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Atomic Structure of Grain Boundaries in Graphene OTHO ULRICH, University of South Florida, Western Michigan University, JOSEPH GONZALEZ, KIEN NGUYEN CONG, IVAN OLEYNIK, University of South Florida — In its pristine form, graphene is one of the strongest materials measured, and possesses a wide range of technologically appealing characteristics. Several recent experiments have explored the mechanical properties of graphene which contains grains, some with contradictory results. To explore the atomic structure of grain boundaries in graphene, we employ a complex of computational approaches. A set of unit cells of graphene bicrystals with variable grain misorientation is generated by applying a conjugate gradient method with periodic boundary conditions using the SEDREBO potential for carbon-carbon interaction. Structures are classified by formation energy and atomic coordination, and identification of physically viable samples is achieved using these statistics. The defective regions constituting the grain boundaries are defined using the atomic energy distribution. Formation energies of any viable structures are normalized according to cell height and compared by indexing misorientation angles. Lack of a functional relationship between misorientation angle and formation energy indicates a greater complexity in the mechanisms of the grain boundaries.

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