Structural and electronic properties of bilayer graphene with biaxial heterostrain

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The study of moiré engineering started with the advent of van der Waals heterostructures, in which stacking 2D layers with different lattice constants leads to a moiré pattern controlling their electronic properties. The field entered a new era when it was found that adjusting the twist between two graphene layers led to strongly-correlated-electron physics [1] and topological effects associated with atomic relaxation [2]. A twist is now routinely used to adjust the properties of 2D materials. This study investigates a new type of moiré superlattice in bilayer graphene when one layer is biaxially strained with respect to the other—so-called biaxial heterostrain [3]. Scanning tunneling microscopy measurements uncover spiraling electronic states associated with a novel symmetry-breaking atomic reconstruction at small biaxial heterostrain [3]. Atomistic calculations using experimental parameters as inputs reveal that a giant atomic swirl forms around regions of aligned stacking to reduce the mechanical energy of the bilayer. Tight-binding calculations performed on the relaxed structure show that the observed electronic states decorate spiraling domain wall solitons as required by topology. This study establishes biaxial heterostrain as an important parameter to be harnessed for the next step of moiré engineering in van der Waals multilayers.

References

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Figures

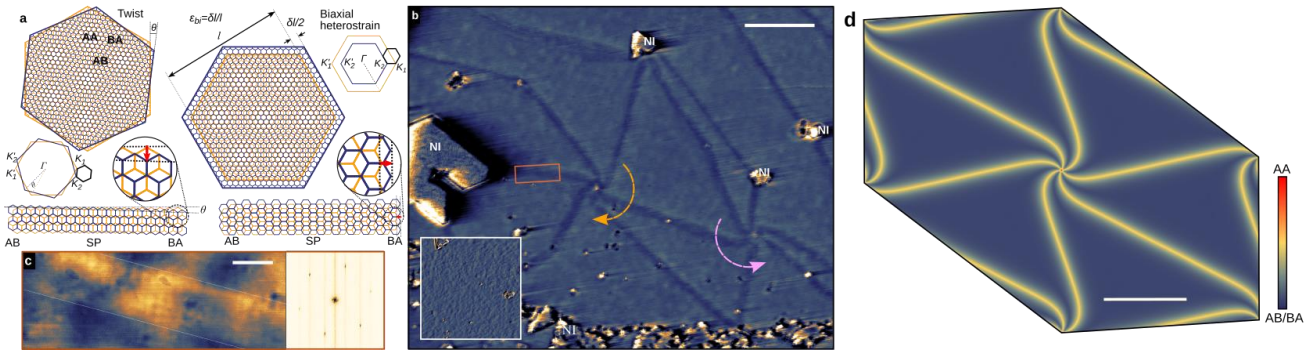

Figure 1: a) Sketch of twist vs biaxial heterostrain moiré. Scanning tunneling microscope image of bilayer graphene with small biaxial heterostrain. c) Atomically resolved image of a domain wall showing that it is parallel to the zigzag crystallographic direction. Local stacking calculated by atomistic simulations.