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Convolutional neural networks for classification and labeling of defects on atomic scale silicon surfaces

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Introduction

Atom-by-atom fabrication allows manufacturing of atomic scale devices, which has broad applications across fields, including digital electronics and quantum computing. This is a complex problem requiring atomic scale precision, and it becomes necessary to know the exact type and location of atoms, structural irregularities, and step edges – amongst other features – on an atomic surface. This project seeks to identify and label these features on silicon surfaces such as those shown in Figure 1.

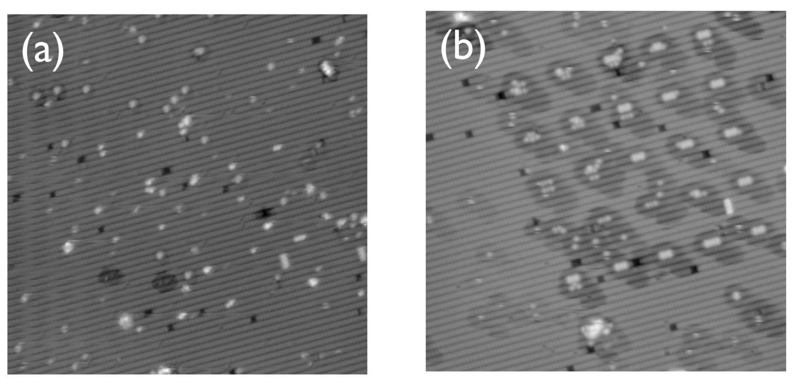

Figure 1: Hydrogen-passivated silicon surface (a) with bright and dark spots marking defects. Same surface (b) after hydrogen atoms are removed in an array.

The model will progressively be adapted to work for publicly available data, test dipole data, and experimental dipole data, before being applied to the STM data.

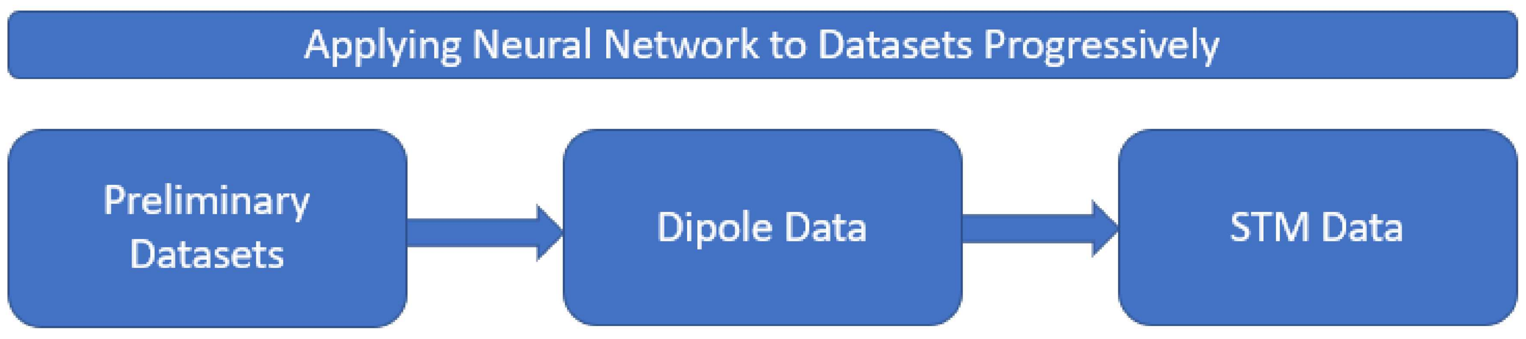

Figure 2: Overall workflow

Preliminary MNIST and SVHN Datasets

To establish a fundamental baseline from which to work, a 3-layer CNN was built for the MNIST dataset, consisting of hand-drawn digits numbering 0-9, and it achieved an accuracy comparable to those of state-of-the-art CNNs in literature as seen in Table 1.

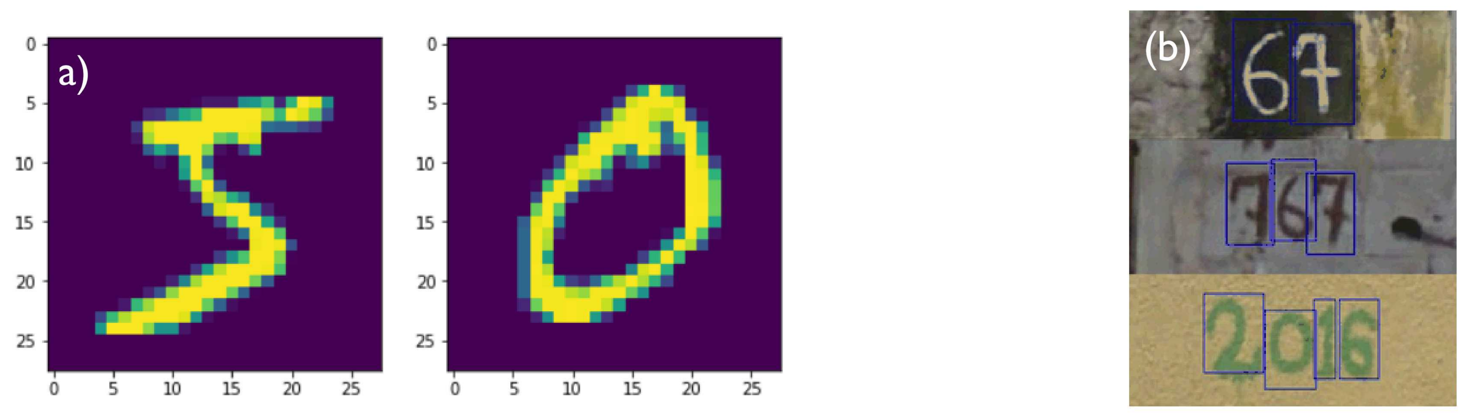

Figure 3: MNIST (a) and SVHN (b) sample images

The SVHN dataset – the next step up from MNIST in complexity – consists of images of real-world street views of sequences of digits. A CNN trained on the cropped images achieved an accuracy comparable to an early result by Netzer et al. (2011) of 0.8970.

Neural Network	Test Accuracy	Test Loss
CNN for MNIST	0.9927	0.0227
CNN for SVHN	0.9116	0.0830

Table 1: Test accuracies and losses for both CNNs

Dipole Data

Following implementation on publicly available data and a basic understanding of the CNNs, more atomically relevant data was used by training on dipole data. In that pursuit, code from Ziatdinov et al. (2020) was adapted to train a reinforced auto encoder on generated dipole test data, to be tested on experimental dipole data.

An example of the training data and its corresponding label are shown in Figure 4. Preprocessing involved:

- one-hot encoding
- Reshaping images to an array of (1600, 128, 128, 1).

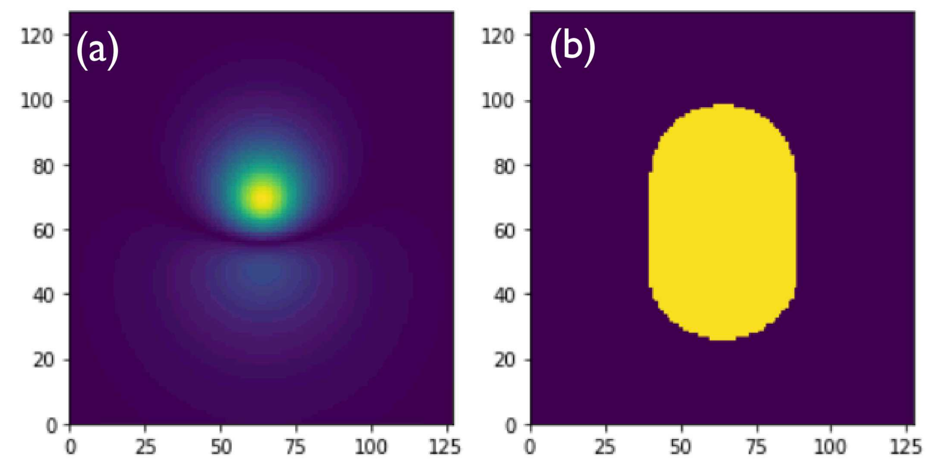

Figure 4: Generated dipole data

Figure 5 shows the result of training the network over 50 epochs.

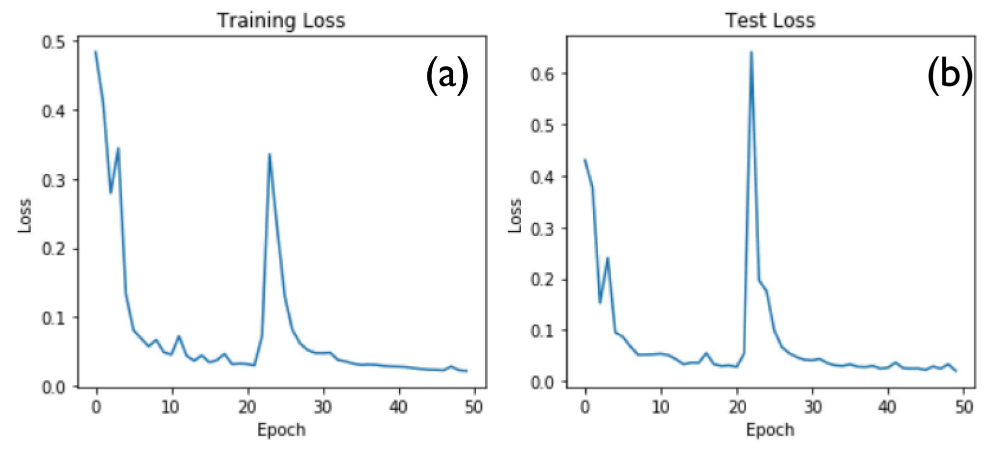

Figure 5: Training and test loss

With the model trained, the next step is to test it on experimental dipole data. Though there are few (<10) such images readily available, they are on the scale of ~1000x1000 pixels each, expanding the somewhat limited testing set by generating dozens of 128x128 sub-images from the originals. One such image is shown below, with output from this step still pending.

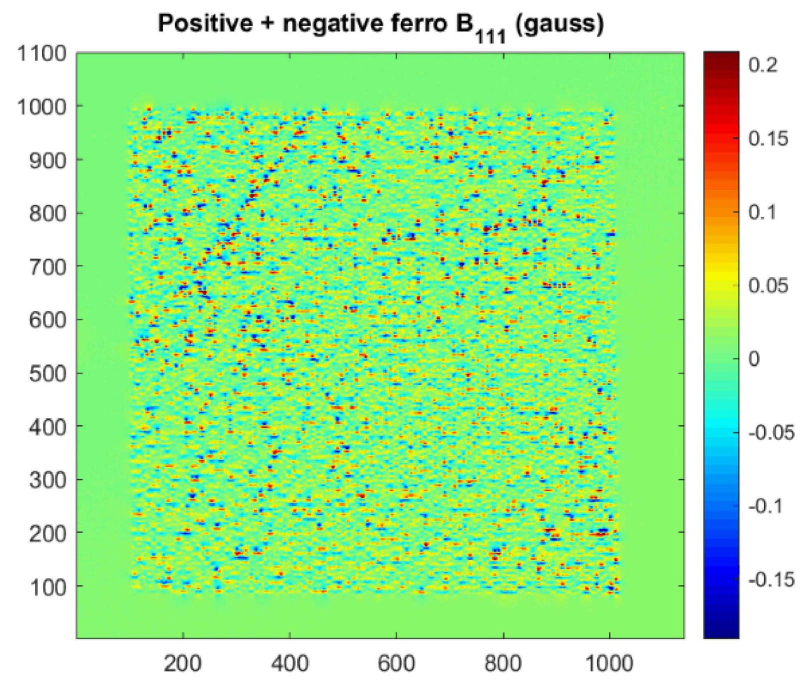

Figure 6: Experimental dipole data

STM Silicon Surface Data

The final step for this project is to apply these techniques to the surface of interest – Scanning Tunneling Microscopy (STM) images of silicon surfaces – to identify the different features on the surface. Some of these include depressions and protrusions (dark and bright spots in 7(a)), and step edges (lines shown in 7(b) and 7(c)). Accurate labeling of these features will facilitate atom-by-atom fabrication.

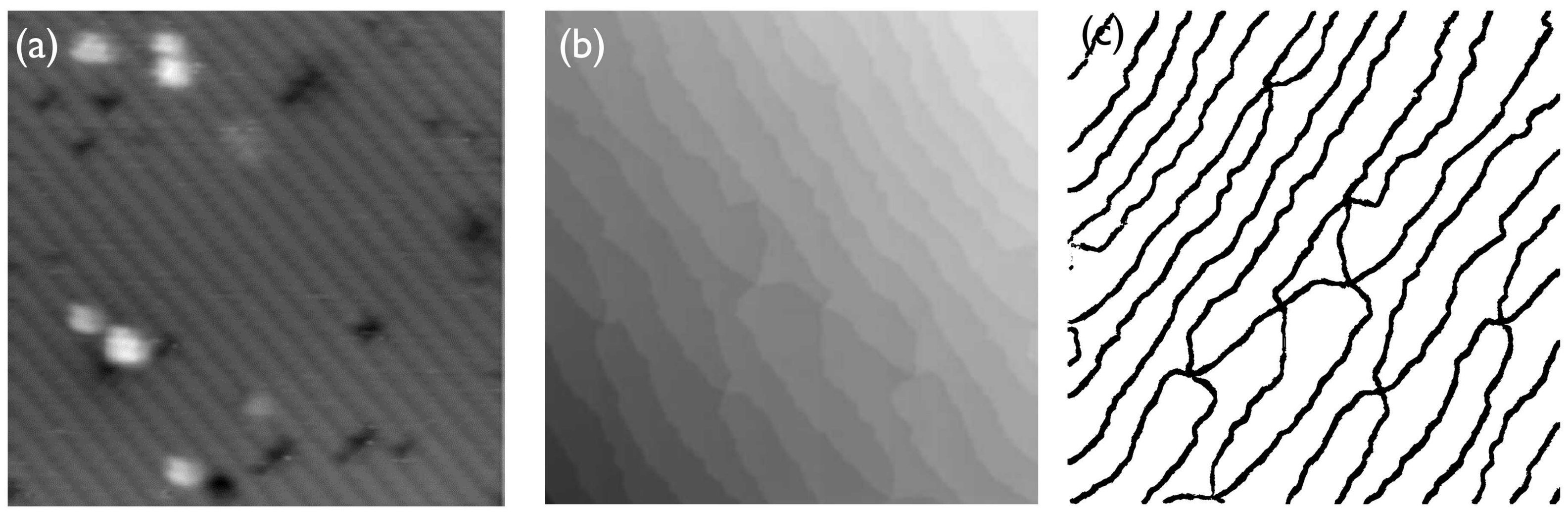

Figure 7: 7(a) illustrates defects in a 50 nm x 50 nm square and 7(b) and 7(c) shows step edges in 1 um x 1 um squares.

References

1. Netzer, Y., Wang, T., Coates, A., Bissacco, A., Wu, B., & Ng, A.Y. Reading digits in natural images with unsupervised feature learning. (2011)
2. Yitamben, E.N., Butera, R.E., Swartzentruber, B.S., Simonson, R.J., Misra, S., Carroll, M.S., & Bussmann E. Heterogeneous nucleation of pits via step pinning during Si(100) homoepitaxy. *New Journal of Physics 19*. (2017)
3. 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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