Accelerating Discovery of Atomistic Defects via Machine Learning

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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.

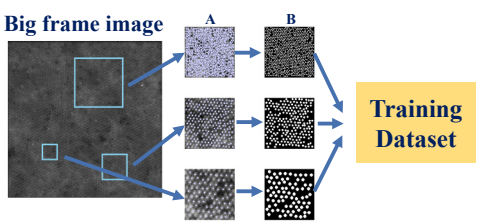

Figure 1: Training Workflow

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

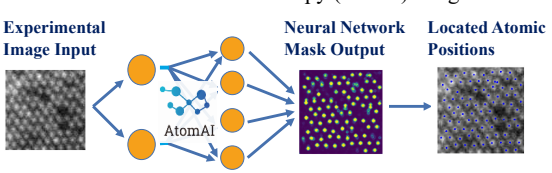

Figure 2: Abstraction of AtomAI Neural Network

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.

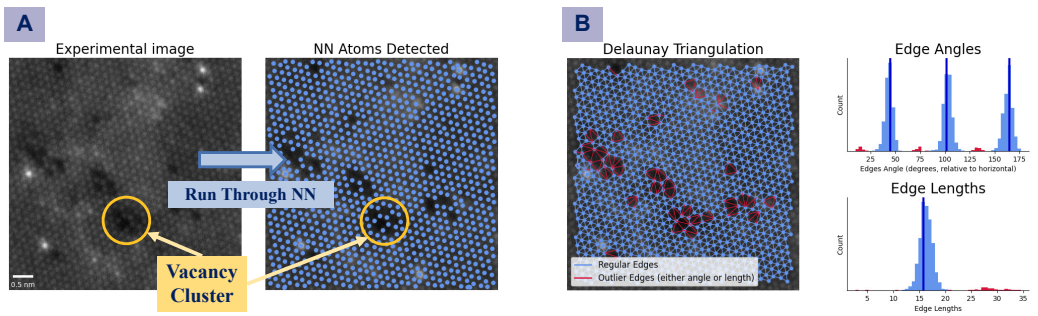

Figure 3: (A) The trained neural network located atomic positions in experimental STEM Mxene image. (B) Using a Delaunay Triangulation, the basis angles of the atomic lattice and the median distance between atoms are calculated.

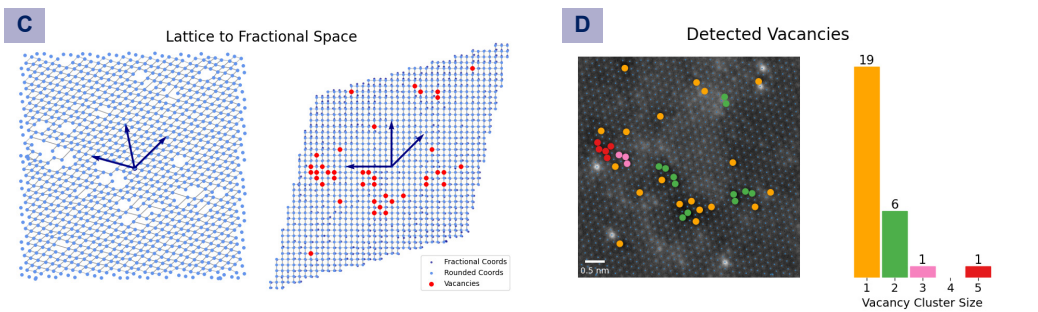

Figure 4: (C) Using the angles and median distance found in (B), a linear transformation is applied to take atoms from lattice to fractional space (integer coordinates). Missing atoms are located, then (D) transposed back into fractional space and grouped by size.

Future Work

- Going forward, we aim to gather a wider field of view of data for a **bigger statistical study** of defects in MXenes. We also wish to map the **strain** in the lattice around different vacancy configurations.
- While we specifically looked at MXenes, the same pipeline can be applied to **other materials systems** in the future.

References

1. X. Sang, Y. Xie, M.-W. Lin, M. Alhabeb, K. L. Van Aken, Y. Gogotsi, P. R. C. Kent, K. Xiao, and R. R. Unocic, Atomic defects in monolayer titanium carbide (ti3 c2 t x) mxene, ACS Nano 10, 9193 (2016).
2. M. Ziatdinov, A. Ghosh, C. Y. Wong, and S. V. Kalinin, Atomai framework for deep learning analysis of image and spectroscopy data in electron and scanning probe microscopy, Nat Mach Intell 4, 1101 (2022).

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