Ultra-flat twisted superlattices in 2D heterostructures

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When 2D materials are layered on top of each other an interference pattern called the Moiré-pattern is formed due to the lattice mismatch and relative rotation between the layers. Moiré-patterns already host a large variety of exciting physical phenomena e.g.: secondary Dirac cones, Hofstadter's butterfly, superconductivity. However, the corrugation stemming from the pattern is still a largely unexplored field and is lacking a comprehensive theoretical description. The way 2D heterostructures relax strain through out-of-plane deformation can highly influence the properties of such systems. The commonly accepted picture is that the corrugation is a monotonically decreasing function of the twist angle. Here we found [1] by lattice relaxation of around 8000 different Moiré-superstructures using large scale Classical Molecular Simulations combined with analytical calculations, that even a small amount of strain can substantially change this picture, giving rise to more complex behavior of superlattice corrugation as a function of twist angle. One of the most surprising findings is the emergence of a topographic ultra-flat phase that can be present for arbitrary small twist angle having a much lower corrugation level than the decoupled phase at large angles. A possible experimental realization of the ultra-flat state is revealed by STM investigations of the graphene/graphite system.

References

[1] Szendrő, M., Süle, P., Dobrik, G., & Tapasztó, L. npj Comput Mater 6, 91 (2020)

Figures

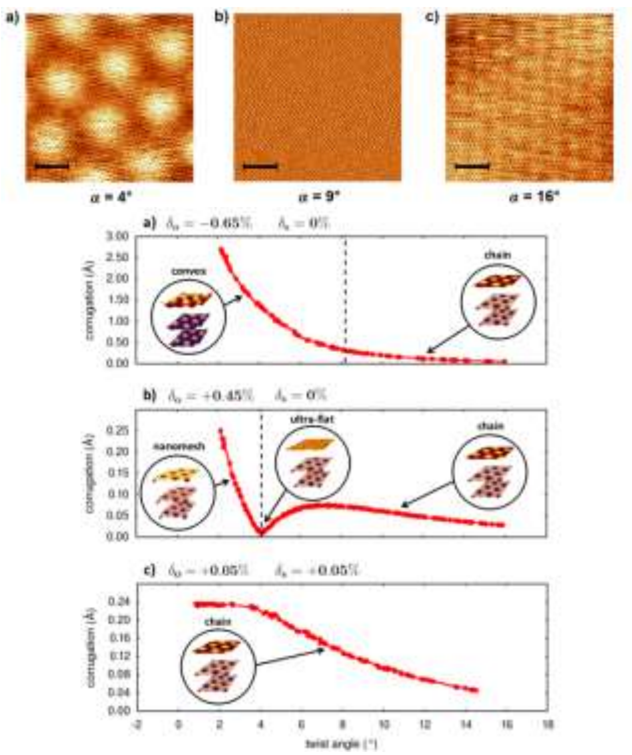

Figure 2: Moiré-superlattice corrugations of the top rotated graphene layer for three differently strained five-layer graphene heterostructures (red dots) from molecular mechanics simulations. Each point represents a commensurate Moiré-superlattice. **a)** The overlayer is externally compressed with ~0.65% during minimization which leads to a phase transition, indicated by dashed lines. **b)** The overlayer is stretched with ~0.45% strain. Near the phase transition (dashed line), the corrugation vanishes and an ultra-flat phase appears. **c)** Both the overlayer and the substrate are stretched with a small 0.05% strain. No phase-transition occurs, each point corresponds to a chain structure. In the range of 0–4° the corrugation is closely constant (plateau-effect). The topographies of the top three layers of the corresponding Moiré-phases are displayed in bubbles.

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Figure 1: Topographic scanning tunneling microscope images of graphene layers deposited on top of a graphite substrate for various relative rotation angles (scale bars: 2 nm). Although the apparent corrugation has a decreasing tendency from a–c, the STM image in panel b reveals an ultra-flat state, much smoother than observed even for high rotation angles (c). The experimental conditions for image acquisition (Itunnel = 1 nA, Ubias = 200 mV), data processing, and graphic display parameters are the same for all panels. The relative rotational angles are indicated under each panel.