Mechanical Properties of Twisted Bilayer Graphene

Jack Gagliardi, Md. Rakib Hassan, and Francis W. Starr

Department of Physics, Wesleyan University, Middletown, CT 06459

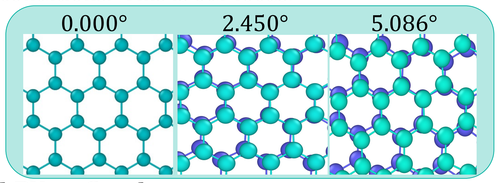
Background

2D Materials

Graphene was the first 2D material discovered in 2004. Subsequently, other 2D sheet materials, such as hexagonal boron nitride (hBN) and molybdenum disulfide (MoS_2), were synthesized. These materials draw interest because they exhibit many unusual properties, including exceptional tensile strength (stronger than steel). These materials are also promising for next-generation electronics, photonics, and energy storage.

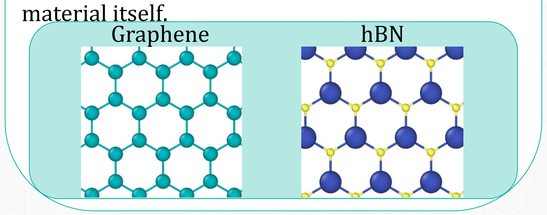
Moiré Twist

Rotating one 2D layer slightly relative to another creates a moiré superlattice. Most research focuses on how the twist angle gives rise to superconducting behavior near absolute zero. Much less attention has been given to thermal properties of these systems at ambient conditions. This is our focus.

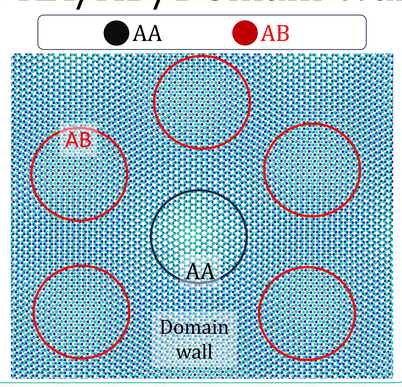


hBN vs. Graphene

Both share the same honeycomb lattice, but graphene is all carbon while hBN alternates boron and nitrogen atoms. hBN is an insulator, while graphene is an excellent conductor. hBN is also flatter and more chemically inert, which is why it is sometimes used as a substrate for graphene devices rather than as the active material itself.



AA/AB/Domain Wall



Goals

Main Goal

- How twist angle affects stiffness (Young's modulus)
- Focus: small angles, ambient temperature

Side Goal

- Link stiffness trends to AA/AB stacking

Methods: ML Modeling

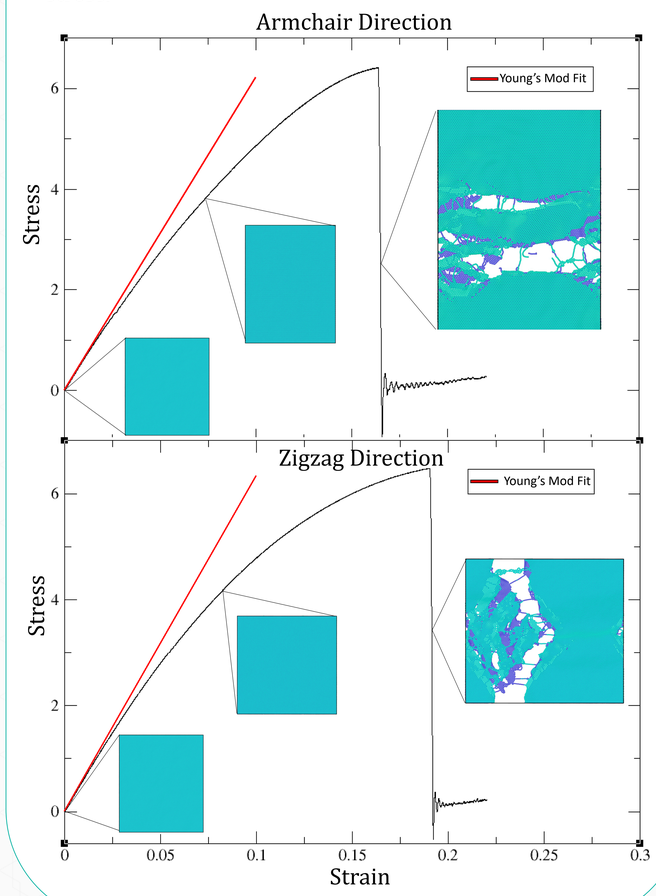
All-atom Molecular Dynamics (LAMMPS) using a machine-learned potential (ACE + van der Waals corrections)

Workflow

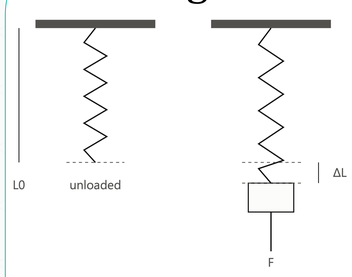
Build twisted structures, equilibrate at ambient temperature, strain along zigzag/armchair directions, record stress to fracture for all 27 twist angles, multiple replicas to improve statistics.

Stress-Strain Curves

We stretch each twisted bilayer at ambient temperature and record the resulting stress until the lattice fractures. Then we can apply a fit to the initial slope to obtain Young's modulus, and its endpoint marks the fracture strain and stress.



Young's Modulus



Strain

$$\varepsilon = \frac{\Delta L}{L0}$$

Stress

$$\sigma = \frac{F}{A}$$

Young's modulus

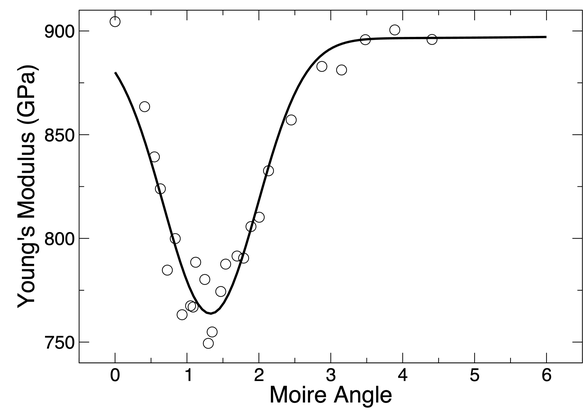
$$Y = \frac{\sigma}{\varepsilon} = \frac{F\,L0}{A\,\Delta L}$$

L0	Original length	F	Applied force
ΔL	Change in length	A	Cross-sectional area

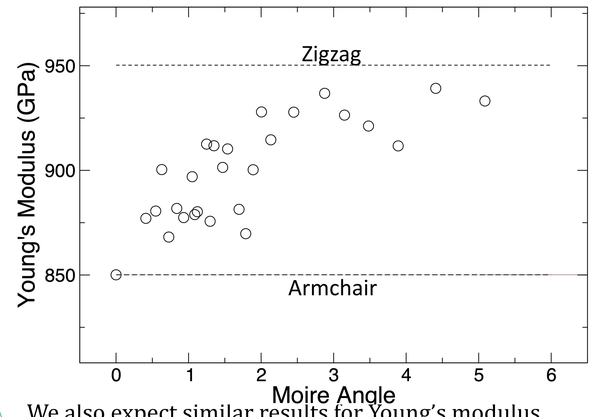
Results

A Trough at Small Angles

Young's modulus displays a large dip near a "magic angle" of 1.5° for dual-layer graphene.



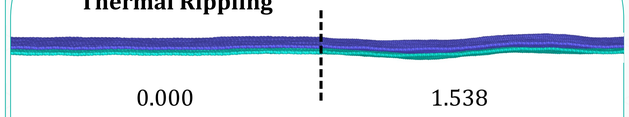
Moreover, for monolayer graphene, there is no dip, indicating this behavior is specifically induced by the moiré layers.



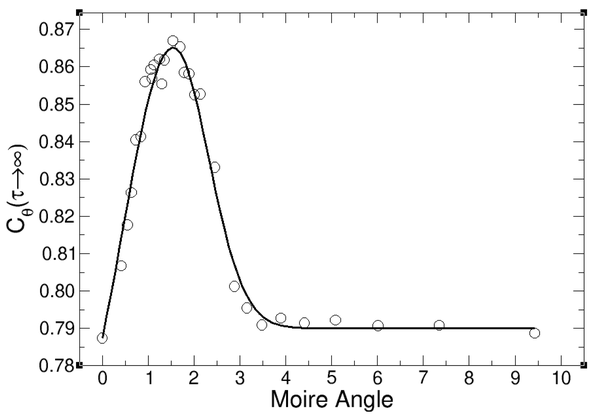
We also expect similar results for Young's modulus in dual–layer hBN.

Explanations

Thermal Rippling



To explain this dip in Young's Modulus, we performed runs on graphene and hBN at a constant ambient temperature. We then used a code that computes the autocorrelation function of the local normal vector to the sheet, which measures how persistent the sheet's out-of-plane corrugation is. We see that this quantity also peaks around the same 1.5° twist angle where Young's modulus dips (both graphene and hBN). At these angles, we see correlations are stronger in AA/AB stacking domains. This persistent, moiré-pinned rippling allows the sheets to initially flatten locally under strain, which we see as a reduction of Young's modulus. At larger twist angles, the domains shrink, the corrugation decorrelates faster, so that both $C_\theta(\tau\to\infty)$ and the modulus recover.



Conclusions + Future

Conclusions

- Twist angle measurably changes stiffness
- Peak near 1.5°
- This moiré effect is caused by thermal rippling.

Future Work

- Continue current work on fracture strain/stress and effective angle vs strain for graphene.
- Utilize similar methods to study mechanical properties of other 2D materials.