

# The Role of Atomic Force Microscopy in 2D Material Characterization: Surface Features, Defects and Strain

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## Introduction

Two-dimensional (2D) materials such as graphene, Transition Metal Dichalcogenides (TMDs), and hexagonal boron nitride (h-BN) have emerged as key materials for next-generation electronics, photonics, and energy storage technologies. Due to their atomic-scale thickness and sensitivity to surface phenomena, precise characterization techniques are essential for understanding their structural and functional properties. Atomic Force Microscopy (AFM), with its nanometer-scale resolution and multimodal capabilities, plays a central role in 2D material research. This article reviews the applications of AFM in identifying surface morphology, defects, layer number, and strain in 2D materials. We also explore how advanced AFM techniques—such as PeakForce QNM, Kelvin Probe Force Microscopy (KPFM), and scanning thermal microscopy—provide complementary insights into the mechanical, electrical, and thermal behavior of atomically thin films.

## Description

The discovery of graphene and other 2D materials has revolutionized materials science due to their exceptional electrical, mechanical, optical, and thermal properties. However, the performance of 2D materials in practical devices depends critically on their nanoscale structural integrity, including the presence of surface irregularities, defects, layer-dependent behavior, and strain fields. Atomic Force Microscopy (AFM) offers a suite of techniques capable of probing the physical and functional characteristics of 2D materials under ambient or controlled environments. Unlike electron microscopy, AFM provides true 3D surface profiling without the need for conductive coatings or high vacuum, making it particularly suitable for fragile or insulating 2D systems. The number of layers in a 2D material significantly affects its band structure, optical absorption, and mechanical properties. AFM can determine layer thickness with sub-nanometer resolution by measuring the height difference between the flake and the substrate. Single-layer graphene typically shows a step height of ~0.4–1.0 nm depending on substrate interactions and imaging mode. MoS<sub>2</sub> and other TMDs: Step heights of ~0.6–0.8 nm per layer allow precise layer counting. AFM is commonly used alongside Raman spectroscopy for unambiguous layer identification.

AFM can quantify surface roughness at the atomic level, helping to evaluate the effects of synthesis conditions, substrate interactions, and post-processing steps. CVD-grown 2D materials often exhibit wrinkles, folds, and particles that affect device performance. High-resolution AFM imaging can identify grain boundaries, terraces, and step edges, which act as scattering centers for

charge carriers. Defects—such as vacancies, dislocations, grain boundaries, and cracks—play a crucial role in modulating the electronic and mechanical properties of 2D materials. AFM operated in non-contact or Ultra-High Vacuum (UHV) environments can achieve atomic resolution, revealing defect structures directly in real space. Defective regions often show altered stiffness and adhesion. This provides indirect yet valuable information about defect location and type. Defects may locally change conductivity and work function. When combined with Conductive AFM (C-AFM) or Kelvin Probe Force Microscopy (KPFM), researchers can correlate mechanical and electrical inhomogeneities with structural defects. Wrinkles, ripples, and buckling patterns observed via AFM often indicate the presence of local or global strain induced by thermal mismatch, transfer processes, or substrate effects. Changes in mechanical stiffness measured via PeakForce QNM or Fast Force Mapping Mode can reflect strain-induced modifications in the elastic modulus. PFM, traditionally used in ferroelectrics, has also been applied to detect piezoelectric responses in strained monolayers of TMDs such as MoS<sub>2</sub> and WS<sub>2</sub>.

C-AFM can visualize local current paths in devices, while Electrostatic Force Microscopy (EFM) reveals trapped charges and dielectric contrast in insulating 2D films. SThM measures thermal conductivity and temperature gradients at the nanoscale, helping to assess heat dissipation in graphene-based and TMD devices. Accurate characterization depends on proper tip calibration and interaction models. Artifacts may arise from tip contamination, finite tip radius, or surface roughness. Ambient humidity, temperature, and contamination affect 2D material behavior and must be controlled during measurement, especially for hygroscopic or oxidizable samples like BP or MoTe<sub>2</sub>. While AFM excels in resolution, it is inherently a serial technique with lower throughput than optical or electron-based methods. Multimodal and correlative AFM systems that combine topography, mechanics, electrical, and thermal imaging. In situ AFM for studying growth dynamics, degradation, or device operation under applied bias or illumination. Machine learning-based analysis for feature extraction, defect classification, and predictive modeling. Probes functionalized for chemical sensitivity, enabling detection of specific molecules or bonds on 2D surfaces. These advancements will enhance AFM's utility in both fundamental research and industrial-scale quality control of 2D materials [1-5].

## Conclusion

Atomic Force Microscopy has become a cornerstone technique in the characterization of 2D materials, offering high-resolution insight into surface features, defects, and strain that govern their properties and performance. As 2D materials continue to evolve from lab-scale discoveries to industrial applications, AFM will remain an essential tool for ensuring material quality, optimizing synthesis, and guiding device engineering.

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## Conflict of Interest

None.

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