Revealing the atomic structure of graphene defects by nc-AFM

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Atomic-scale defects are ubiquitous in graphene and often determine its ultimate electronic, thermal, and mechanical performance. In this talk, I will show how cantilever-based non-contact AFM (nc-AFM) operated in UHV at 5 K enables direct, atom-by-atom identification of defect structures with unprecedented real-space resolution, bridging the gap between idealized models and experimentally relevant interfaces. Using nc-AFM (without CO tip functionalization), we resolve a broad variety of defects in graphene grown on SiC(000-1), from topological point defects to extended grain boundaries. High-resolution imaging reveals that many defect cores are built from alternating pentagon/heptagon rings. For grain boundaries, we uncover an unexpected structural duality: stable, flat boundaries coexist with metastable configurations featuring irregular pentagon/heptagon motifs and out-of-plane corrugation [1]. First-principles modeling and simulated nc-AFM contrast attribute these metastable phases to uniaxial compressive strain, and we demonstrate in situ tip-induced switching that drives them toward the minimum-energy structure. Strikingly, although the geometric distortions are confined to only a few atoms, their influence extends over much larger length scales, highlighting how atomic defects can impact device-scale behavior.

[1] Haojie Guo et al., *Advanced Materials* e10899 (2025).