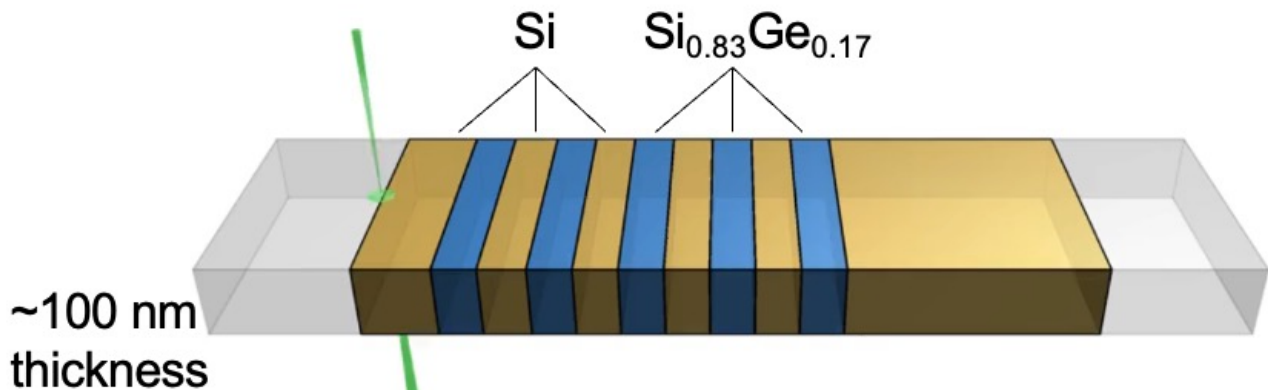
Diffraction pattern from using large convergence angle, thick sample



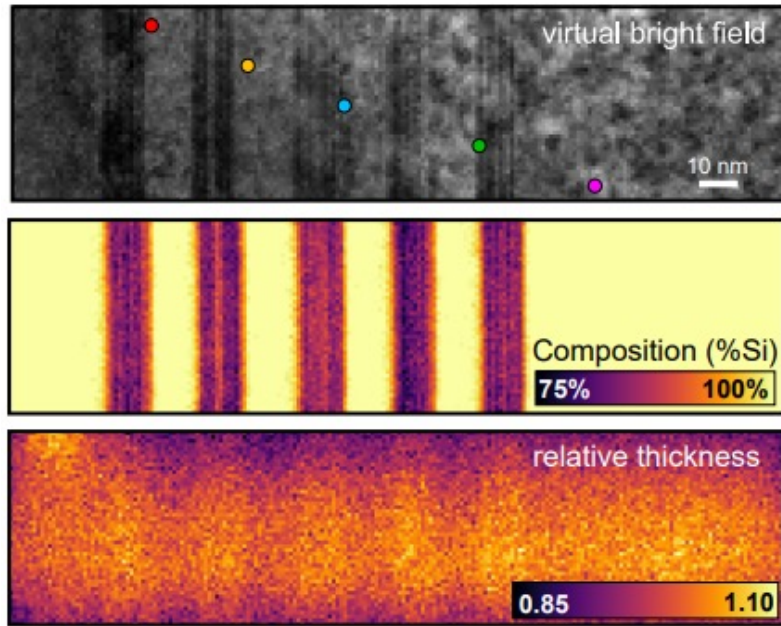
Solving Diffraction with Deep Learning – FCU-Net



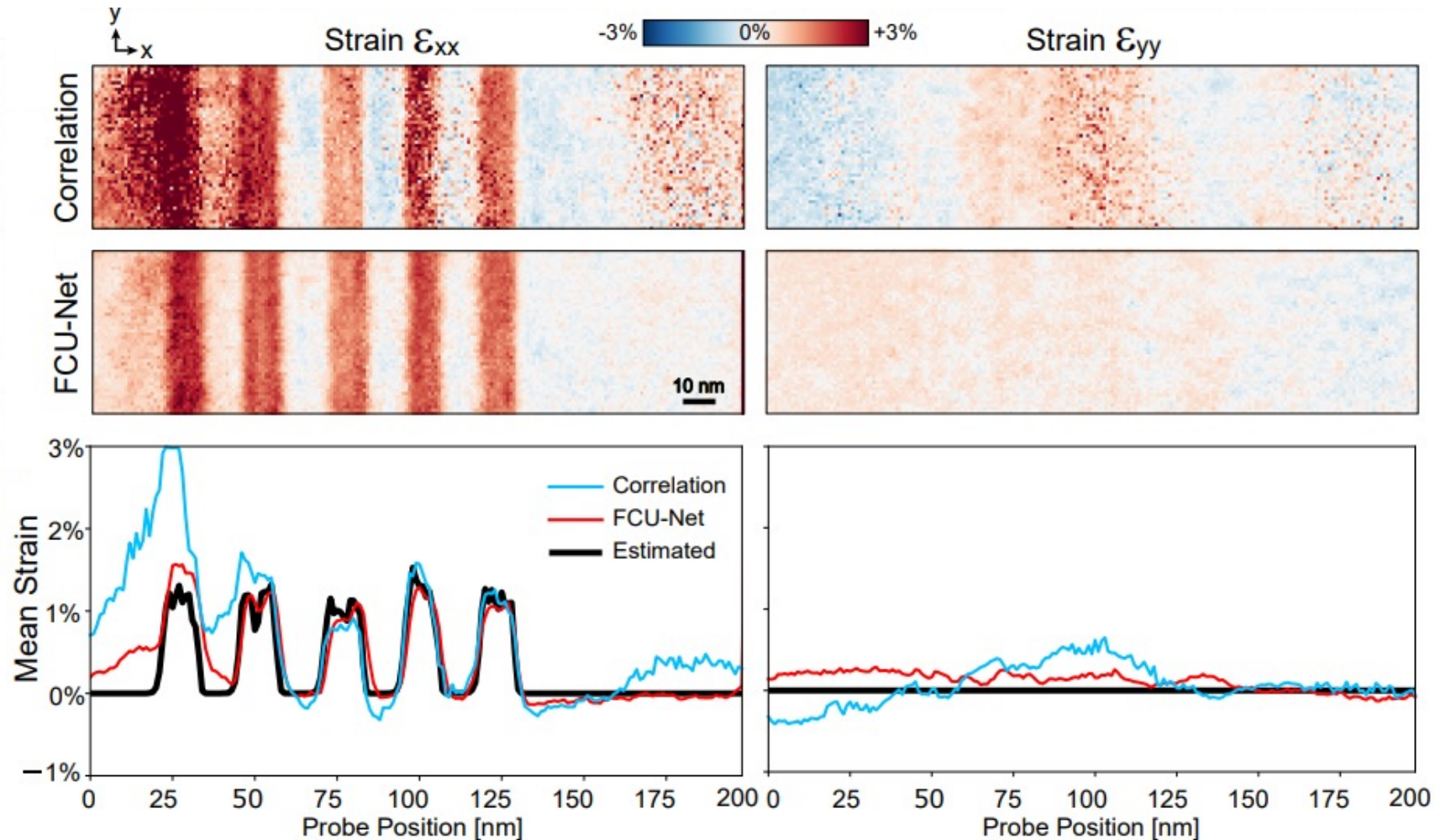
Strain Mapping of SiGe Multilayers w/ Deep Learning



Strain Mapping of SiGe Multilayers w/ Deep Learning



Strain mapping of alternating multilayers of Si and SiGe.

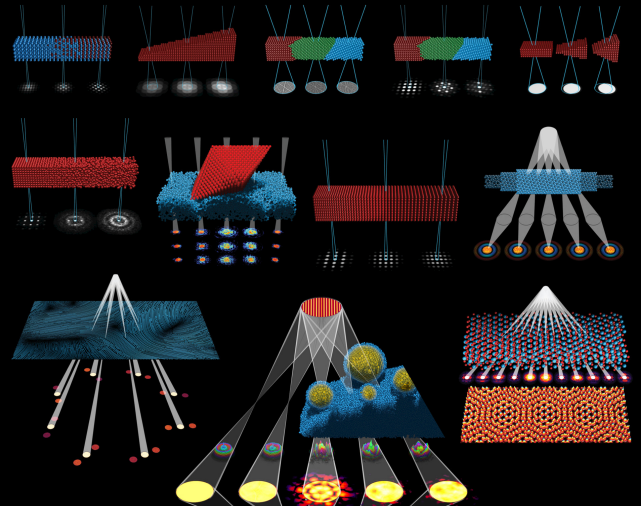


- Our deep learning approach significantly improves the **measurement accuracy** over conventional correlation, and **does not require** any **labeled training data**.

More Info – clophus@lbl.gov – ncem-lbl.slack.com

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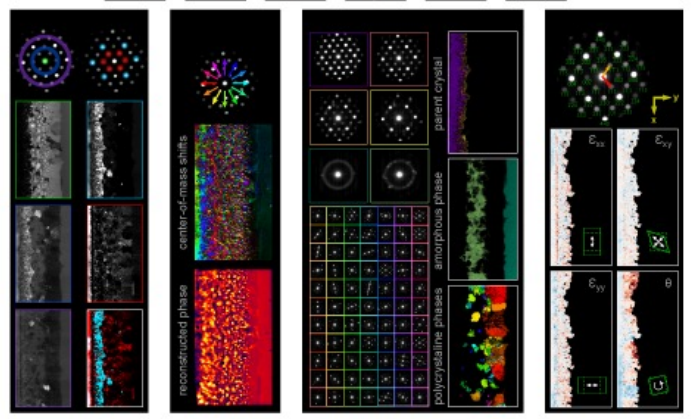
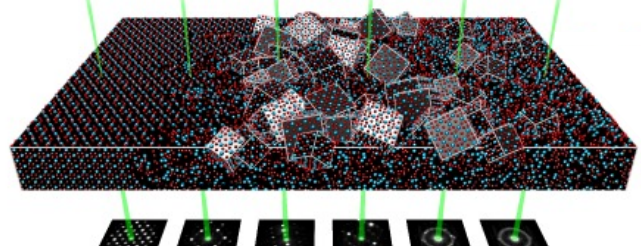


4D-STEM Review

C Ophus, Microscopy and Microanalysis **25**, 563 (2019)

4D-STEM analysis: py4DSTEM

github.com/py4dstem/py4DSTEM
github.com/py4dstem/py4DSTEM_tutorials



www.prism-em.com



Prismatic

STEM Image Simulation

Fast 4D-STEM Simulation Code

Source code, GUI programs for Windows, OSX, Linux, tutorials

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