Van der Waals epitaxy induced thermodynamically stable octahedral (1T') phase in single layer MoS_2

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Selective reversible structural switching of a material among its various polymorphs is the ultimate goal of atomic scale crystal engineering. This has never been achieved in van der Waals (vdW) crystals. It is of particular importance for molybdenum disulfide (MoS_2), where the exited state octahedral polymorphs exhibit remarkable range of physical properties, ranging from ferroelectricity [1] to quantum spin hall effect [2]. We show in this work, for the first time, that octahedral 2x1 1T' phase is obtained as the thermodynamic ground state of single layer MoS2 in heterostructure with another lattice-incommensurate van der Waals material. Temperature dependent Raman spectroscopy, conducting-mode atomic force microscopy and electrical transport studied confirms 1T' forms a network of patches/strips in the overall background of 1H phase. At room temperature, area fraction of 1T' phase can be tuned in the range 0-25%, which is reversibly switchable to 1H phase at elevated temperatures ~ 500 K. The octahedral phase in heterostructure is completely stable under repeated thermal cycling at temperatures < 500 K. We attribute the 1H to 1T' structural transition, with support from our density functional theory calculations, to incommensurability driven interfacial strain fields in the van der Waals heterostructure. Our work stablishes van der Waals epitaxy as a novel tool for atomic scale structural engineering in vdW crystals.

References

[1] Shirodkar, S. N. & Waghmare, U. V *Phys. Rev. Lett.* **112** (2014), 157601.
[2] Qian, X., Liu, J., Fu, L. & Li, J. *Science* **346** (2014), 1344–1347.

Figures

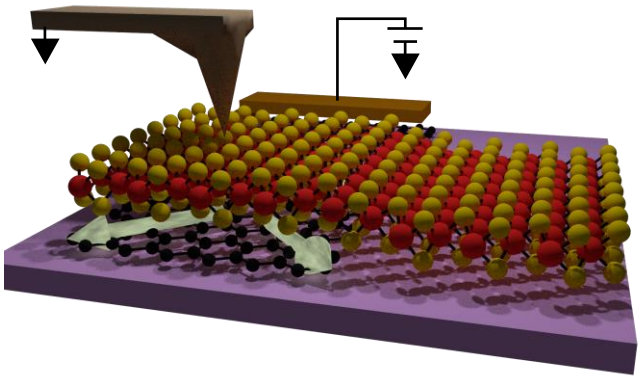

Figure 1: Schematic presentation of conducting mode AFM on MoS_2 in presence of strained van der Waals epitaxy.