Deep Learning of Solid-State Transformations and Reaction Pathways in 2D Materials

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Introduction

Background:
Recent advances in scanning transmission electron microscopy (STEM) have allowed unprecedented insight into the elementary mechanisms behind the solid-state phase transformations and reactions.

Challenge:
Rapid physics-based analysis of large, high-resolution STEM images and movies.

Solution: ***DefectFinder***
A convolutional-neural-network(CNN)-based framework for automated localization, classification and visualization of the defects in 2D materials from dynamic STEM data.

Workflow:

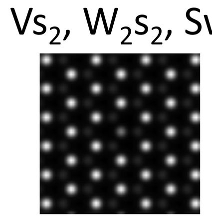
Defect Localization
- Train CNN on experimental STEM movie with pixel-wise labels(defect/not defect)
- Localize defect area and cut them out from the movie

Defect Classification
- Train CNN on simulated STEM images with image-wise labels(defect types)
- Classify the defects we cropped in last step

Visualization and Analysis
- Use Class Activation Map(CAM) to visualize the region that CNN "focus on"
- Map the predicted defect types back onto the STEM movie
- Analyze defect reaction pathways

Data Processing

Theoretical data:
45 simulated STEM images of WS_2 with shape of 64*64.
Each image contains only one type of defect.
6 Defect types: Mo, Vw, Vs_2, W_2s_2, Sw, Ws.



Experimental data:
Dynamic experimental STEM data(movie) of 2D WS_2 material.

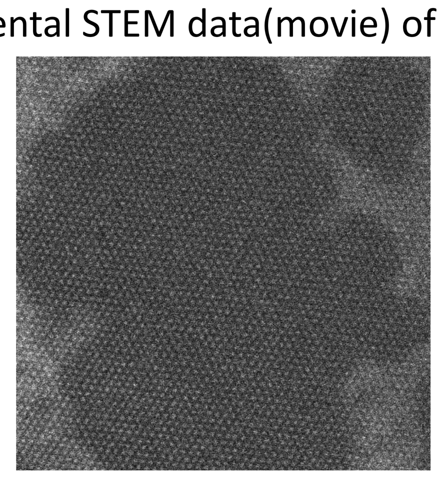
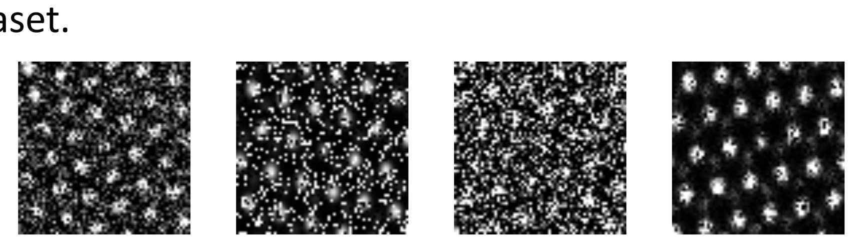
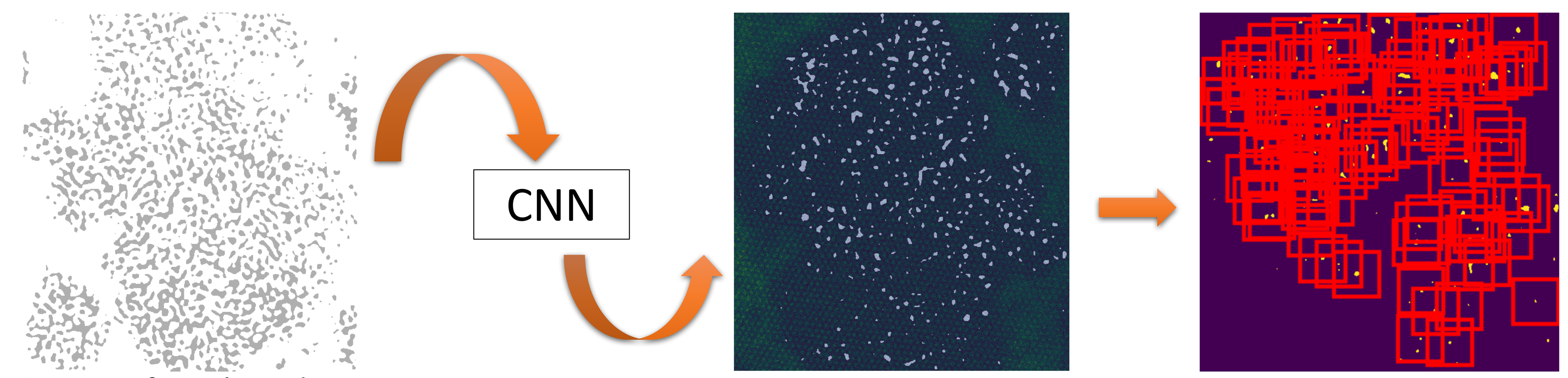


Image Preprocessing:
Do data augmentation on theoretical data to generate a dataset with 50178 images. Gaussion, salt & pepper, speckle and mixed types of noise are added. Each image is image-wise labeled with its defect type.
This dataset is split into 80% training dataset and 20% testing dataset.



Defect Localization

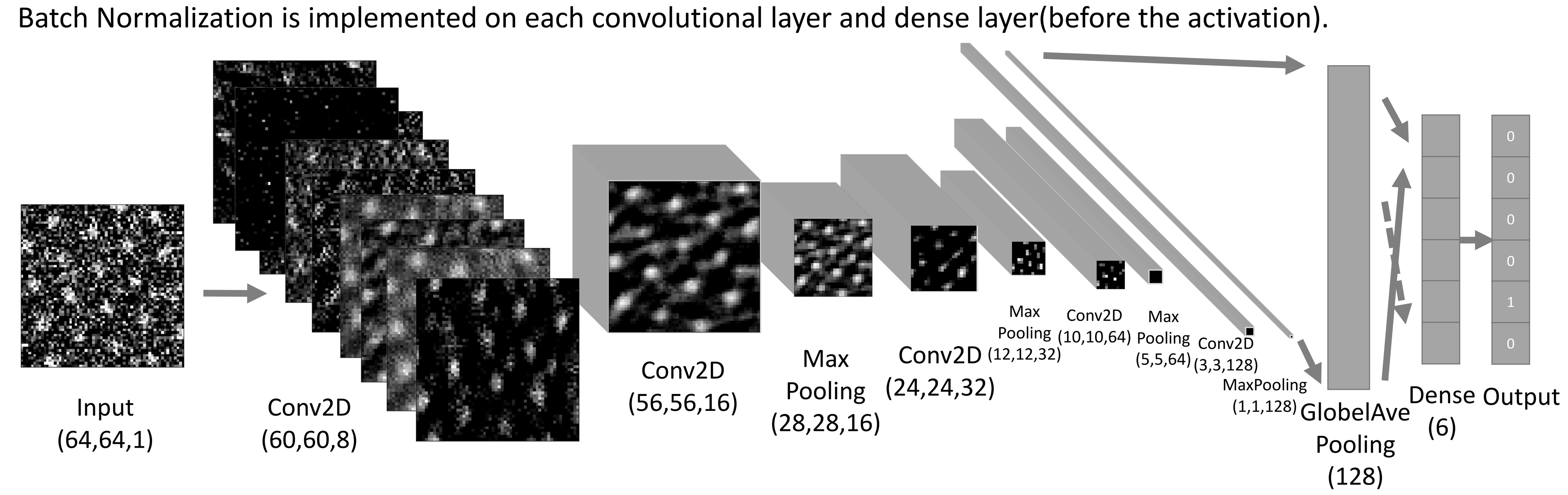
Defect localization on experimental data
A CNN is trained on the first frame of STEM movie and make prediction on the remaining frames.



- A Fourier-transform-based method is performed to locate the non-periodic lattice area(in deep color) on the 1st frame.
- A CNN is trained on the 1st frame to output pixel-wise classification map (The light area are the pixels classified into defect)
- The defect area are cut out by windows with shape of (64*64).

Defect Classification

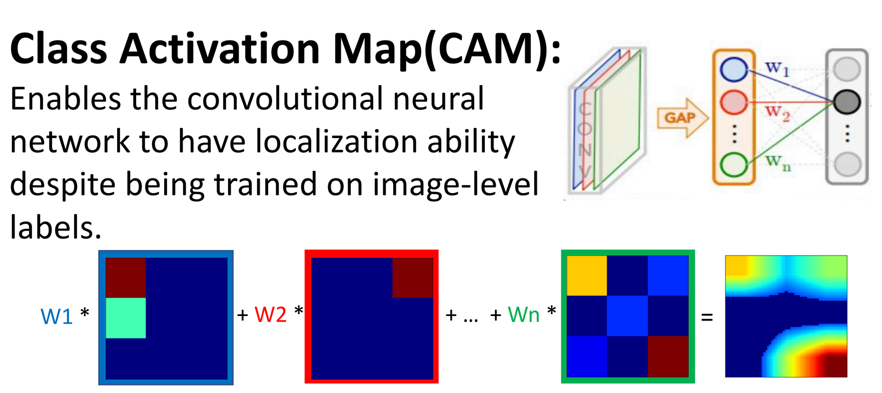
Defect Classification on theoretical data
A CNN structure is developed as shown below. It is trained on 67% and validated on 33% of the training dataset we generated from image preprocessing.
- Each Max pooling layer is followed with a dropout layer(Not shown on the graph).
- 2D convolutional layers(Conv2D) are activated with 'relu' and Dense layer is activated with 'Softmax'.
- Batch Normalization is implemented on each convolutional layer and dense layer(before the activation).



Hyperparameters Tuning:
The learning rate and dropout rate are tuned by gridsearch method. The table below shows part of tuning results.
With respect to the validation accuracy, the CNN model with learning rate of 0.00034 and dropout rate of 0.2 is the best.
When test on the testing dataset, the accuracy of this model reaches 95.68%.

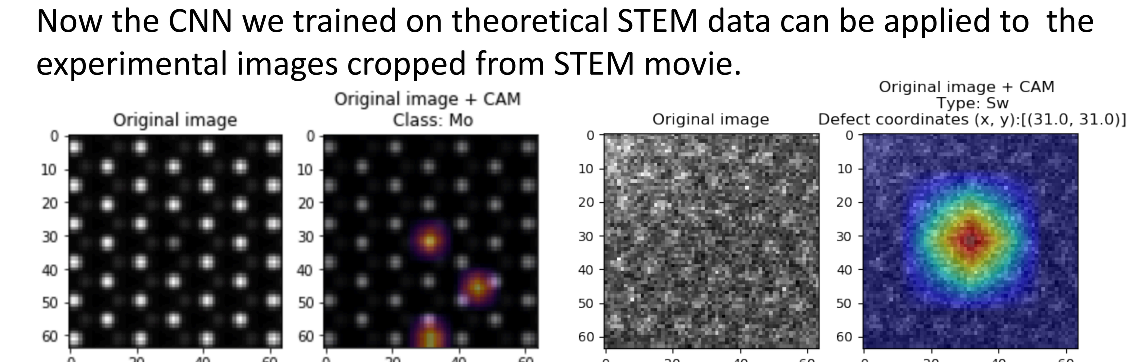
Learning Rate	0.000016		0.00034		0.0047	
DropoutRate\Accuracy	Training	Validation	Training	Validation	Training	Validation
0.2	0.85	0.88	0.97	0.96	0.88	0.90
0.4	0.74	0.80	0.92	0.93	0.75	0.80

Class Activation Map(CAM):
Enables the convolutional neural network to have localization ability despite being trained on image-level labels.



W1 to Wn are the output weights of Global Average Pooling layer, each of them are multiplied with the corresponding output of final Convolutional layer.

Make Prediction on theoretical/experimental data:
Now the CNN we trained on theoretical STEM data can be applied to the experimental images cropped from STEM movie.

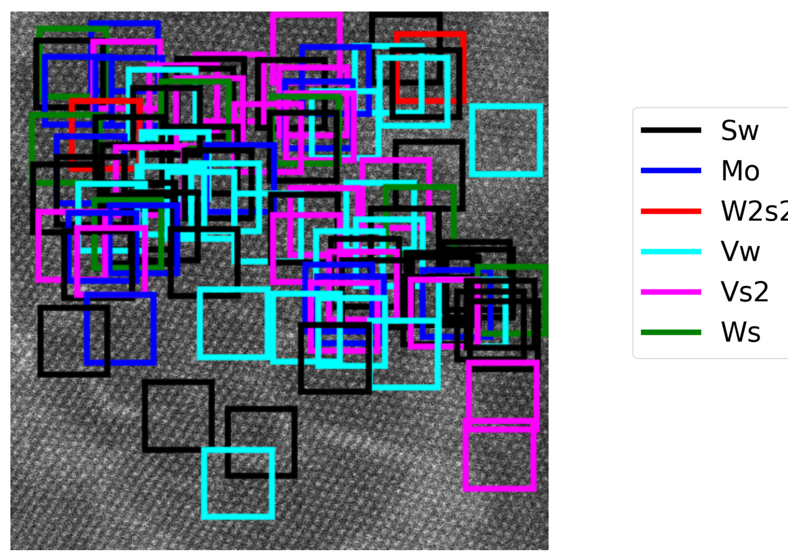


Defect Type: Mo
Defect coordinates: (63.0, 31.0), (46.0,46.0), (31.0,31.0)

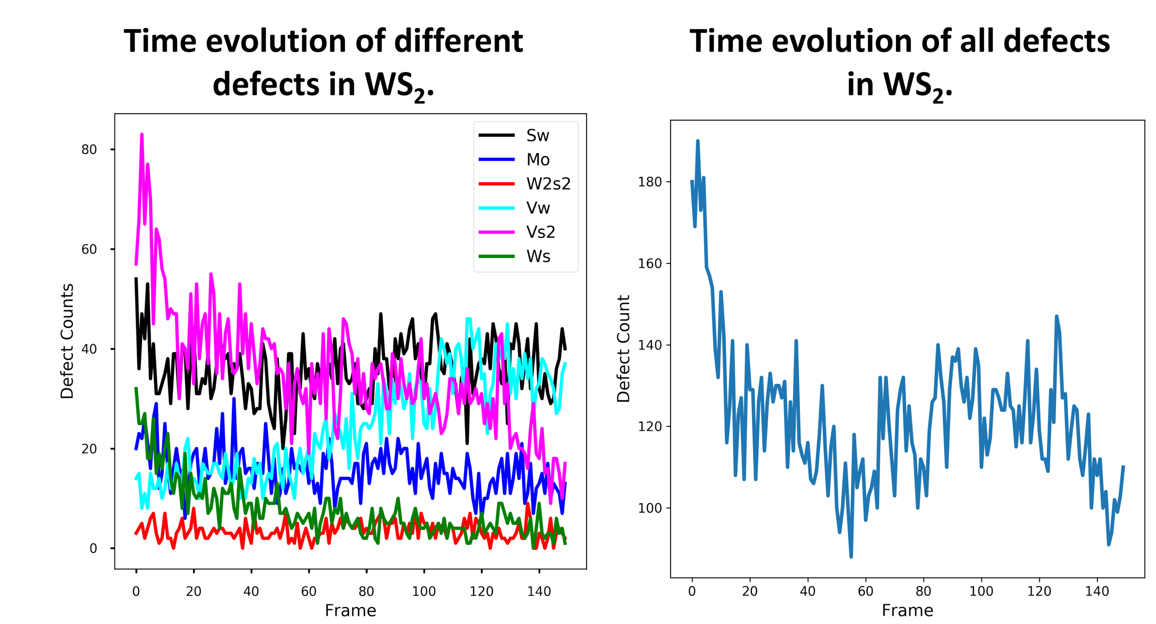
Defect Type: Sw
Defect coordinates: (31.0,31.0)

Visualization

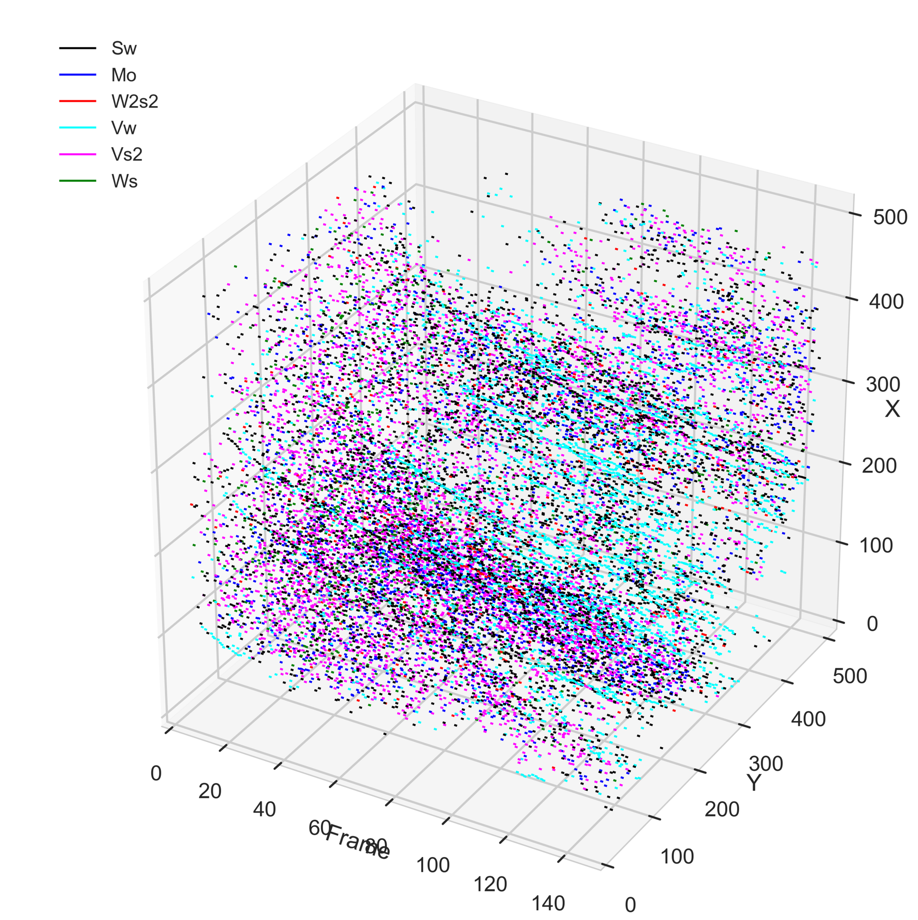
The predicted defects can then be visualized along with its dynamic STEM data as shown in the figure below.



Furthermore, we can also gain insight into the time evolution of the different defects as shown in the figures below.



We can also visualize the spatial-temporal evolution of different defects using a broom graph as shown in the figure below.



Reference:
B. Zhou, A. Khosla, A. Lapedriza, A. Oliva, and A. Torralba. Learning Deep Features for Discriminative Localization. CVPR'16 (arXiv:1512.04150, 2015).