Strain-Driven Defects and Ripple Networks in Layered Two-Dimensional Materials: From Atomistic Mechanisms to Mesoscale Behaviour

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Layered two-dimensional materials such as bilayer graphene and bilayer hexagonal boron nitride (h-BN) exhibit a distinctive mechanical response arising from the interplay between strong in-plane covalent bonding and comparatively weak interlayer van der Waals interactions. This competition gives rise to a rich spectrum of deformation pathways, in which in-plane strain is accommodated not only through dislocation climb and glide but also via out-of-plane buckling, delamination, and the formation of complex ripple and structures. Using large-scale molecular dynamics (MD) simulations, we access deformation regimes that bridge atomistic and mesoscale behaviour.

Several interatomic potentials are systematically evaluated to assess their reliability in describing both interlayer interactions and defect energetics, ensuring robust and transferable insights across material systems. We begin by examining the role of partial basal dislocations of mixed screw and edge character, introduced as dipoles within bilayer systems. Structural optimisation reveals that the edge component of these dislocations plays a dominant role in driving out-of-plane buckling, with 60° mixed partials adopting energetically favourable buckled configurations consistent with experimental observations. Building on this, we explore how dislocation pile-ups lead to surface ripple formation under increasing compressive strain, identifying a critical threshold beyond which flat configurations become unstable and ripple structures emerge as the preferred state.

Extending beyond isolated defects, we investigate heterostrained bilayer graphene to uncover the emergence of dense 2D ripple networks. We demonstrate that heterogeneous in-plane strain induces confined buckling and local delamination, resulting in self-organised arrays of dislocations and ripples that evolve into extended mesoscale patterns. The insights gained provide a predictive basis for tailoring mechanical and structural properties in 2D heterostructures.