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Probing the Strain Fields of Single-Atom Defects in 2D materials with Sub-Picometer Precision

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Analyzing large volumes of data using machine learning can make it possible to access hidden information in electron microscopy data. In our work, we use this approach to detect picometer-scale displacements that result from single atom defects, such as vacancies and substitutional dopants in 2D materials [1]. This work utilizes deep learning techniques based on fully convolutional networks (FCN) to locate, classify, and segment defects in aberration-corrected scanning transmission electron microscopy (STEM) images [2]. First, we use simulated data to train the FCNs to identify each defect type with high accuracy in experimental data –comparable to or even exceeding human labeling. Next, we acquired large atomic resolution dataset on 2D materials samples transferred using large-area, clean transfer techniques. Then, we identify hundreds or thousands of individual point defects, screen them for the presence of long-range strain fields, and then align and sum images from nominally equivalent defects. This approach allows us to overcome the fundamental limits set by electron beam damage and measure the 2D coordinates of atoms with up to 0.3 pm—comparable to the precision of density functional theory (DFT) simulations, and sufficient to measure the strain field of a single atom more than a nanometer away from the defect core. Using this combination of atomic resolution and sub-picometer precision, we are able to detect radially oscillating strain fields that deviate clearly from a continuum elastic model, which we attribute to defect-induced charge redistribution. Moving beyond single atoms, we study defect clusters to study how the strain fields from different defects couple with one another. By carefully benchmarking uncertainties and potential sources for error in our data, we find that mechanical drifts and the gaussian fitting process we use to determine atomic positions are current limiters for the precision we achieve, indicating potential routes to even further improve the ultimate precision at which atomic coordinates can be measured in the STEM. Our methods can readily be extended to other beam-sensitive materials and other types of atomic resolution datasets.

References

[1] C. H. Lee *et al.*, Nano Letters **20** (2020), p. 3369-3377

[2] Code available at: https://github.com/ClarkResearchGroup/stem-learning

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