Atomic Structure of Grain Boundaries in Graphene

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Motivation

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, and have left us with contradictory results. Atomic-scale modeling of the material can elucidate trends in the strength of the material as a function of misorientation angle and provide clues into the mechanism responsible for the strengthening of the grain boundaries. Atomic-scale modeling is highly dependent upon how one treats the interatomic potentials. Much of the current theoretical work uses descriptions that were built for pristine conditions. However, the applicability of these potentials is not guaranteed when simulating defective graphene.

Objectives

- Study the formation energy graphene bicrystals as a function of misorientation angle.
- Determine trends between formation energies of certain grain boundaries and their effect on mechanical properties.
- Determine breaking strength and Young's modulus as a function of misorientation angle.

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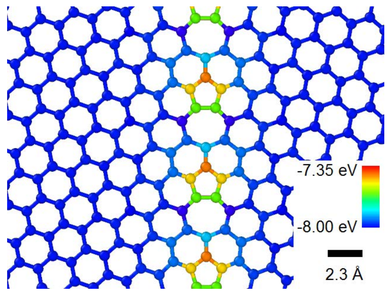
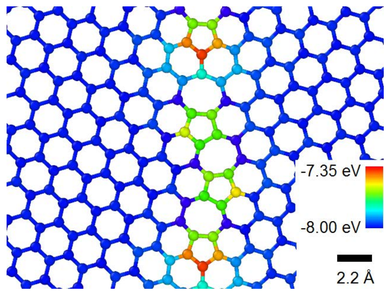
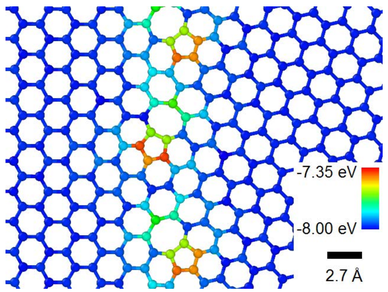
Structure of Grain Boundaries



θ=21.8˚



θ=27.8˚

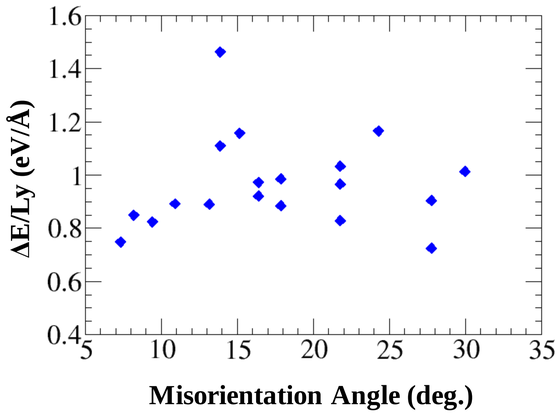


θ=13.9˚

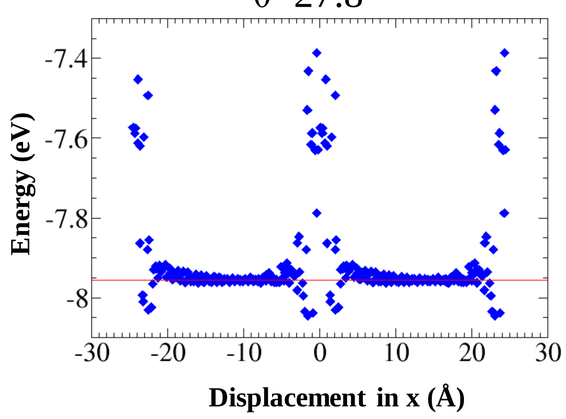
- Grain boundaries are generated by merging misoriented crystals.
- Periodic lengths in x dimension are restricted to avoid interaction between grain boundaries.
- In accordance with recent experimental findings, we only investigate boundaries formed by pentagon-heptagon pairs and hexagonal rings.

Analysis of Grain Boundaries

Formation Energy Distribution



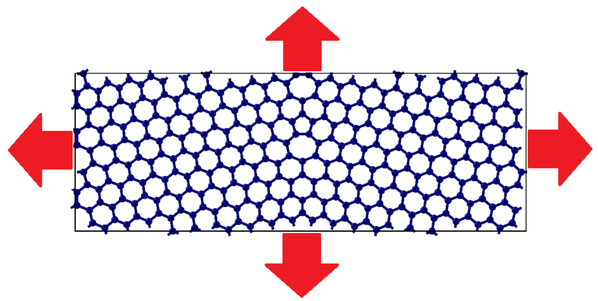
Atomic Energy Distribution
θ=27.8˚



Computational Details

- Geometric relaxation with periodic boundary conditions: Conjugate-gradient method.
- Classify and rank structures based on energy.
- SED-REBO: Interatomic potential to describe carbon-carbon interactions.
  - ➢ Screening function to preserve only nearest neighbor interactions are taken into account
  - ➢ Large cutoff distance beyond the spinodal bond length
  - ➢ Analytical pairwise attractive and repulsive functions

Future Studies



- Each unit cell will be subjected to hydrostatic biaxial strain.
- Stress-strain curves will yield predictions for Breaking strength and Young's modulus.