Imaging 2D materials, atom by atom, on the million-atom scale*

Pinshane Y. Huang
Materials Science and Engineering
University of Illinois at Urbana-Champaign

Abstract

Analyzing large volumes of data using machine learning can make it possible to access hidden information in electron microscopy data. In particular, two-dimensional (2D) materials present an unprecedented opportunity to probe structure-property relationships because, in projection we can characterize almost every individual atom, making 2D materials well-suited for high precision defect analysis. Understanding the types and densities of point defects in 2D materials is important for producing 2D materials that can achieve tailored properties, such as materials that reach the theoretical limits of charge mobility and quantum yield for high quality optoelectronics. In our work, we use a combination of automated image acquisition, electron scattering simulations, and machine learning to develop workflow for acquiring and processing large volumes of atomic resolution images acquired using aberration-corrected scanning transmission electron microscopy. Using a combination of fully convolutional networks (FCNs) [1] and generative adversarial networks (GANs), we rapidly and adaptively train models to identify defects of interest with a high accuracy and precision that can rival or exceed human-based defect identification. We apply our approach to large, atomic resolution datasets of 2D materials in order to study the strain fields of single defects in a 2D layer and long-range defect-defect interactions [2].

References:

[1] Code available at: https://github.com/ClarkResearchGroup/stem-learning
[2] C. H. Lee et al., Nano Letters 20 (2020), p. 3369-3377
[3] This work is supported primarily through DOE BES under DE-SC0020190. Additional support from AFOSR FA9550-7-1-0213, ONR grant numbers N00014-17-1-2973 and N00014-18-1-2605, NSF OCI-0725070 and ACI-1238993, and the state of Illinois. This work was carried out in part in the Materials Research Laboratory at UIUC.

* Title and Abstract of an Invited Presentation at the Workshop: AI/ML for Particle Accelerator, X-Ray Beamlines and Electron Microscopy at Argonne National Laboratory, November 1-3, 2021.