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Conserved Bonding Sequences and Atomic Strain Fields of Graphene Grain Boundaries HAIDER RASOOL, UC Berkeley, COLIN OPHUS, Lawerence Berkeley National Laboratory, ZIANG ZHANG, Rice University, MICHAEL CROMMIE, UC Berkeley, BORIS YAKOBSON, Rice University, ALEX ZETTL, UC Berkeley — Grain boundaries in polycrystalline materials have significant impact on their bulk mechanical properties. The detailed arrangement of atoms and bonding at the boundary dictate these properties and their differences from bulk single crystal behavior. In this work, we use aberration corrected high resolution transmission electron microscopy imaging to study the structure of graphene grain boundaries. By mapping the exact atomic positions of the carbon lattice, we visualize atomic scale strain organization in the material. We find that grain boundaries are comprised of conserved bonding sequences that can appear as periodic or aperiodic building blocks that give rise to similar strain behavior at the boundary. Using molecular dynamics fracture simulations, we predict that experimentally observed grain boundary structures will maintain strengths that are comparable to ideal theoretical grain boundaries.

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