Electronic Behaviour at Commensurate Interfaces between Semi-Infinite Graphite Crystals

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The two common stackings in graphite crystals are Bernal (ABA) and rhombohedral (ABC), distinguished from each other by the relative position of every third layer. The electronic behaviour on the surface of multilayer graphene stacks and semi-infinite graphite crystals of both stacking types has previously been investigated [1], with localised electronic states known to arise due to rhombohedral stacking faults [2]. Here, we study the electronic properties of the interfaces between infinite crystals of either stacking using Green's functions to derive embedding potentials that capture the influence of layers far away from the interface. We discuss all 13 distinct interfaces which we group into six categories based on the characteristic density of states features in the interfacial region. We also investigate the charge redistribution induced in the vicinity of the interface by the breaking of translational symmetry in the out-of-plane direction. We show that for some interfaces the impact of the latter can lead to on-site energy shifts ~10 meV. These studies provide a foundation for future work on surfaces misaligned by a small twist angle, with the aim to exploit the rich moiré-induced physics observed in twisted bilayer graphene [3-4] in a truly 3D structure.

References

[1] V. Kaladzhyan et al, *Phys. Rev. B* **104** (2021) 155418.
[2] J. Muten et al, *Phys. Rev. B* **104** (2021) 035404.
[3] Y. Cao et al, *Nature* **556** (2018) 43–50.
[4] Y. Cao et al, *Nature* **556** (2018) 80–84.

Figures

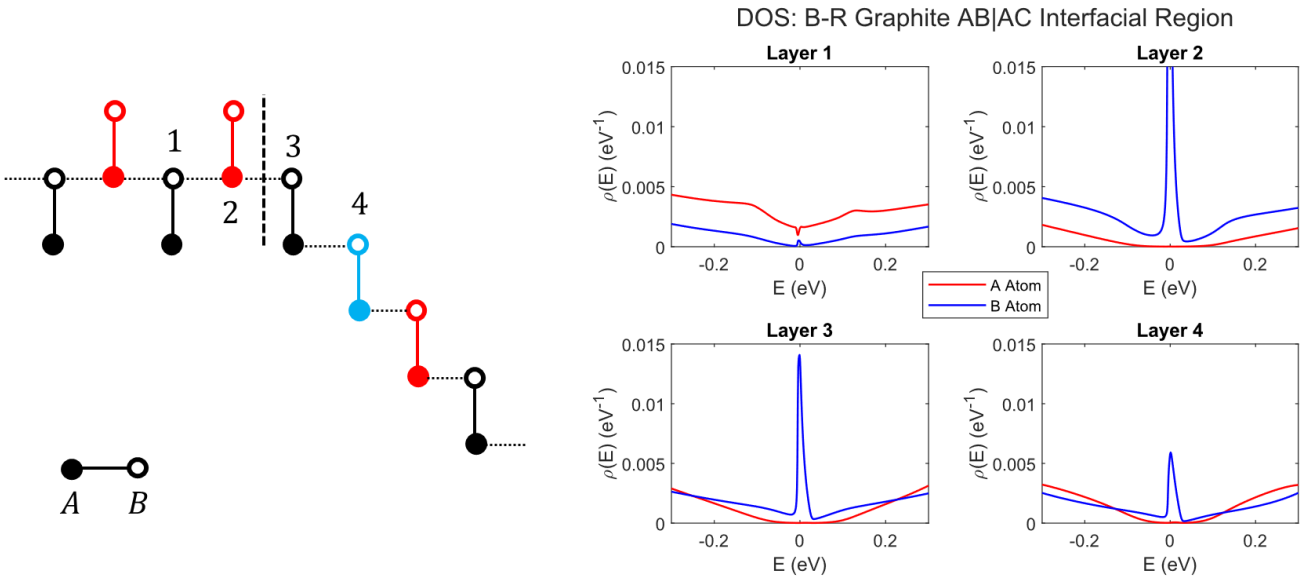

Figure 1: Side view of one of the possible infinite crystals formed from the commensurate stacking of two semi-infinite graphite crystals. In this example, the crystal on the left is Bernal stacked, the crystal on the right is rhombohedral stacked, and the dashed line represents the physical interface between the two surfaces. A region of ABAC stacking is formed near the interface, and the electronic density of states in this region is shown on the right.