Scanning Tunneling Microscopy (STM) Image Segmentation Using Unsupervised and Few-shot Learning

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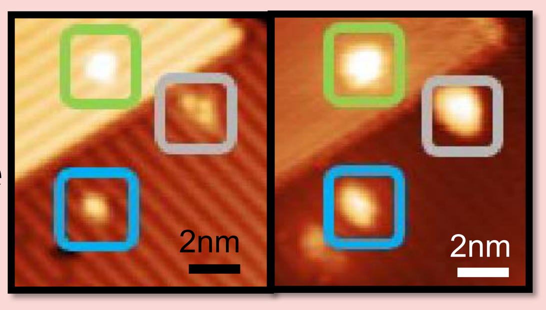
- Scanning tunneling microscopy (STM) is a powerful technique for imaging surfaces with atomic resolution, providing invaluable insights into surface structure and physical and chemical processes occurring on surfaces. A regular task of STM image analysis is detecting and labelling features of interest against the background of the unperturbed surface. Performing this segmentation manually is a labor-intensive task, requiring significant human effort.
- We propose an automated approach to the segmentation of STM images that leverages few-shot learning and unsupervised learning to remove the requirement for large manually annotated datasets.

(1) STM imaging

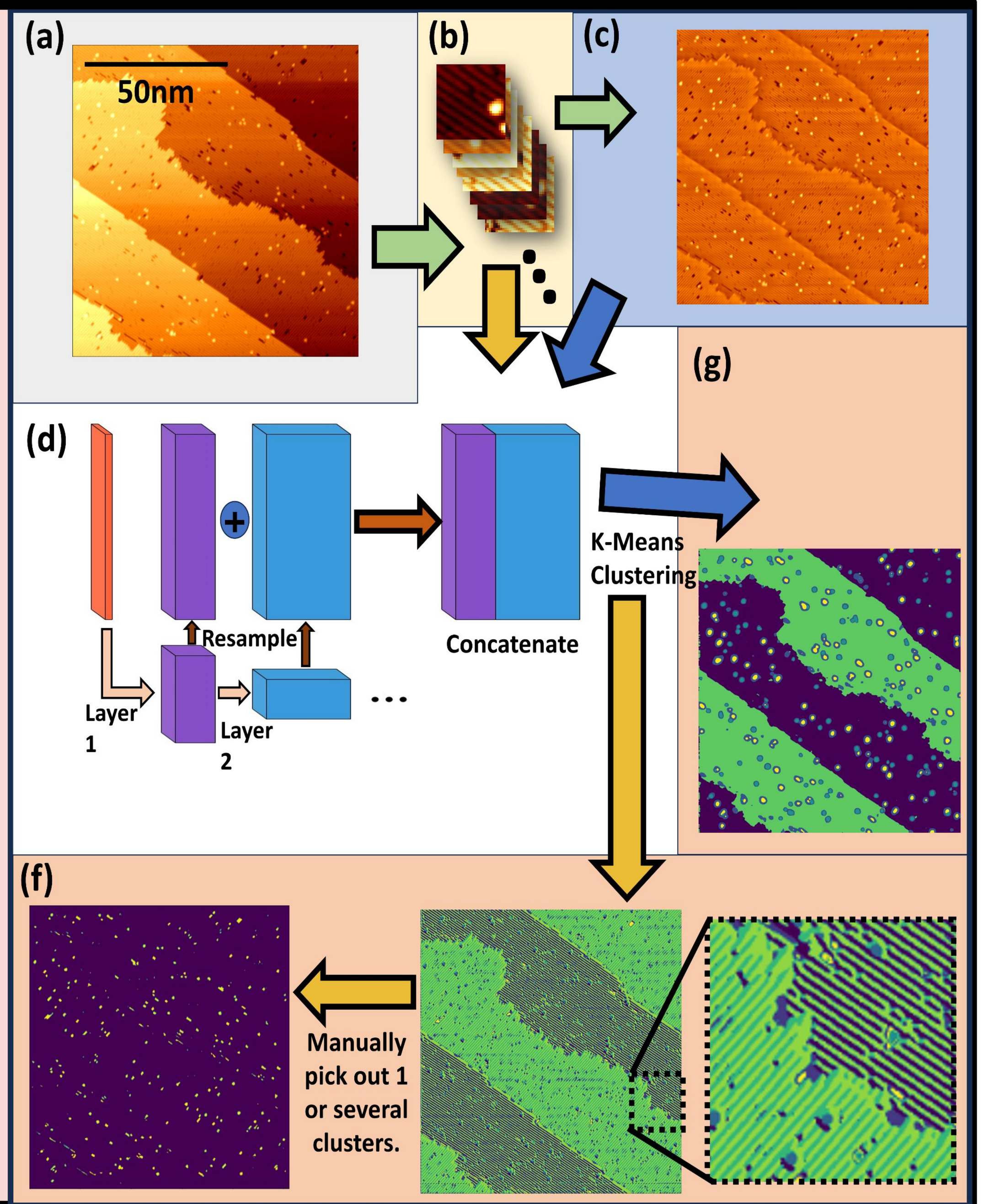
- A microscopy technique used to image conducting surfaces with **atomic resolution**. It can also **manipulate single atoms** on the surface.
- Each pixel in an image represents the height of the density of electron states at that point. We can measure either the filled or empty states, producing 2 channels.

Images of the Si(001) surface with different defects (the size of a few atoms) highlighted.



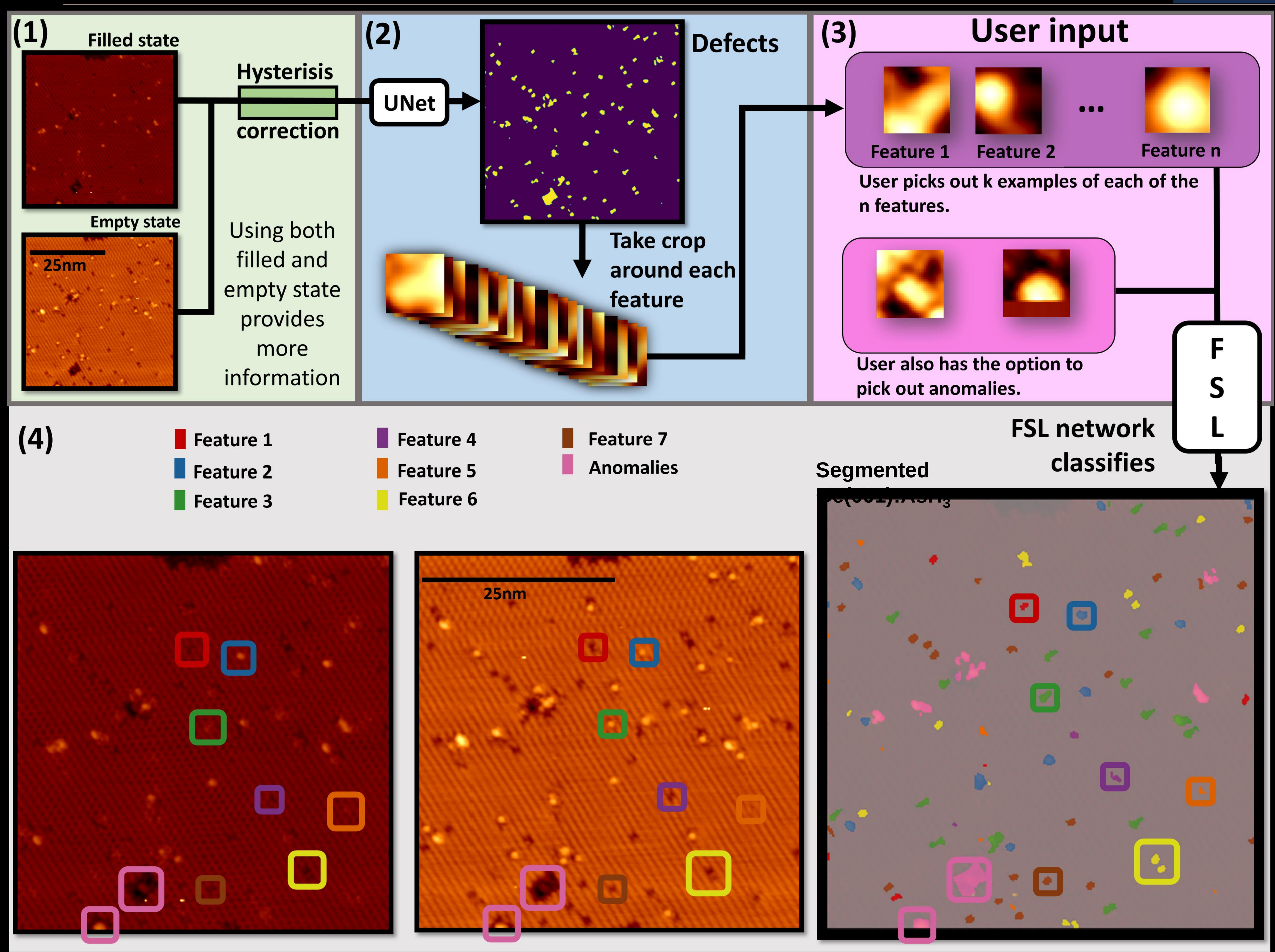
(2) – UNet & Automated Labelling of training data

- UNet is used to produce a **binary map** of the all the defects on the surface (like the one shown in f).
- We want to **reduce** the time spent **manually** labelling training data for the UNet:
  - Use a pretrained network (FCNResnet101) to extract feature vectors for each pixel.
  - These are then clustered using k-means clustering to produce a segmented image.
  - By **varying the resolution** of the input, we can change how **detailed** the segmentation is: higher resolution highlights features such as **atomic rows and defects**, lower resolution focuses more on **phase domains.**
  - These images are then augmented, and **extra experimental noise** is added to train a UNet. In this way, we get a more **robust**, and **faster**, segmentation network.



(3) – FSL networks

- We test multiple few-shot learning (FSL) networks.
- The prototypical, matching, relation, and simple shot (conv4) all have a **Conv4 backbone** and are trained using episodes on **subject specific data**.
- We test a simple shot network with a pretrained (**non-subject specific**) Resnet18 backbone.
- Are the embeddings **useful/meaningful**? - We compare to the accuracy of KNN on the **bare** pixels.



(4i) – Si(001):H:AsH_3

- Surface is of especial significance for the **semiconductor** and **quantum computing** industry [1][2].
- FSL allows for flexibility to implement new dopant atom precursor types with as little as one new labelled data point.
- Models are trained and tested on data from the same surface.

Model	Training Set	Acc (4-way, 1-shot)
Prototypical	Si defects	**95.567±0.013%**
Matching	Si defects	94.950±0.009%
Relation	Si defects	93.400%±0.014%
Simple shot (conv4)	Si defects	92.933±0.010%
Simple shot (Resnet18)	ImageNet	66.873±0.030%
KNN (K=1) on bare pixels	Si defects	76.567±0.020%

(4ii) – Ge(001):AsH_3 and TiO_2

Results for all tables are accuracies averaged over 100 episodes and with 95% confidence interval.

Model	Training Set	Acc (4-way, 1-shot)
Prototypical	Si defects	61.25±0.02%
Matching	Si defects	**61.61±0.02%**
Relation	Si defects	25.07%±0.01%
Simple shot (conv4)	Si defects	48.18±0.01%
Simple shot (Resnet18)	ImageNet	43.00±0.02%
KNN (K=1) on bare pixels	Ge defects	46.64.±0.02%

Classification on Ge(001):AsH_3 data. **Trained on defects from non-Ge(001):AsH_3 data.**

Model	Training Set	Acc (2-way, 1-shot)
Prototypical	Si & Ge defects	**70.03±0.03%**
Matching	Si defects	61.60±0.02%
Relation	Si defects	30.93%±0.03%
Simple shot (conv4)	Si defects	54.47±0.02%
Simple shot (Resnet18)	ImageNet	65.03±0.02%
KNN (K=1) on bare pixels	TiO_2 defects	57.40±0.03%

Classification on TiO_2(110) data. TiO_2(110) data has only filled state images. **Trained on defects from non-TiO_2(110) data.**

- The technique offers greater flexibility compared to previous supervised methods, being easier to adapt to an unseen surface while maintaining high accuracy, reaching up to 90%. This will make it useful for research which is constantly studying new substrates and adsorbates.
- Right hand column of tables shows accuracy of classification of the networks. It demonstrates the effectiveness of our approach on three distinct surfaces: Si(001):H:AsH_3, Ge(001):AsH_3, and TiO_2(110). We show that our model exhibits strong generalization capabilities, adapting well to unseen surfaces with only as little as one additional labeled data point after initial training.
- Different FSL-networks are tested, with the prototypical performing the best overall. The relation network shows signs of overfitting.
- Currently, no standardized dataset to use for benchmarking exists within the STM community. We believe this would be a worth while, but time consuming, venture.
- An ablation study (not included) showed simple manipulations to the data to generate new classes allowed for a better feature embedding and therefore accuracy.

[1] Stock, T.J., Warschkow, O., Constantinou, P.C., Li, J., Fearn, S., Crane, E., Hofmann, E.V., Kölker, A., McKenzie, D.R., Schofield, S.R. and Curson, N.J., 2020. Atomic-scale patterning of arsenic in silicon by scanning tunneling microscopy. ACS nano, 14(3), pp.3316-3327.

[2] Stock, T.J., Warschkow, O., Constantinou, P.C., Bowler, D.R., Schofield, S.R. and Curson, N.J., 2024. Single-Atom Control of Arsenic Incorporation in Silicon for High-Yield Artificial Lattice Fabrication. Advanced Materials, p.2312282.

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