Machine learning detection and classification of defects in STM lithography data

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Introduction

Atom-by-atom fabrication using scanning tunneling microscopy (STM) has great potential to revolutionize materials synthesis for digital electronics. Key to the fabrication process is the ***automatic*** localization and classification of intended or unintended defects – seen in Figure 1(a) below – in STM data.

Auto defect detection and classification:
1. STM Lithography data
2. Defect detection neural network
3. Defect classification neural network

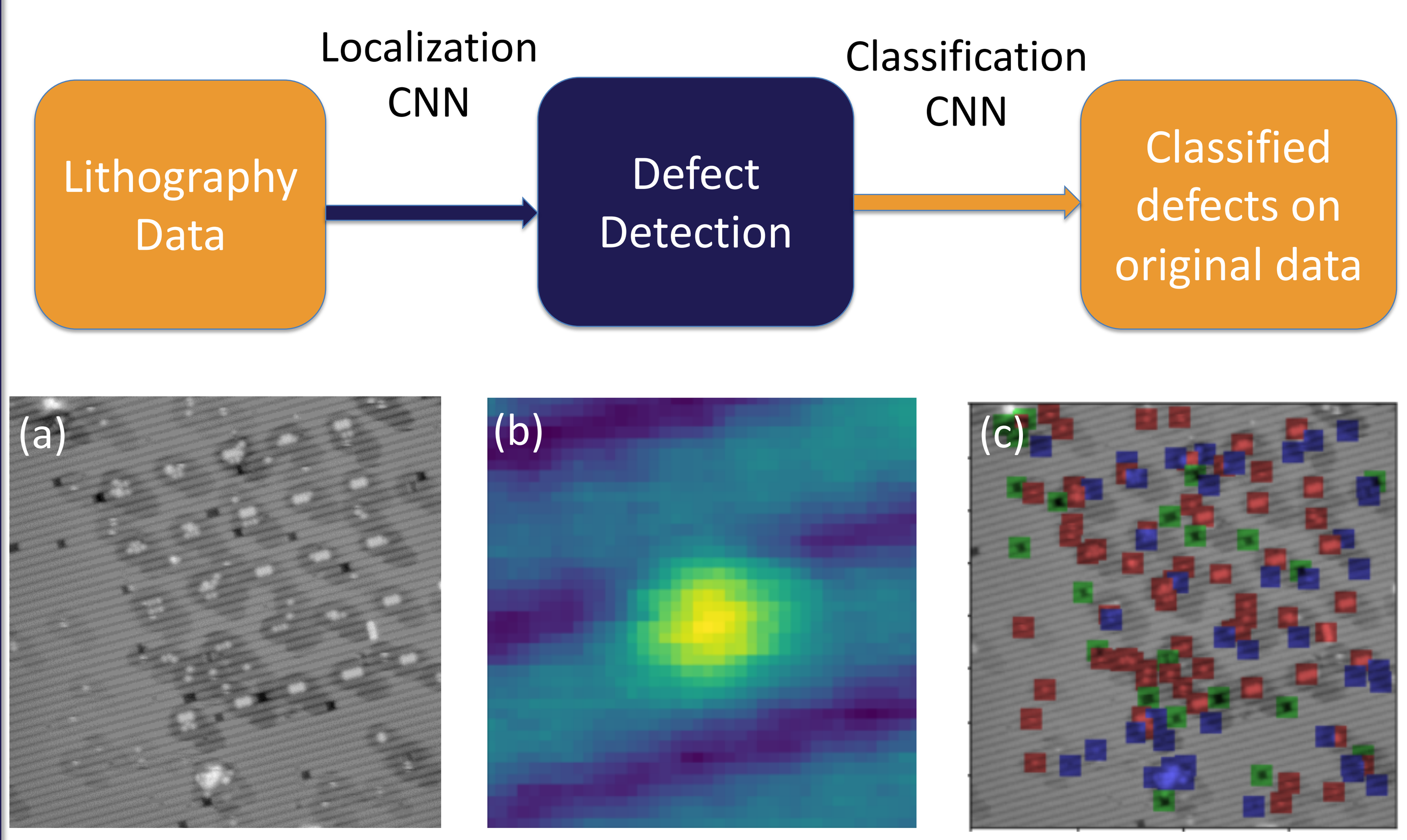
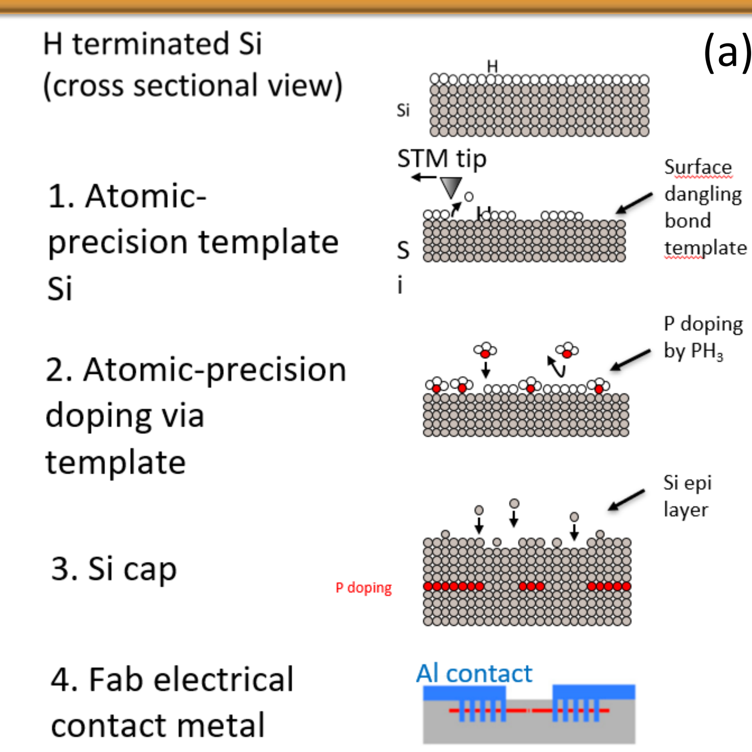


Figure 1: Machine learning workflow showing the input and output data for each network

1. STM Lithography Data

- Scanning Tunneling Microscopy is used to generate images like those seen in Figure 2 (b and c)
- Bright and dark spots are types of defects
- Hydrogen depassivation as seen in Figure 2(a) leads to an array of stripped hydrogen as seen in Figure 2(c)



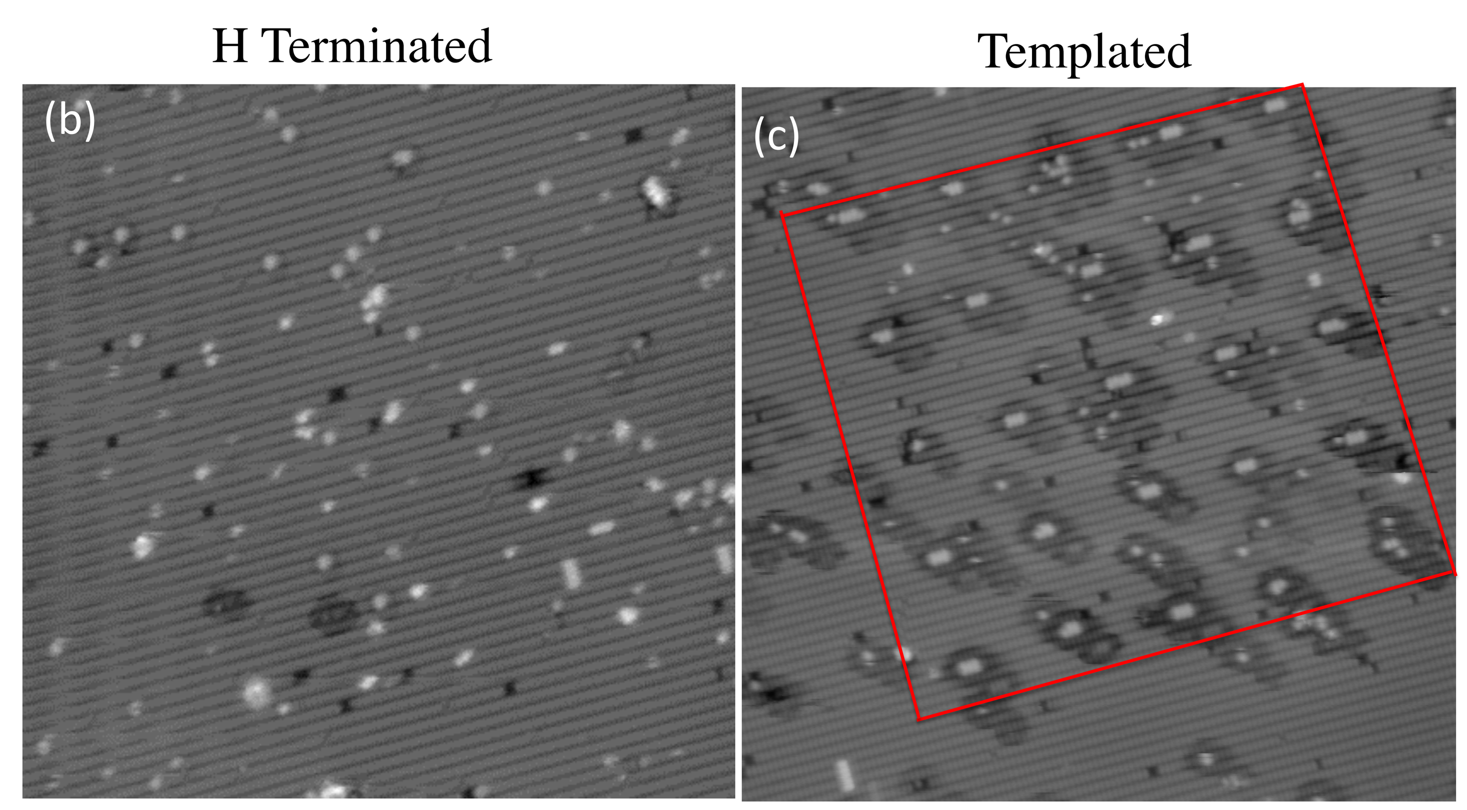


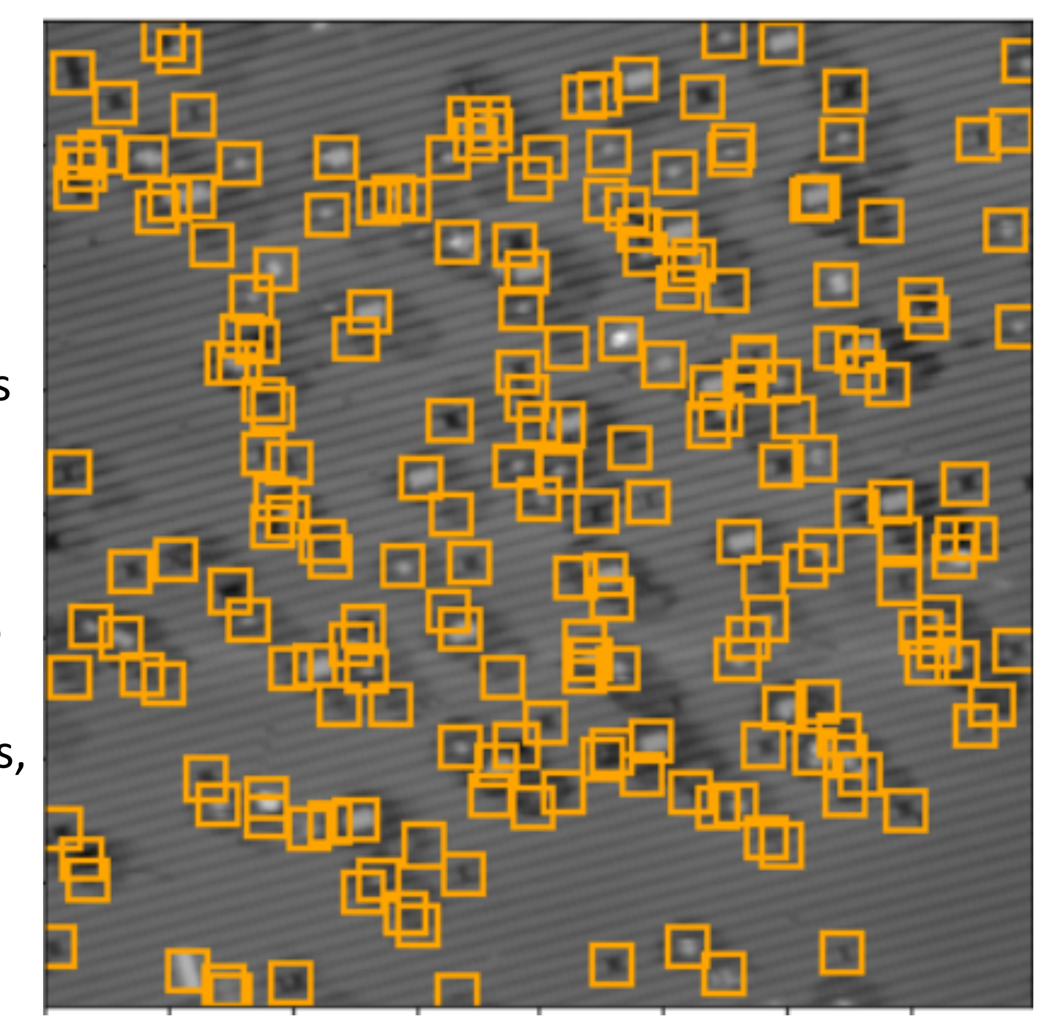
Figure 2: Hydrogen depassivation (c) is the process by which H atoms are removed. A hydrogen-passivated silicon surface (b) and another that has been depassivated (c), displaying an array of hydrogen-removed areas, both show varieties of defects.

2. Defect Detection Neural Network

Broadly speaking, the first step of the machine learning workflow entails feeding an input image into a convolutional neural network that returns as its output the coordinates of any identified defects.

- Autoencoder topology
- Pre-trained on separate data
- Binary classification of pixels as defect or lattice
- Defect pixels' location returned

Figure 3: The image shows the output of the localization CNN, with the pixels marked as defects now bearing a bounding box over. These locations can also be used to obtain defect sub-images, to be used in the next part of the workflow.



3. Defect Classification Neural Network

- Convolutional Neural Network takes defect sub-images as input
- Classifies as lattice or 1 of 3 defect classes
- Training accuracy of 0.98 is promising
- Limited training set of 180 images
- Tested on 20 labeled images with 0.91 accuracy

Figure 4: Current training accuracy of network is around 0.98

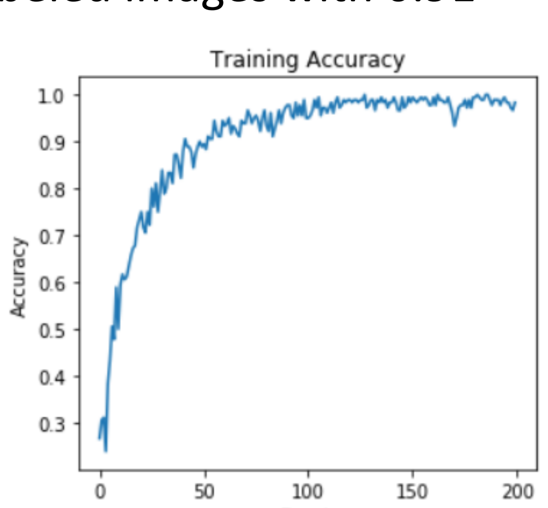
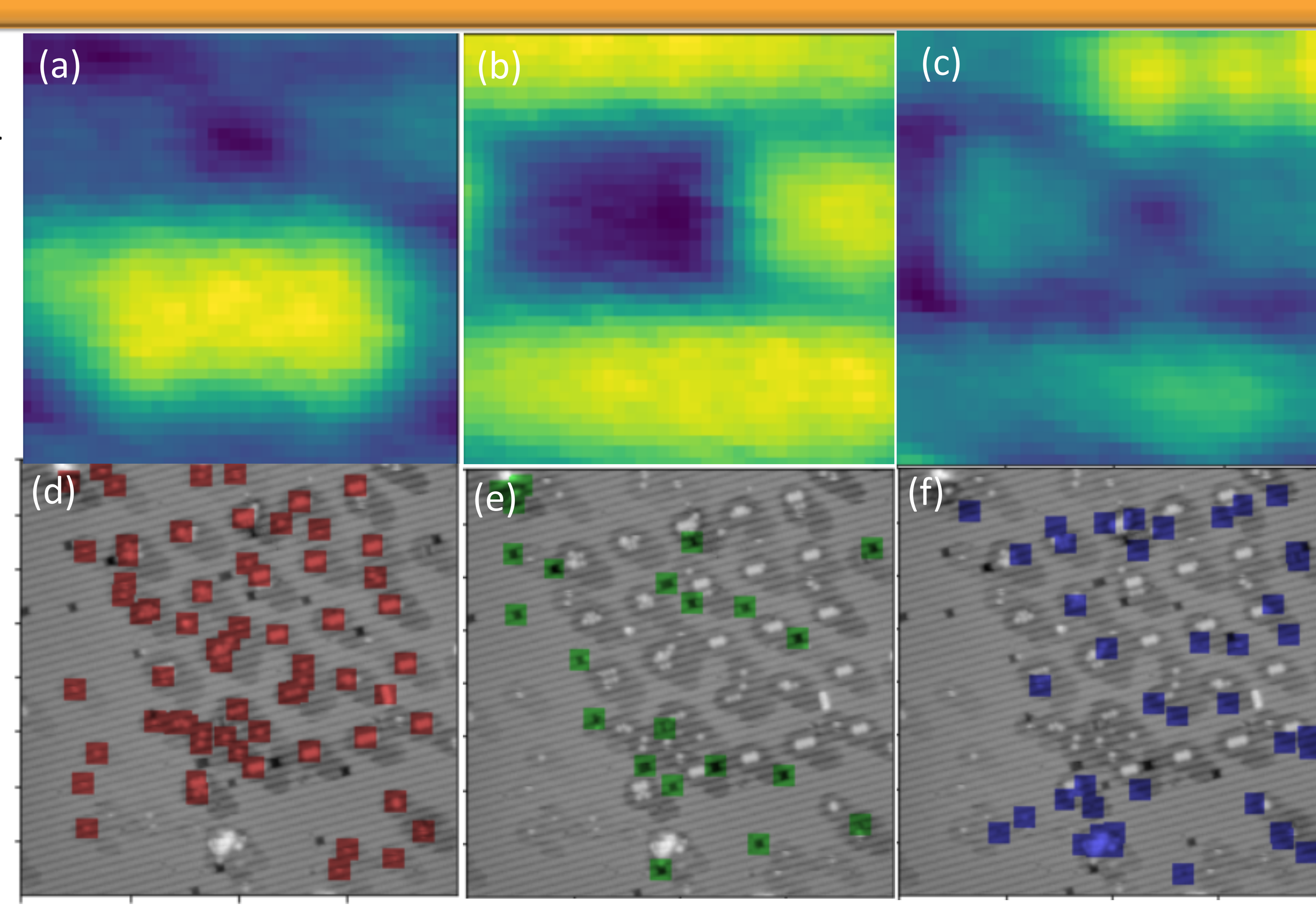


Figure 5:The three types of defect sub-images are shown in (a), (b), and (c), showing instances of classes 1, 2, and 3 respectively. Classification results overlaid on the original STM image are seen in (d), (e), and (f), showing defect classes 1, 2, and 3 respectively.



Conclusions & Future Steps

Immediate next steps will focus on the second part of the workflow. Although results from the classification network are promising, there are significant improvements yet to be made. During training, testing accuracy was shown as 0.91 on a very limited testing set, so expanding the data available for training will likely lead to significant improvement.

Three areas for future direction:

- More training
- Human verification
- More labeled data

1. Ziatdinov, M., Fuchs, U., Owen, J.H.G., Randall, J.N., & Kalinin, S.V. Robust multi-scale multi-feature deep learning for atomic and defect identification in Scanning Tunneling Microscopy on H-Si(100) 2x1 surface (2020)

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