ABSTRACT:

Analytical Theory of Stress-Driven Lattice Relaxation in Moiré Materials

Shaffique Adam

Department of Physics, Washington University in St. Louis, St. Louis, Missouri 63130, USA

Van der Waals heterostructures are composed of atomically thin crystals that behave mechanically more like elastic membranes than rigid solids. When two layers are twisted or have slightly different lattice constants, the resulting spatial variation of atomic registry produces nonuniform interlayer adhesion forces. The layers respond by developing in-plane displacement and strain fields—and, in some cases, out-of-plane deformation—that reconstruct the moiré pattern and can qualitatively alter the electronic properties.

I will present an analytical continuum theory of this stress-driven lattice relaxation. The theory couples the elastic energy of the individual layers to a stacking-dependent interlayer adhesion energy and provides closed-form descriptions of the displacement and strain fields. For twisted homobilayers, we first obtain a single-parameter analytical model describing the weak- and intermediate-relaxation regimes [1]. In the marginal-twist, strong-coupling regime, the structure reorganizes into large domains of energetically favorable stacking separated by narrow soliton domain walls [2]. The crossover between these regimes is governed by a dimensionless parameter that can be interpreted as the ratio of the moiré period to the characteristic domain-wall width. This reveals a degree of universality across systems including twisted bilayer graphene and both parallel- and antiparallel-stacked transition-metal dichalcogenides.

We then generalize the framework to heterobilayers, where twist and lattice mismatch generate distinct rotational and dilational components of the displacement field [3]. Applications include graphene on hexagonal boron nitride and TMD heterobilayers such as $MoTe_2/WSe_2$ and WSe_2/WS_2. Near crystallographic alignment, lattice mismatch can produce substantial compressive strain, and the theory predicts a transition from predominantly in-plane relaxation to an out-of-plane buckled state.

Finally, I will discuss how the reconstructed stacking and strain fields enter electronic-structure calculations. Applications include the moiré potential and band-gap formation in graphene/hBN [4,5], interaction-driven magnetic phases in twisted WSe_2 [6], and direct measurements of the graphene/hBN electrostatic potential using an atomic single-electron transistor [7]. These examples illustrate how analytical descriptions of mechanical relaxation provide both physical

insight and quantitatively accurate structural inputs for modelling electronic and quantum phenomena in moiré materials.

References

[1] M. M. Al Ezzi, G. N. Pallewela, C. De Beule, E. J. Mele, and S. Adam, Analytical model for atomic relaxation in twisted moiré materials, Physical Review Letters 133, 266201 (2024).

[2] C. De Beule, G. N. Pallewela, M. M. Al Ezzi, L. Peng, E. J. Mele, and S. Adam, Theory for lattice relaxation in marginal twist moirés, Physical Review B Letter (2026, in press; Editors' Suggestion).

[3] C. De Beule, Y. Lai, L. Peng, D. Bennett, and S. Adam, Lattice relaxation in moiré heterobilayers, submitted (2026).

[4] J. Jung, A. M. DaSilva, A. H. MacDonald, and S. Adam, Origin of band gaps in graphene on hexagonal boron nitride, Nature Communications 6, 6308 (2015).

[5] M. Yankowitz et al., Dynamic band-structure tuning of graphene moiré superlattices with pressure, Nature 557, 404 (2018).

[6] L. Peng et al., Itinerant magnetism in twisted bilayer WSe_2 and $MoTe_2$, Physical Review B 113, L161119 (2026).

[7] D. R. Klein et al., Imaging the sub-moiré potential using an atomic single electron transistor, Nature 650, 875 (2026).