Stacking Domains in Strained and Twisted Van der Waals Materials

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Introducing strain or twist between the individual layers of Van der Waals (VdW) heterostructures is yet another handle to tailor their properties, opening the route towards more refined device concepts and exotic, correlated electron effects. The formed supercells, however, are often thermodynamically metastable leading to the formation of domains with crystallographic stacking order and dislocation lines in between.
Here we demonstrate this effect for two VdW systems. We show that graphene layers grown in argon atmosphere on silicon carbide (SiC) are, in contrast to the current consensus, composed of such domains of the AB and AC versions of Bernal stacking. They are intrinsically formed during growth by nucleation dynamics and in-plane strain. The dislocation networks between domains dominate the (de)intercalation dynamics of hydrogen at the graphene/SiC interface [1]. We find very similar behaviour for twisted layers of molybdenum disulphide and explore local band structure changes due to this rearrangement using angular-resolved reflected-electron spectroscopy [2,3].

References

[1] T.A. de Jong *et al.*, Phys. Rev. Mater. 2, 104005 (2018).
[2] 1. J. Jobst, *et al.*, Nature Commun. 6, 8926 (2015).
[3] J. Jobst *et al.*, Nature Commun. 7, 13621 (2016).

Figures

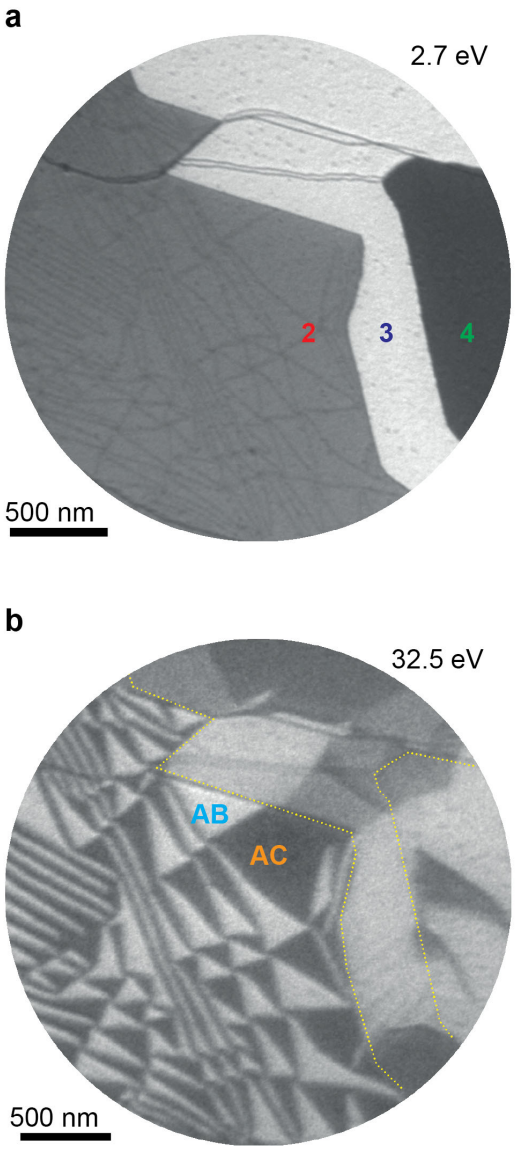

Figure 1: a, Bright-field LEEM shows homogeneous areas of constant graphene layer number (indicated) grown on silicon carbide under argon atmosphere. **b,** Dark-field LEEM of the same area, reveals that the film is, in fact, strongly structured into domains of Bernal AB and AC stacking order.