Atomic reconstruction in twisted transition metal dichalcogenide heterostructures

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The interlayer van der Waals (vdW) interactions enable two single layers of a two-dimensional material to vertically stack together and form van der Waals heterostructures (vdWHs). If the two layers have different distinct symmetries or lattice sizes or if they are twisted with respect to each other, a moiré pattern with much larger length scale than the periodicity of each layer is formed. The moiré superlattice can be further modified by twist angle, which means moiré superlattice is also formed in twisted homostructures. As moiré patterns deeply alter the physical properties of bilayer systems, the controllable design of twisted heterostructures clearly allows for new physics and engineering directions. In this case, lattice reconstruction will be vital for further understanding electronic and optical properties of these complicated moiré interfaces. Here, we performed structure relaxation for MoS2/MoSe2 vdWHs with different twist angles using the force-field method[1] employing the Stillinger-Weber (SW) and Kolmogorov-Crespi (KC) potential to capture the intralayer and interlayer interaction. Standard energy minimization and classical molecular dynamics simulations using the canonical ensemble were adopted. Significant in-plane and out-of-plane deformation can be observed for certain twist angles. Furthermore, domain-wall patterns are formed, where areas with matching lattice constants are separated by domain walls that accumulate the generated strain. This can be also observed in twisted bilayer graphene[2] and graphene/h-B heterostructures[3].

References

[1] Naik, M. H. et al, *J. Phys. Chem. C*, 123 (2019) 9770–9778.
[2] Woods, C. R. et al, *Nat. Phys.*, 10 (2014) 451-456.
[3] Zhang, K. et al, *J. Mech. Phys. Solids*, 112 (2018) 225-238.

Figures

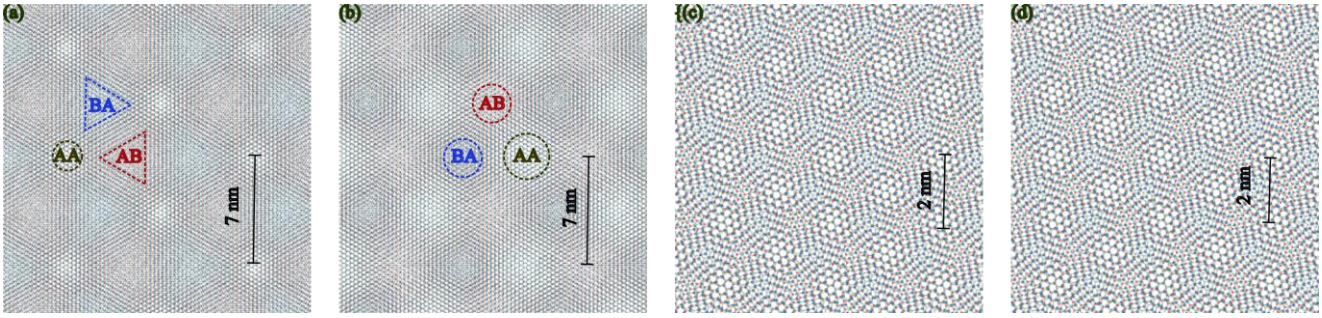

Figure 1: Lattice reconstruction of $MoS_2/MoSe_2$ bilayer, (a) parallel alignment and (b) antiparallel alignment without twist, commensurate domains with different stacking orders are highlighted by dashed lines, (c) parallel alignment and (d) antiparallel alignment with twist angle 7.3 degree.