Describing Point Defect Topology in 2D Energy Materials Through Computer Vision

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Introduction

- Point defects such as **vacancies** and impurity atoms strongly impact the performance of materials.
- 2D transition metal carbides (Ti_3C_2, **MXenes**) exhibit valuable defect-defined electrochemical properties, but we lack statistical understanding of defect topology needed to fully harness these materials.
- Here we employ state-of-the-art **computer vision** approaches to detect, classify, and describe the distribution of point defects in MXenes.

Methods

- A **previously published image** from Sang et. al. (2016) was randomly cropped to create the training dataset.
- 2-D Gaussian fitting was used to find ground truth atomic positions.
- **AtomAI**, a python package for deep learning in microscopy, was used to create masks.

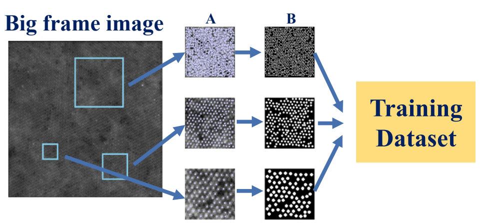

Figure 1: Training Workflow

- An AtomAI **Neural Network** (U-Net) was trained for semantic segmentation of experimental scanning transmission electron microscopy (STEM) images.

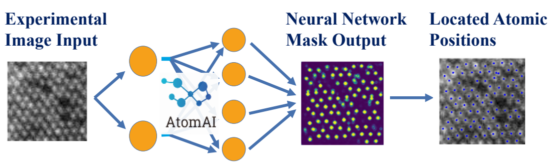

Figure 2: Abstraction of AtomAI Neural Network

Results

We successfully trained a neural network to identify atomic positions in experimental STEM images and investigated vacancy topology.

Data augmentation (rotation and Gaussian noise) greatly improved the neural network's performance.

Vacancies were located using Delaunay Triangulation and fractional coordinate mapping of atomic positions.

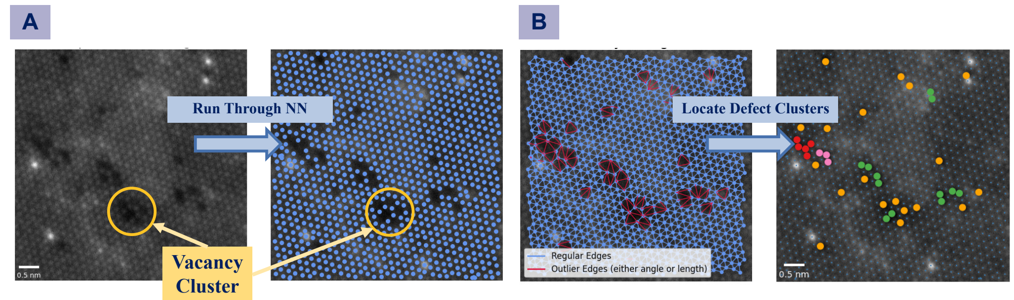

Figure 3: (A) The trained neural network located atomic positions in experimental STEM Mxene image. (B) Using a Delaunay Triangulation and by translating from lattice to fractional space, we locate defect clusters and classify them by size.

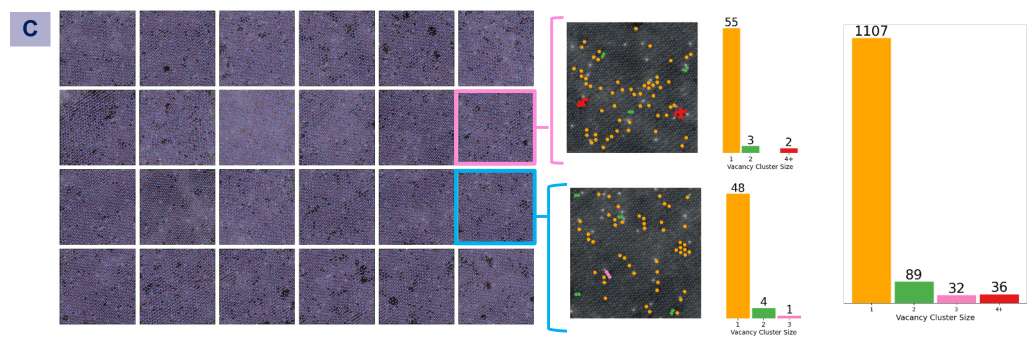

Figure 4: (C) The neural network located atomic positions across a grid of images *(left)*. Select single-frame defect configurations and histograms are shown *(middle)*. Finally, a histogram of defects across the whole grid is pictured *(right)*, showing the statistical importance of ML in this project.

Future Work

- Going forward, we aim to gather a wider field of view of data across multiple etching conditions for a **bigger statistical study** of defects in MXenes. We also wish to use the NN to examine the **3-D structure** of our samples
- While we specifically looked at MXenes, the same pipeline can be applied to **other materials systems** in the future.

References

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