THE UNIVERSITY of TENNESSEE KNOXVILLE

Lecture 22: Policies and Actions in Microscopy Experiments

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Definitions:

- **Objective:** overall goal that we aim to achieve. Not available during or immediately after experiment.

- **Reward:** the measure of success available at the end of experiment

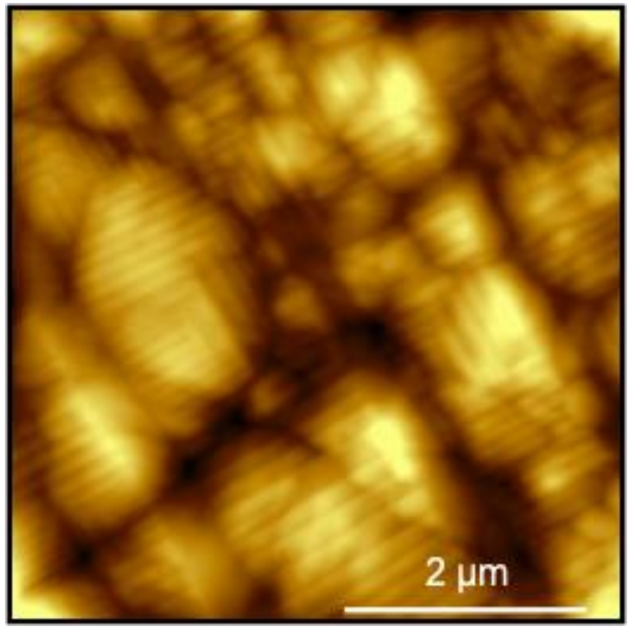
- **Value:** expected reward. Difference between reward and value is a feedback signal for multiple types of active learning

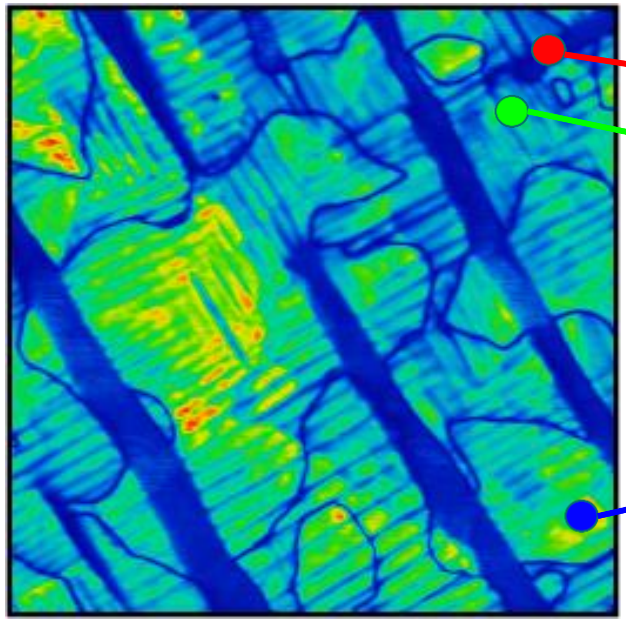
- **Action:** how can ML agent interact with the system

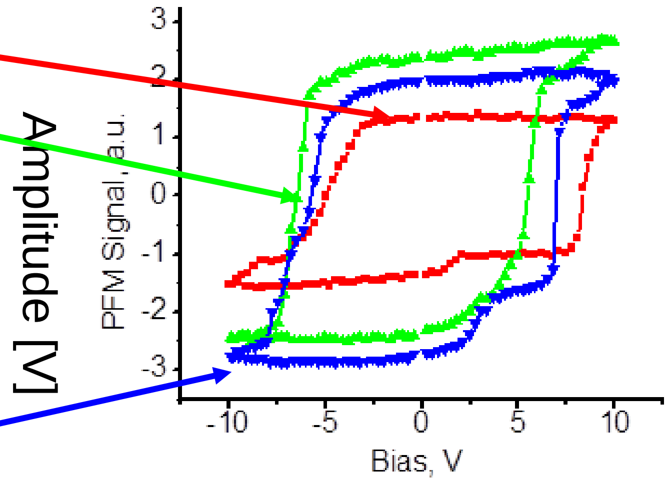
- **State:** information about the system available to ML agent

- **Policy:** rulebook that defines actions given the observed state

Rewards and policies in microscopy world

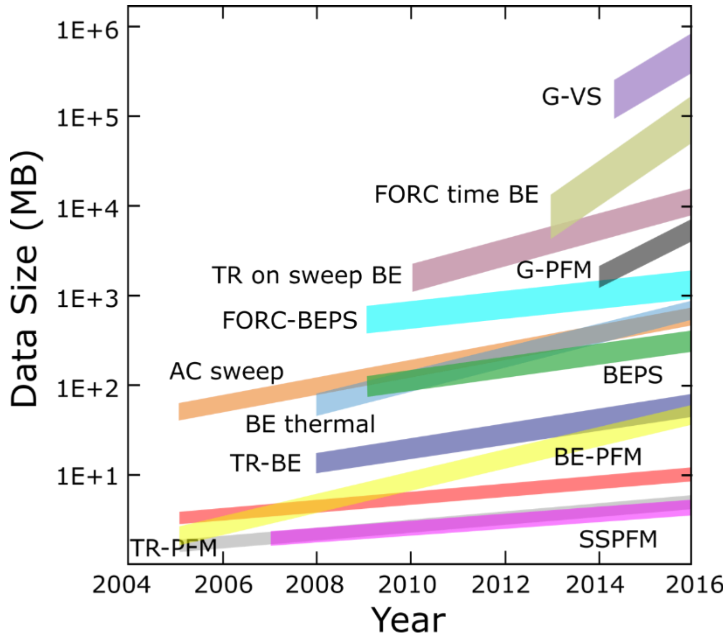






- Interesting functionalities are expected at the certain elements of domain structure
- We can guess some; we have to discover others

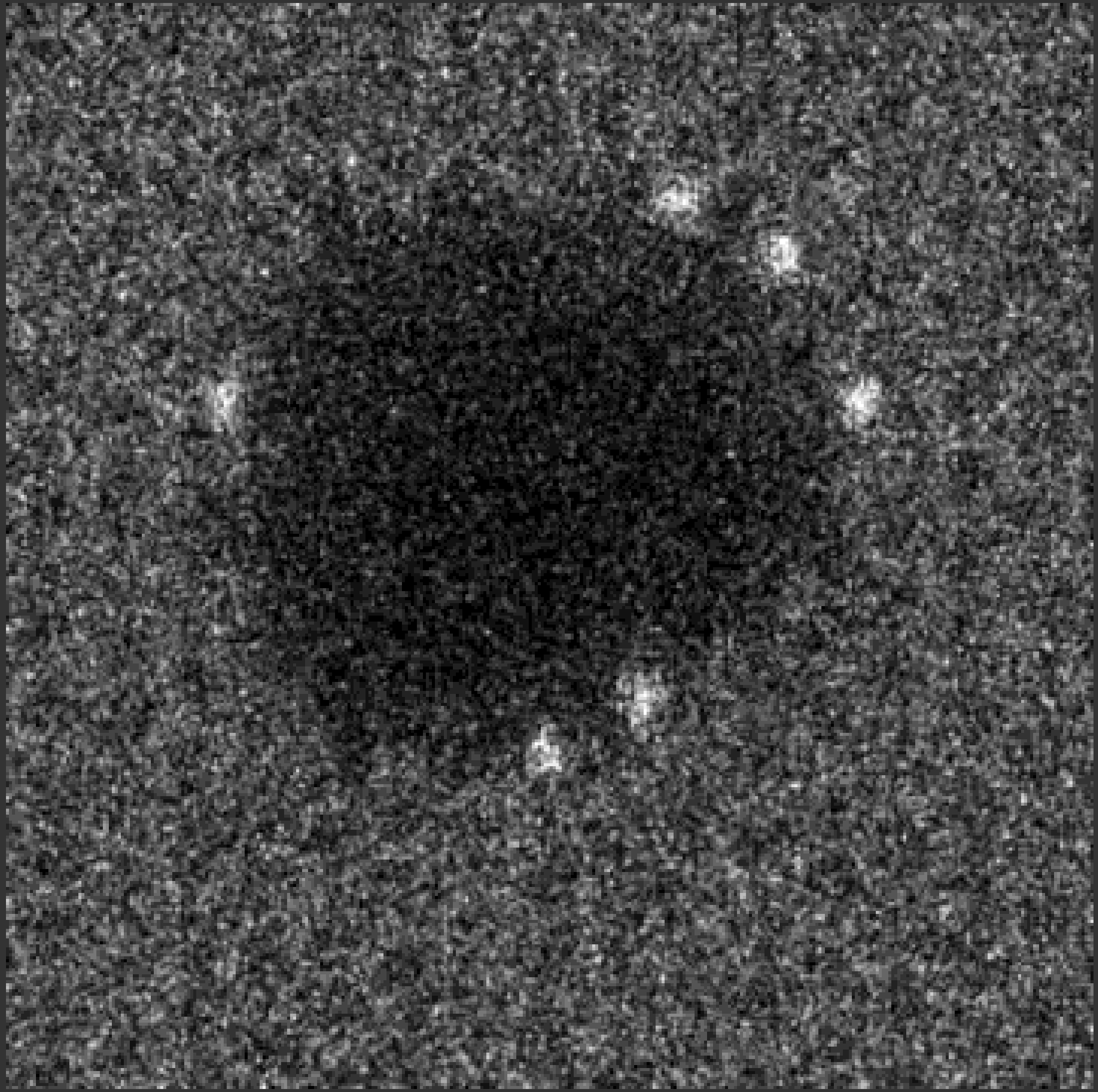
- **Experimental objectives → ML Rewards**
  - Microscope optimization
  - Properties of a priori known regions of interest
  - Discovery of regions with interesting properties
  - Physical theory falsification

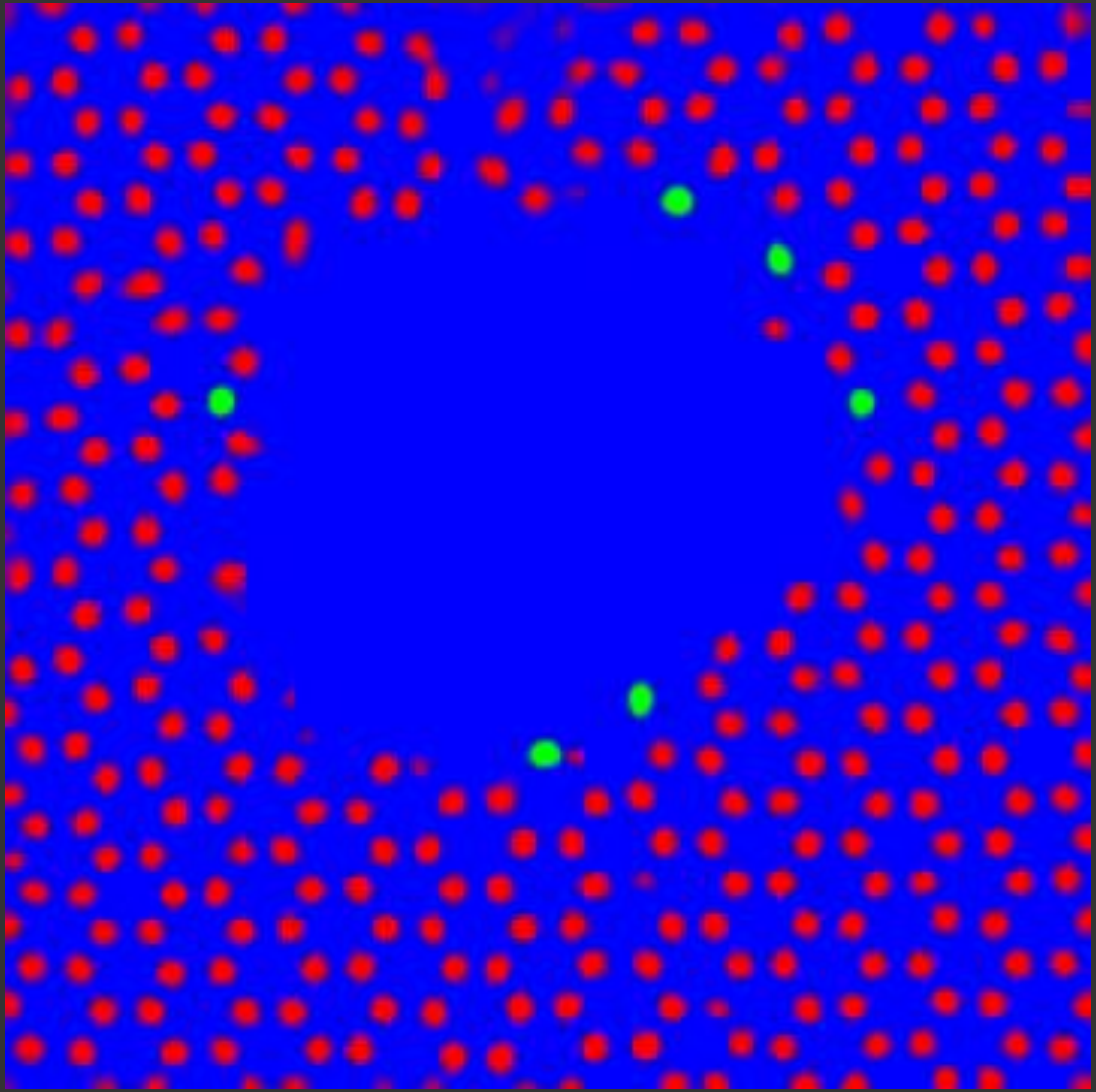


Fixed policy experiments

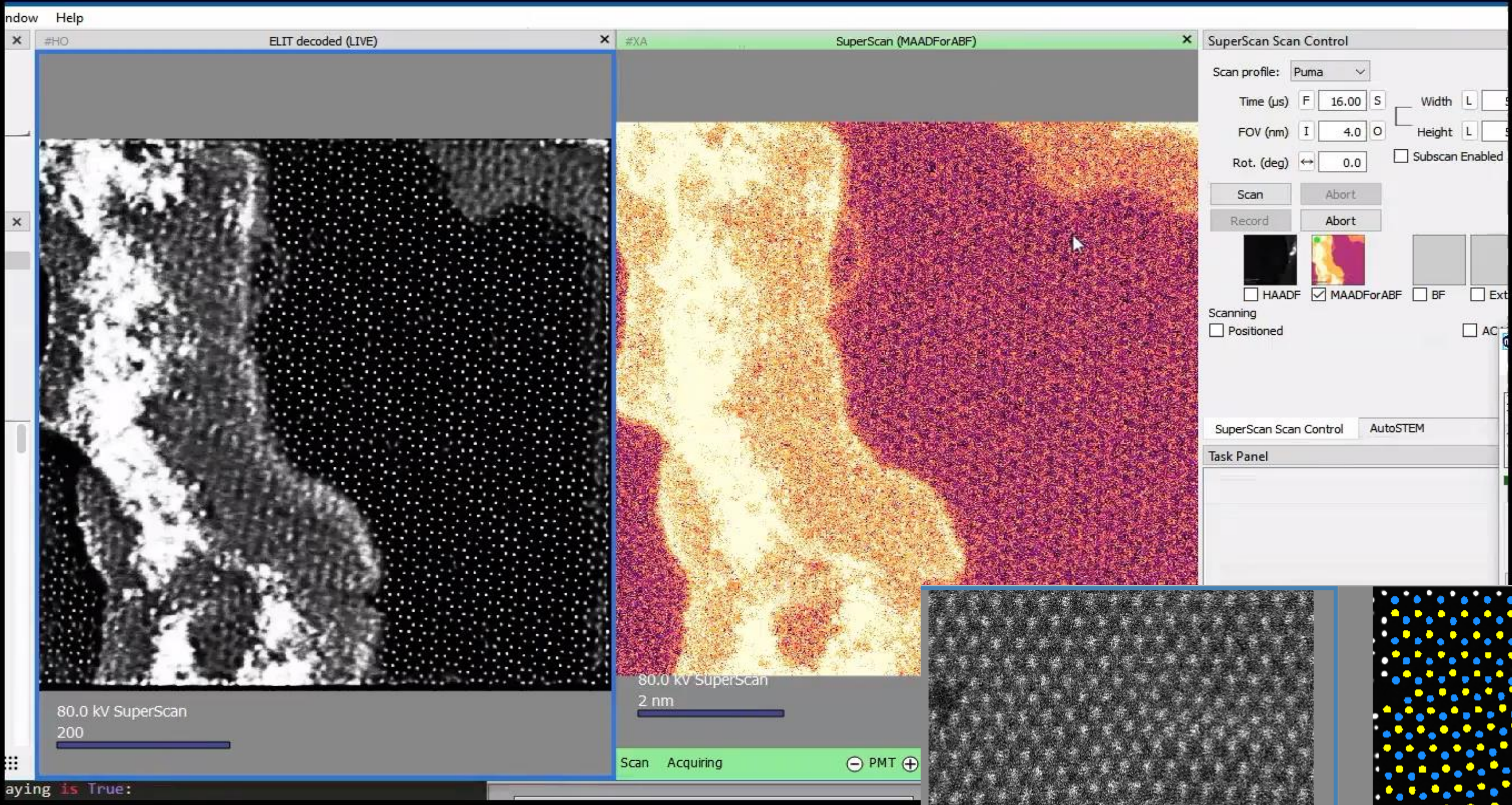
Deep learning works like a charm for:

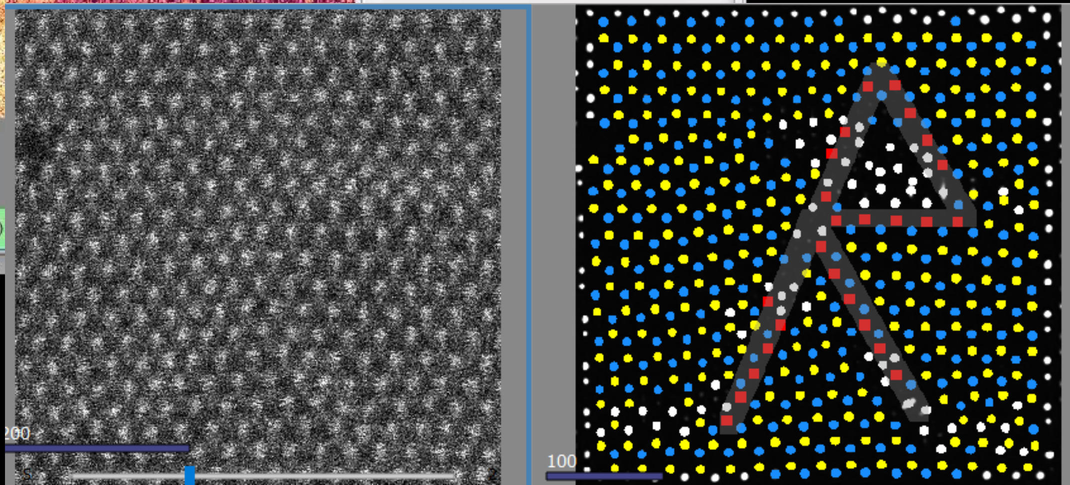
- Drift correction
- Denoising
- Data processing/dimensionality reduction
- Feature finding (physics is in the training set)





AE with Fixed Policies



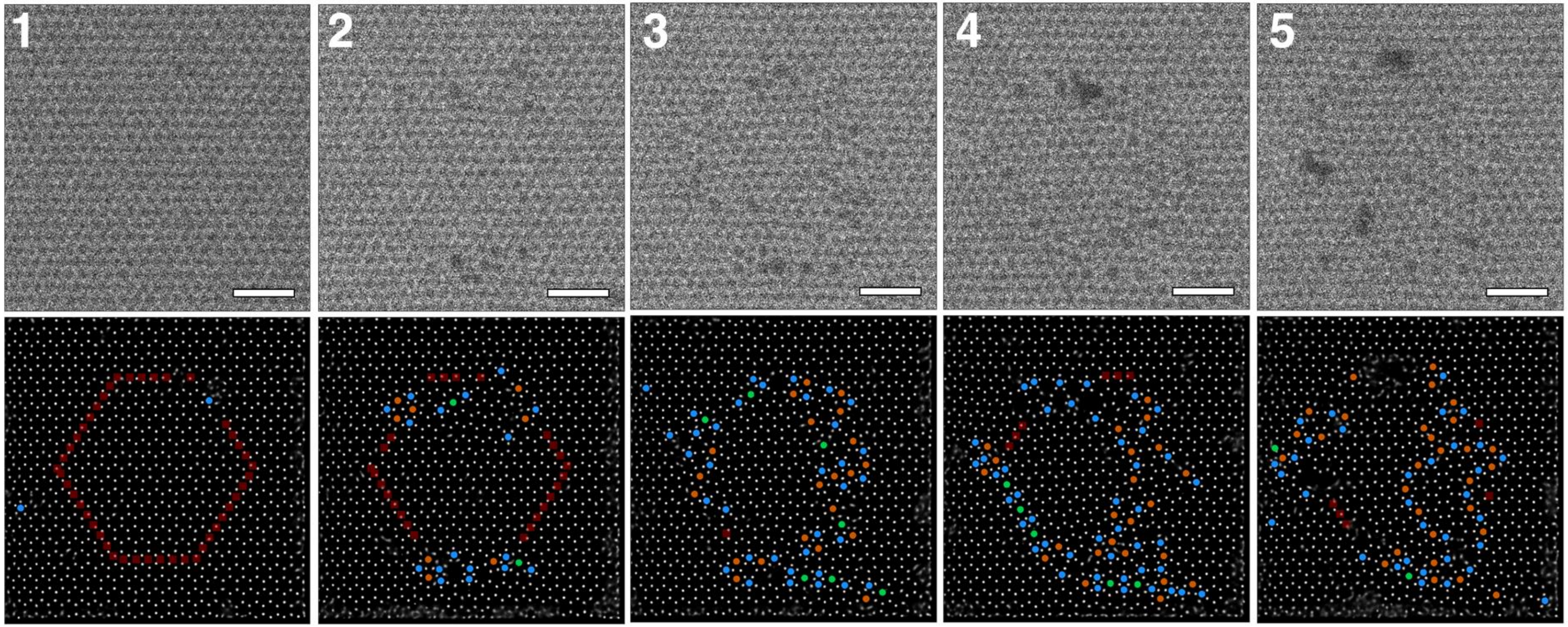


Automated control

Implementation: Kevin Roccapriore, Ayana Ghosh, Sergei V. Kalinin & Maxim Ziatdinov, 2021

Defect patterning in graphene

- Locate atomic coordinates (and defects)
- Direct beam in predetermined path to generate defects (vacancies) – unclear if they form / remain in place
- Repeat scan path, but avoid formed defects
- **Hexagon pattern**



What were we doing?

- **Objective(s):**
  - Understanding electronic and vibrational properties of defects
  - Building structures on the atomic level for biological sequencing and quantum sensing
  - … and so on. We will find out later!

- **Reward:**
  - The number of discovered defects (not used as feedback)
  - Atom moved in desired location

- **Value:** expected reward

- **Action:** position electron beam at given location, take EELS spectrum

- **State:** image

- **Policy:** fixed action table (if detect defect, take EELS)

File Edit View Insert Cell Kernel Widgets Help

Trusted | gpuenv

Run | Code

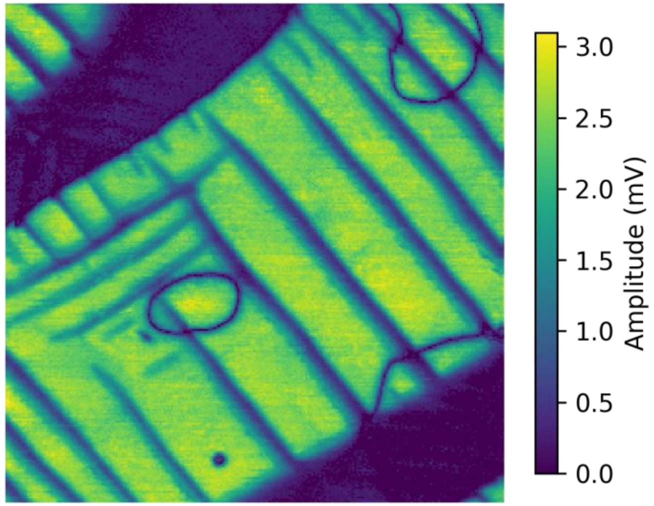
```
move_(-volt*2-(offsetvx), 0, 0-offsetvy, 0, move_speed)
```

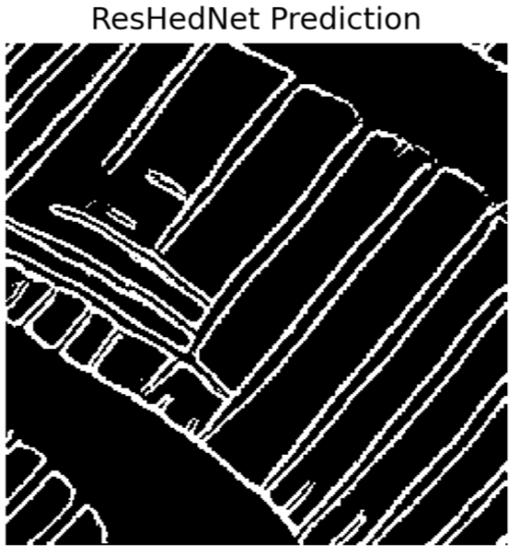

```
scanning line #56
```

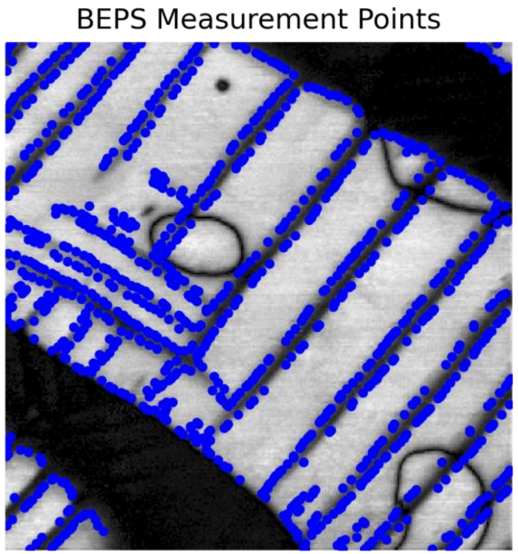
In [ ]:

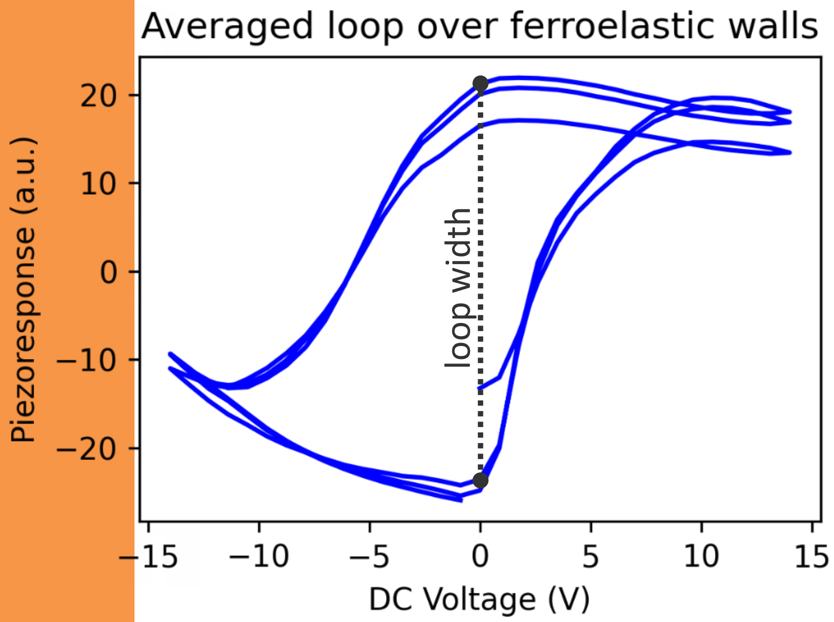
In [ ]:

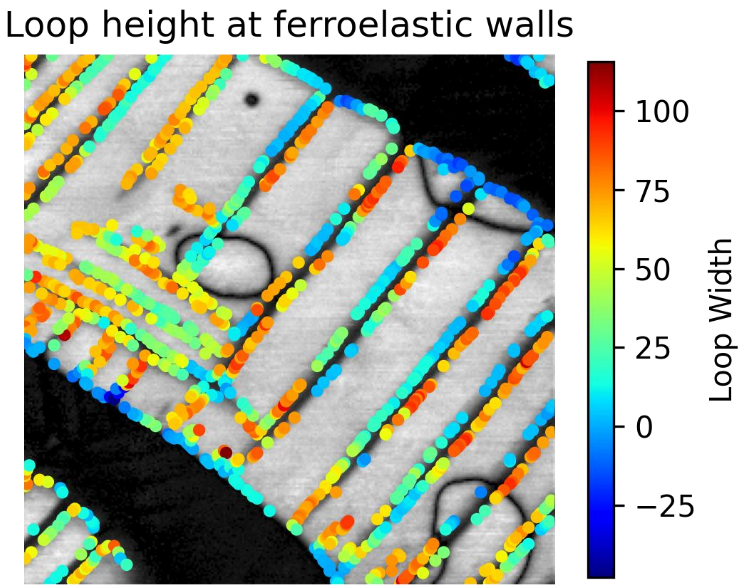
Mapping Activity of Domain Walls

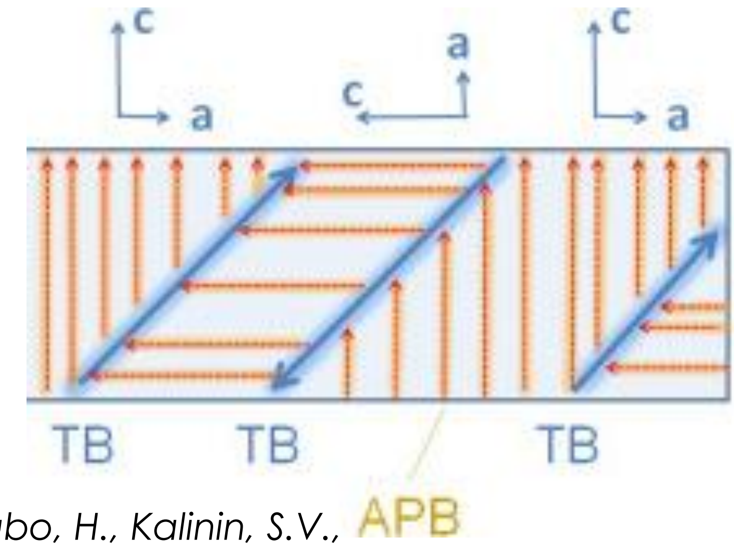












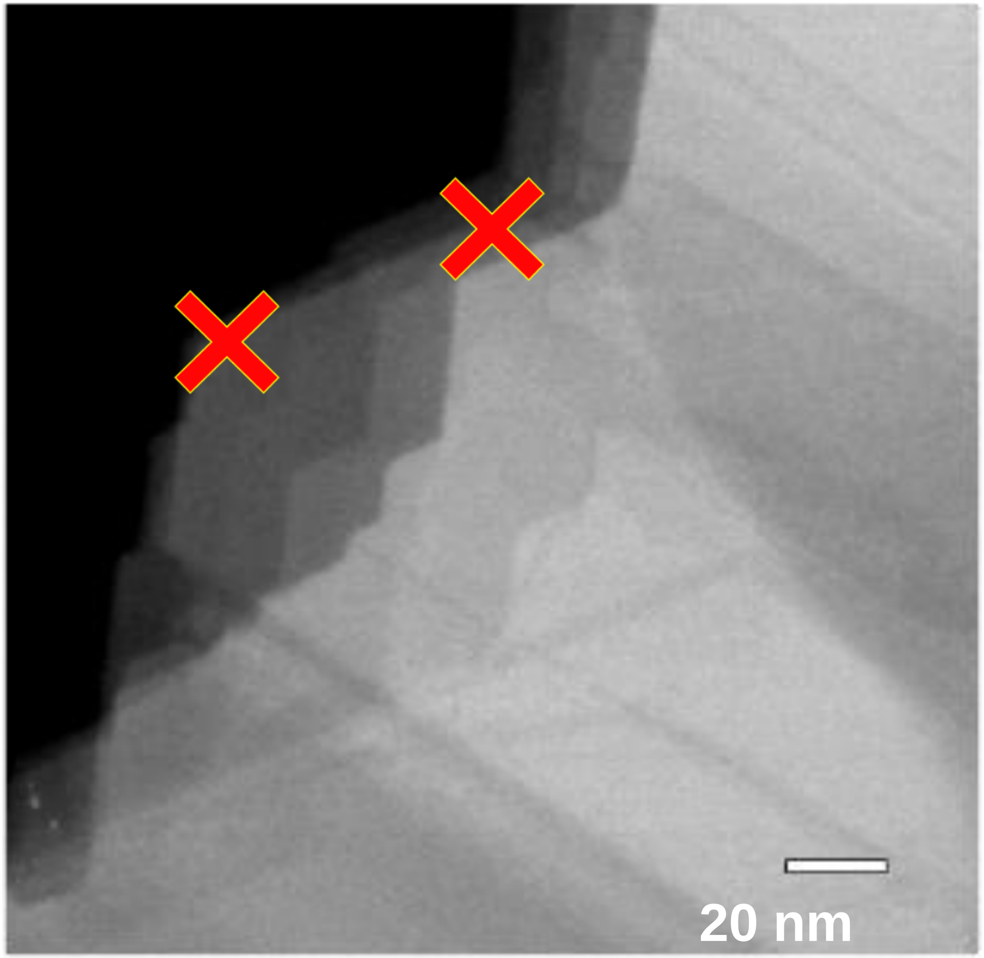
Liu, Y., Kelley, K.P., Funakubo, H., Kalinin, S.V., Ziatdinov, M., Arxiv, submitted

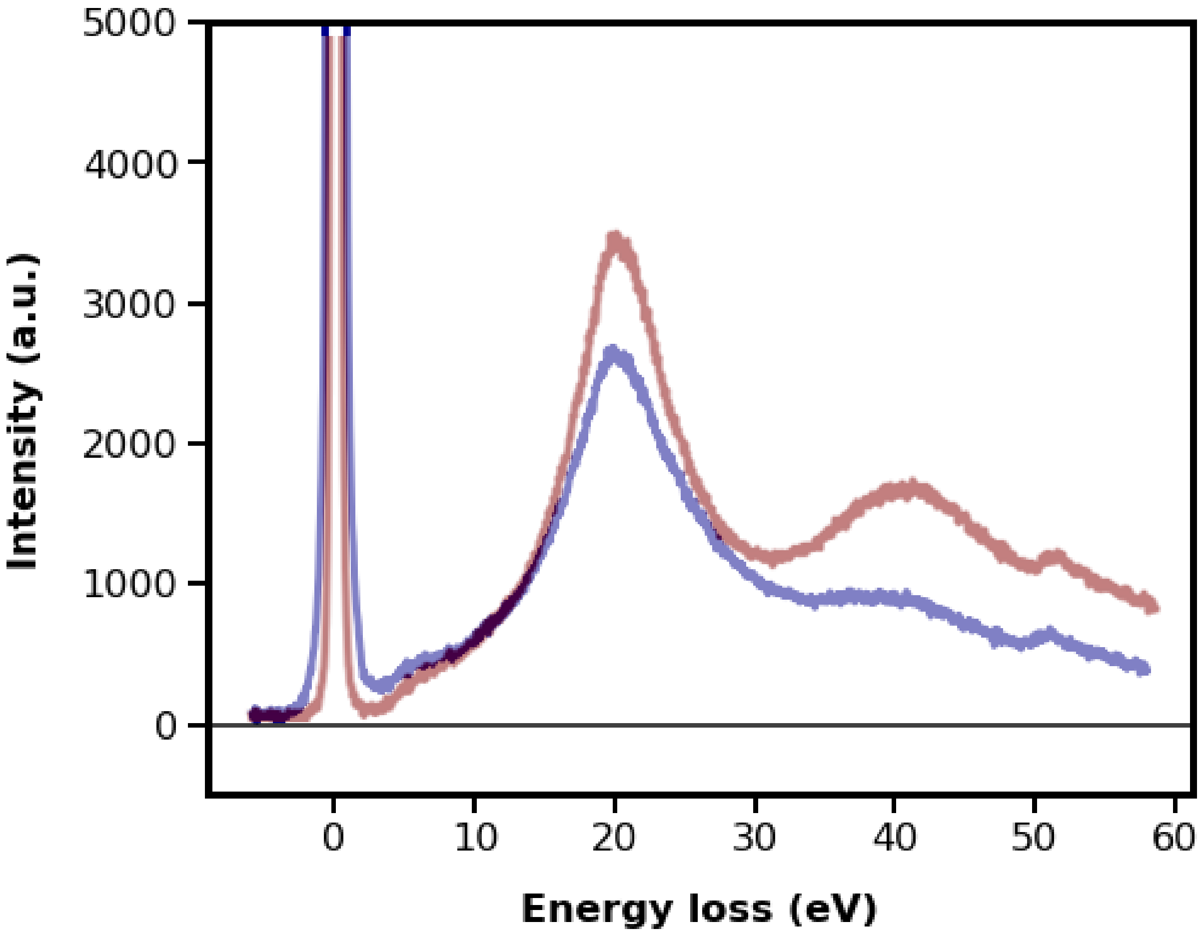
What were we doing?

- **Objective(s):**
  - Understanding the role of domain walls on polarization switching
  - Discover what makes these materials good piezoelectrics
  - … and so on. For fundamental research, vey often impact is clear later!
- **Reward:**
  - The number of explored domain walls (not used as feedback)
- **Value:** expected reward
- **Action:** position SPM probe at a given location, take PFM spectrum
- **State:** image
- **Policy:** fixed action table (if detect wall, take spectrum)

Myopic policy experiments (basically, bandits)

From Static to Active Learning

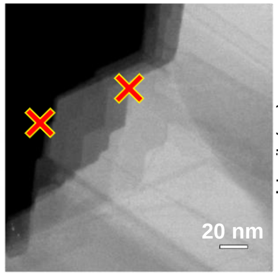


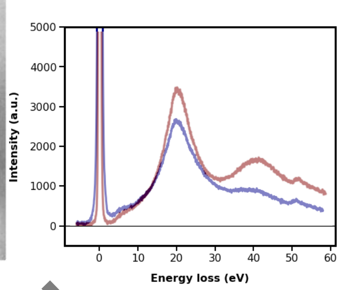


1. What if we have full access to structural information
2. And want to choose locations for (EELS, 4D STEM, CL, EDX) measurements
3. So as to **learn** relationship between structure and spectrum fastest
4. Or **discover** which microstructural elements give rise to specific **desired** spectral features?

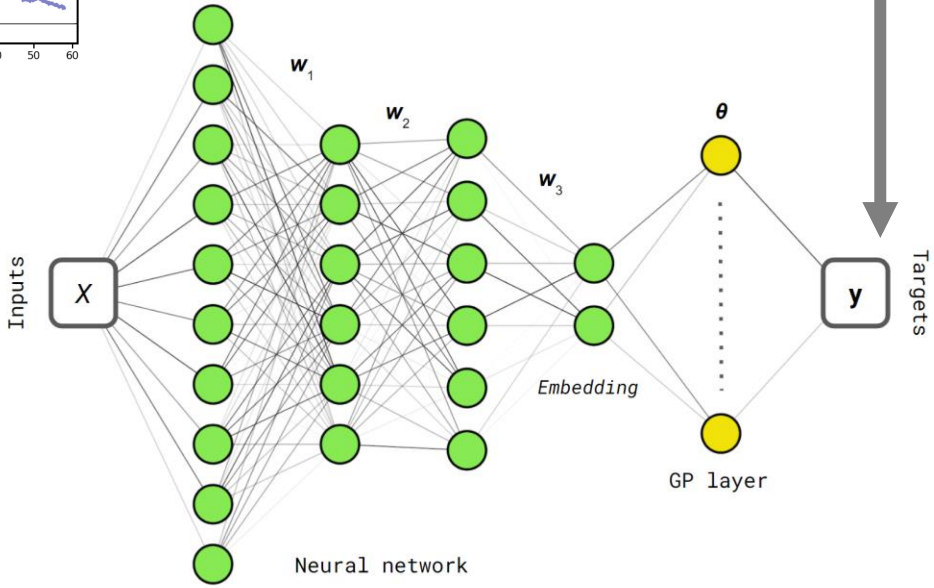
Deep Kernel Learning

- All image patches are available in the beginning of the experiment
- We measure spectra one by one
- And are interested in some specific aspect of spectra
- We aim to learn the relationship between structure and this aspect





Reward
(scalarizer)



Allows navigation of the system to search for physics

<u>Specify physics criteria</u>

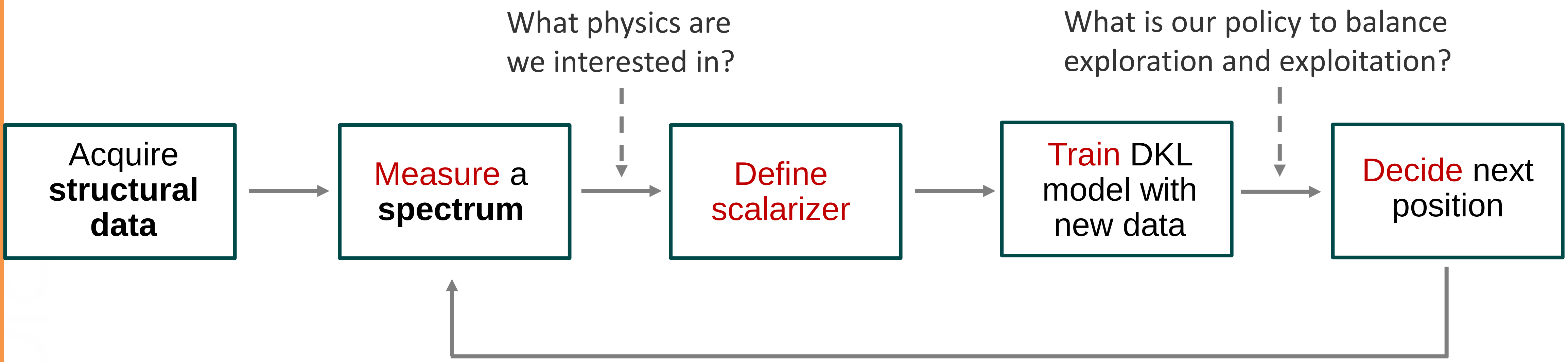
Acquire **structural data**

Measure a **spectrum**

Train DKL model with new data

Decide next position (optimize physics criteria)

Deep Kernel Learning based BO



Key concepts:

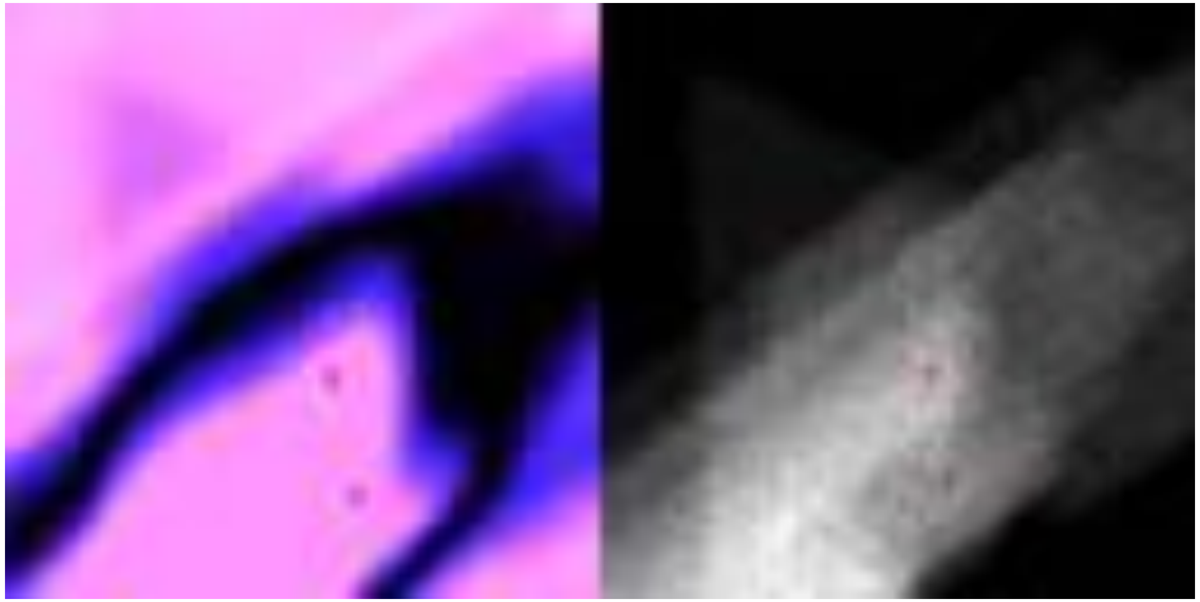
- **Scalarizer:** (any) function that transforms spectrum into measure of interest. Can be integration over interval, parameters of a peak fit, ration of peaks, or more complex analysis

- **Experimental trace:** collection of image patches and associated spectra acquired during experiment. Note that we collect spectra, not only scalarizers

Discovering Regions with Interesting Physics

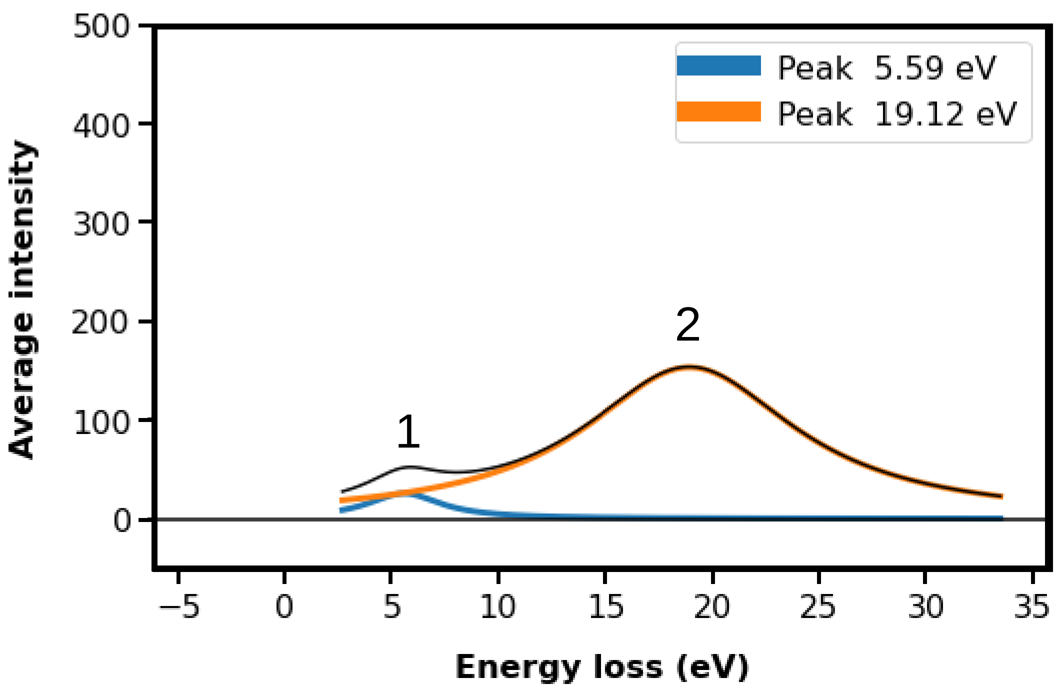
- **Discovering physics in a "new" material $MnPS_3$**
- **Curve fitting** to help enforce physical processes

"Acquisition function" HAADF-STEM



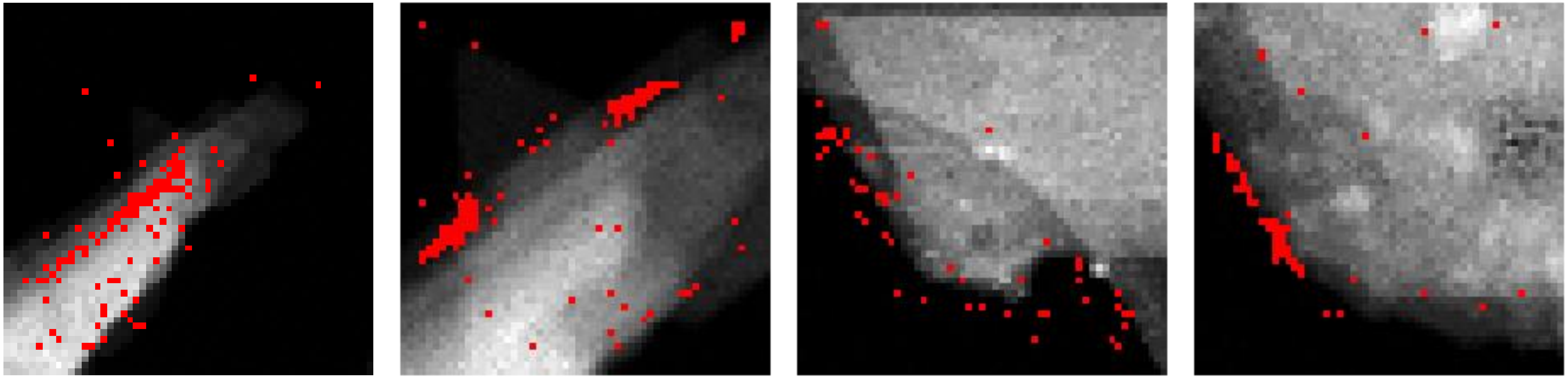
Physics search criteria:

$$\boldsymbol{Ratio = Peak\,1\,/\,peak\,2}$$



More Examples of Physics Discovery

- Very similar behavior when searching for the same criteria!
- Success!

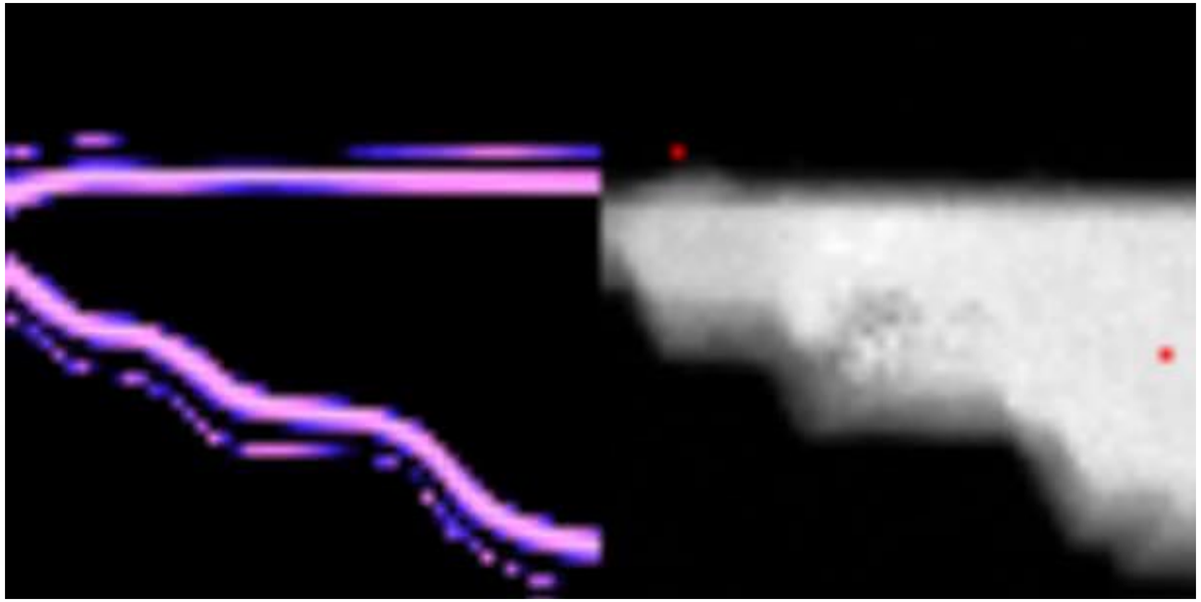


Discovery pathway depends on the reward structure (scalarizer that defines signature of physics we want to discover)!

Changing the scalarizer

- (Same region) **Simple physics search:** peak max in selected region

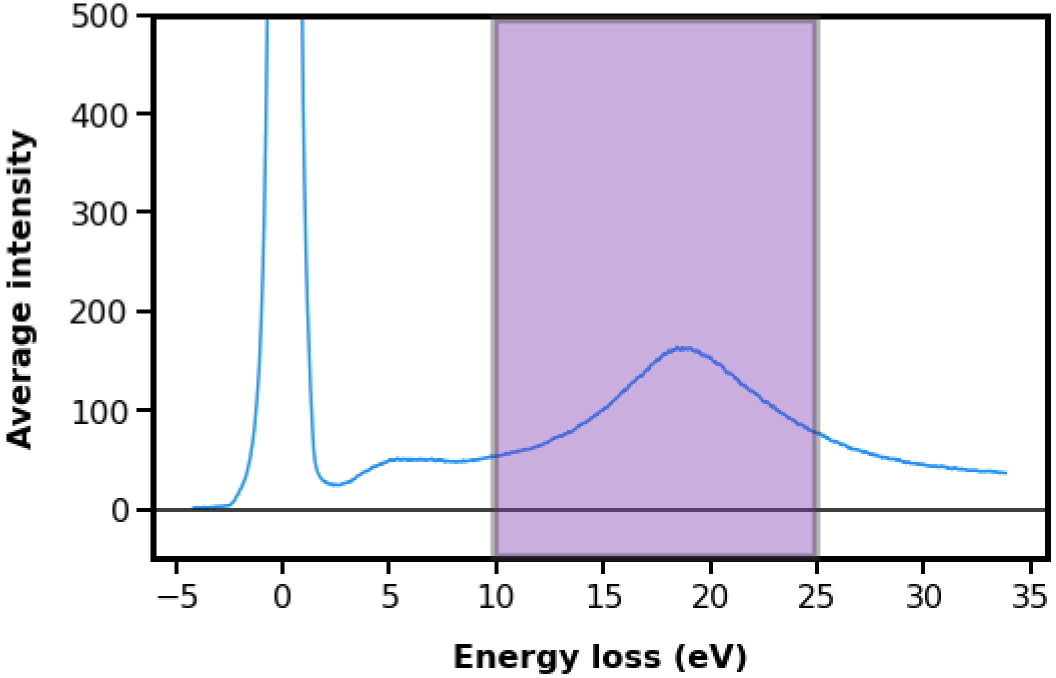
“Acquisition function” HAADF-STEM + points visited



Physics search criteria:

$$\boldsymbol{Maximize(f)}$$

(Specific peak intensity)



What were we doing?

- **Objective(s):**
  - Understanding the emergence of the nanoplasmonic behaviors
  - For understanding physics, optical interfaces to quantum devices, etc.
  - … and so on. For fundamental research, vey often impact is clear later!

- **Reward:**
  - Minimizing uncertainty in structure-property relationships (can we predict expensive EELS from cheap structure)
  - Discovering structures that maximize certain aspect of nanophotonic behavior (have maximal intensity of certain peak, peak area ratio, etc.)

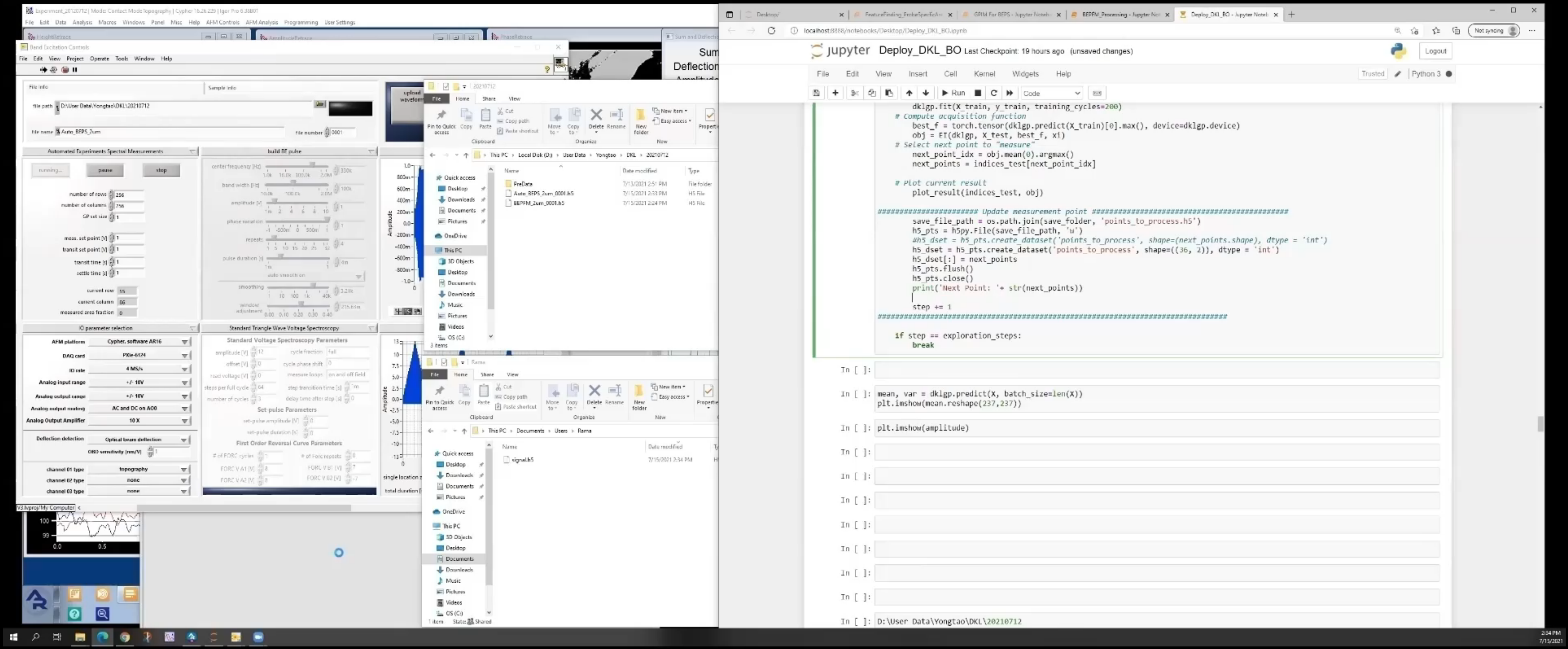
- **Value:** expected reward. Here – predicted scalarizer

- **Action:** position STEM probe at a given location, take EELS spectrum

- **State:** image patch

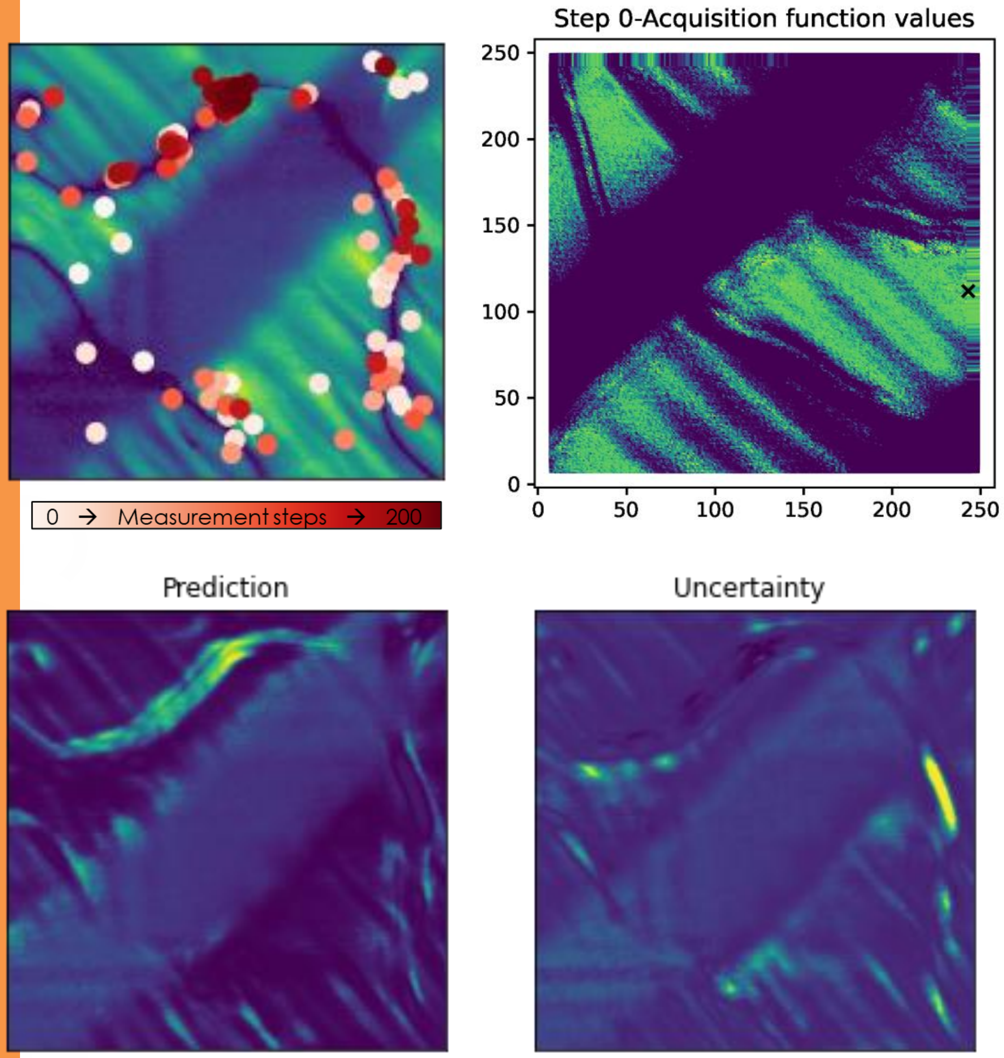
- **Policy:** myopic optimization (actually, upper confidence bound) with defined exploration-exploitation balance

Deep Kernel Learning AE SPM

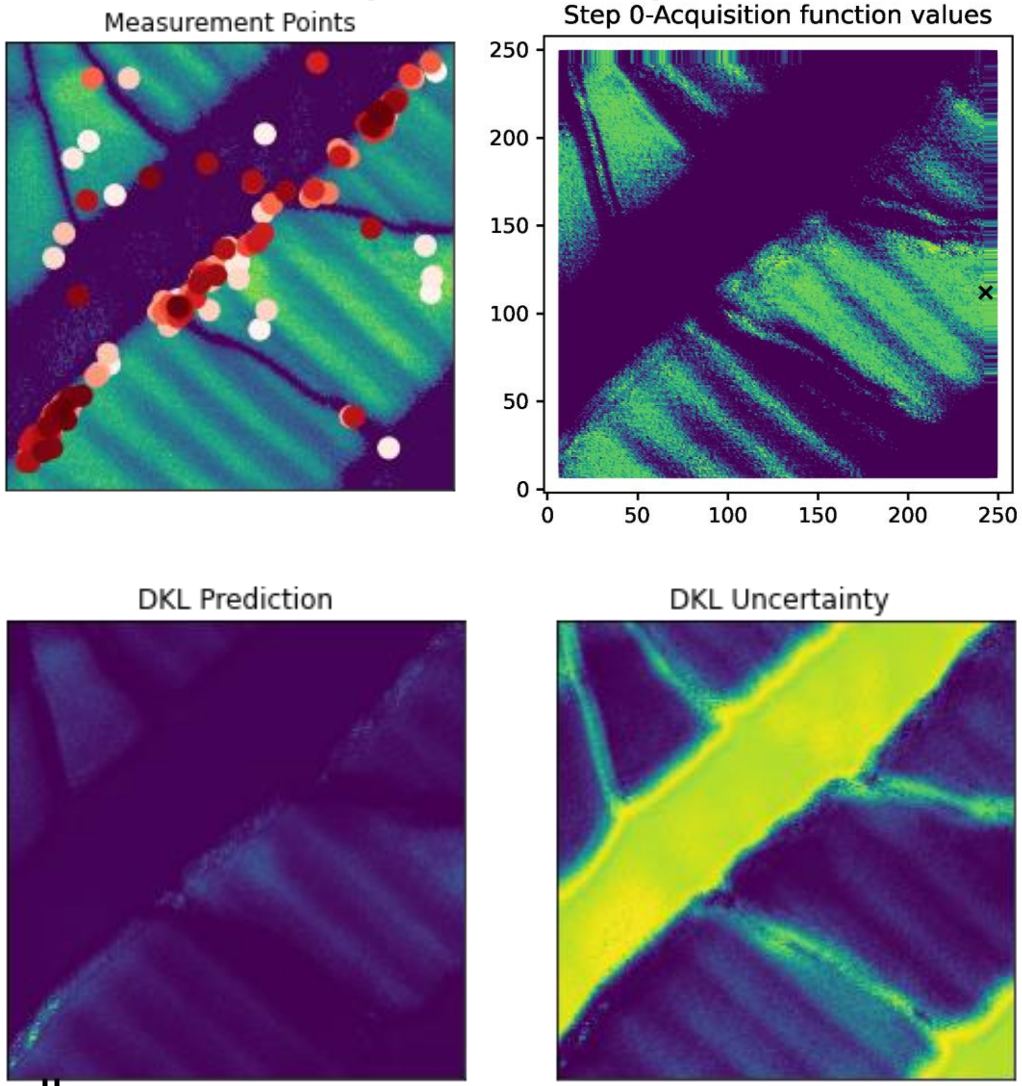


DKL SPM

Guided by: On field loop area



Guided by: Off field loop area

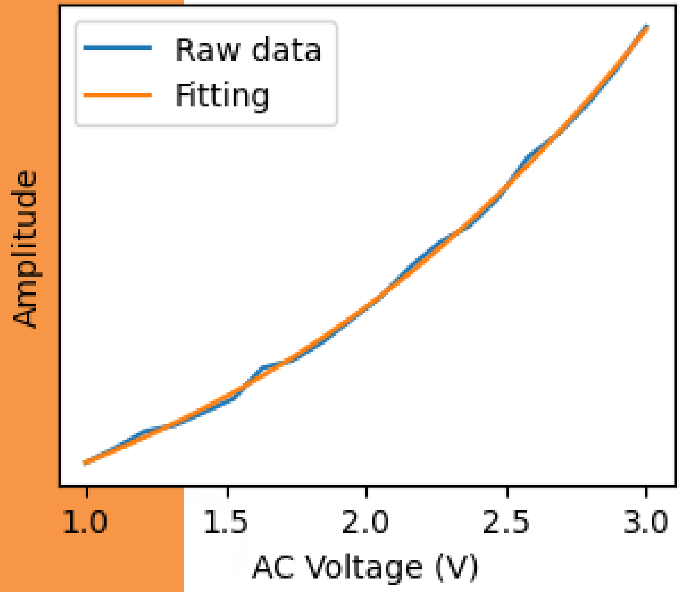


- ➢ Large loop opening corresponding 180º domain walls
- ➢ This behavior can be attributed to the large polarization mobility of 180º walls

Liu, Yongtao, et al, Nature Machine Intelligence 4, 4 (2022): 341-350.

Exploring Non-Linearity

- Shown are 200-step measurements of PTO and HZO thin films
- PFM amplitude was used as structure image; A/B was used to guide the measurement.

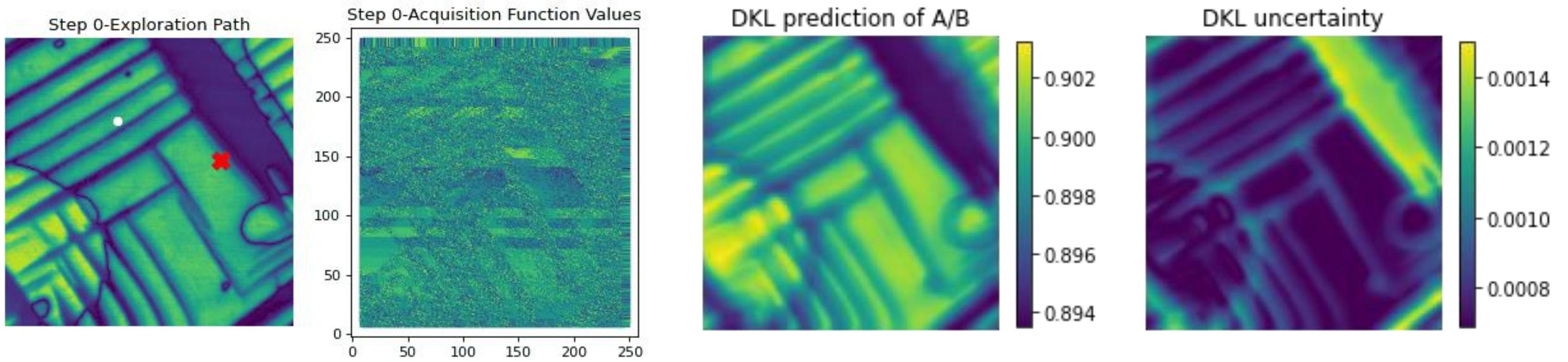


V_{AC} sweep curve at each location was fitted as $y = Ax^3 + Bx^2 + Cx$

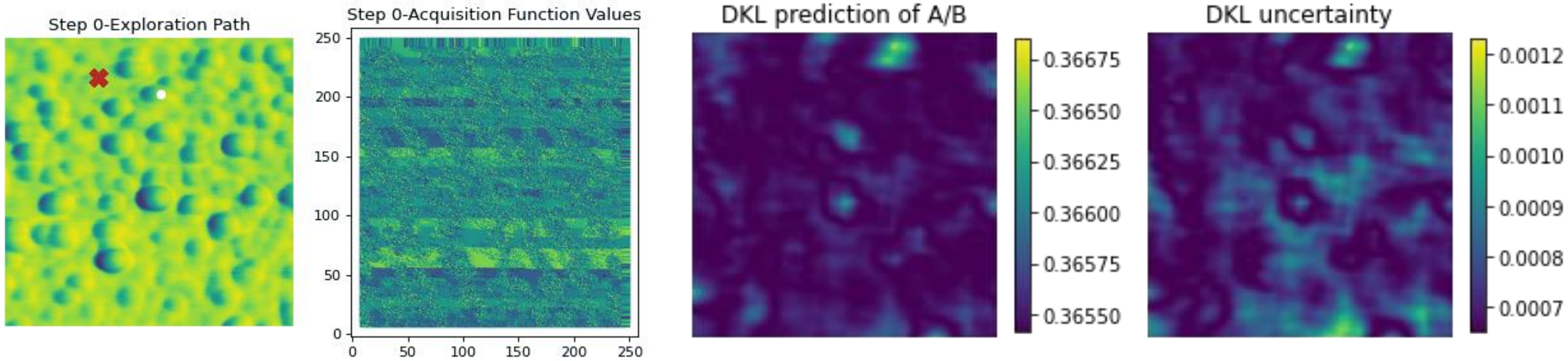
A, B, C, and A/B were us as the target function to guide DKL-V_{AC} measurement.

PTO and HZO thin films were studied.

PTO experiment process and results



HZO experiment process and results



- In conventional microscopy experiment, human runs everything directly – defines scan, positions the probe, defines measurement parameters.

- In AE SPM, the policies are defined before the experiment and do not change. Sometimes it works – but not always.

- How would we:
  – (a) explain the AE progression after the experiment and
  – (b) control it during the experiment ?

Is there a problem with this type of automated experiment?

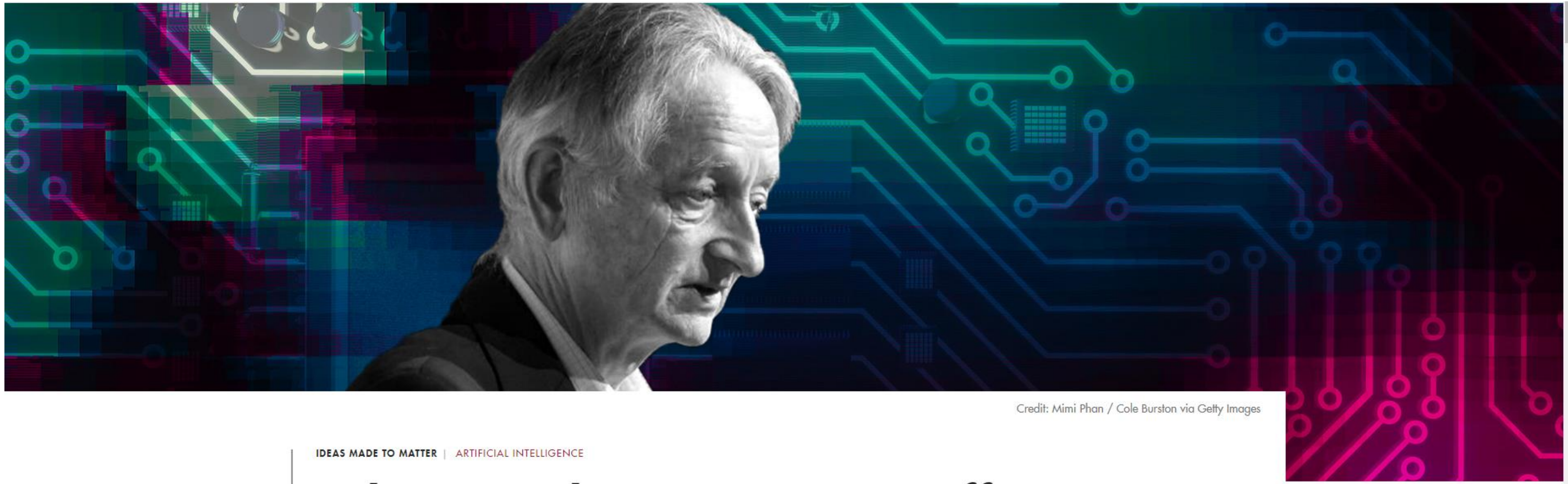
Taking the Human Out of the Loop: A Review of Bayesian Optimization

Citation

Shahriari, Bobak, Kevin Swersky, Ziyu Wang, Ryan P. Adams, and Nando de Freitas. 2016. “Taking the Human Out of the Loop: A Review of Bayesian Optimization.” Proc. IEEE 104 (1) (January): 148–175. doi:10.1109/jproc.2015.2494218.

Published Version

doi:10.1109/JPROC.2015.2494218



Credit: Mimi Phan / Cole Burston via Getty Images

IDEAS MADE TO MATTER | ARTIFICIAL INTELLIGENCE

Why neural net pioneer Geoffrey Hinton is sounding the alarm on AI

Solution: if we can monitor in real time, we can adjust rewards and policies!

Interactive AI

Human-in-the-loop Automated Experiment

Future homework:

- Identify objectives, rewards, policies, values in the publication of your choice (or from suggested list)
- Suggest possible rewards for battery/fuel cell/etc. optimization problem