Atomic Force Microscopy for Routine, Fast, and Reliable Defect Quantification in 2D Materials

Matthew R. Rosenberger Aerospace and Mechanical Engineering University of Notre Dame

Routine defect characterization is a critical capability for understanding defect-property correlations and optimizing growth of two-dimensional (2D) materials. High throughput optical methods for defect characterization, such as Raman spectroscopy, are useful for graphene, but are insufficiently sensitive to defects in some other 2D materials, such as transition metal dichalcogenides (TMDs), particularly for defect densities of about 10¹² cm⁻² or less. Typical methods for directly detecting defects at the atomic scale, such as scanning transmission electron microscopy (STEM) and scanning tunneling microscopy (STM), are effective, but they are slow and often require arduous sample preparation. There is a need for 2D material defect characterization techniques that are routine, fast, and reliable. Here, we demonstrate two atomic force microscopy (AFM)-based techniques for locating and quantifying atomic-scale defects in 2D materials. First, we show that conductive AFM can locate and differentiate the same defects as STM by comparing conductive AFM and STM on the same region of a TMD crystal¹. Our work establishes conductive AFM as a higher-throughput alternative to STM for defect quantification. Second, we show that lateral force microscopy (LFM) can locate atomic-scale defects through a direct comparison of LFM with conductive AFM on a TMD crystal². Importantly, we show that LFM can also identify atomic-scale defects in insulators, such as hexagonal boron nitride, because LFM is a purely mechanical technique. The AFM-based methods presented here enable routine defect characterization, which will facilitate rapid investigations of defect-property relationships and speed up the development of new growth processes.

- (1) Xu, K.; Holbrook, M.; Holtzman, L. N.; Pasupathy, A. N.; Barmak, K.; Hone, J. C.; Rosenberger, M. R. Validating the Use of Conductive Atomic Force Microscopy for Defect Quantification in 2D Materials. *ACS Nano* **2023**, *17* (24), 24743–24752. https://doi.org/10.1021/acsnano.3c05056.
- (2) Yang, Y.; Xu, K.; Holtzman, L. N.; Yang, K.; Watanabe, K.; Taniguchi, T.; Hone, J.; Barmak, K.; Rosenberger, M. R. Atomic Defect Quantification by Lateral Force Microscopy. ACS Nano 2024, 18 (9), 6887–6895. https://doi.org/10.1021/acsnano.3c07405.