MIP: 2DCC at Penn State University, DMR-1539916

In-house Research - 2019

Orientation control of epitaxial transition metal dichalcogenides on hexagonal boron nitride via defects

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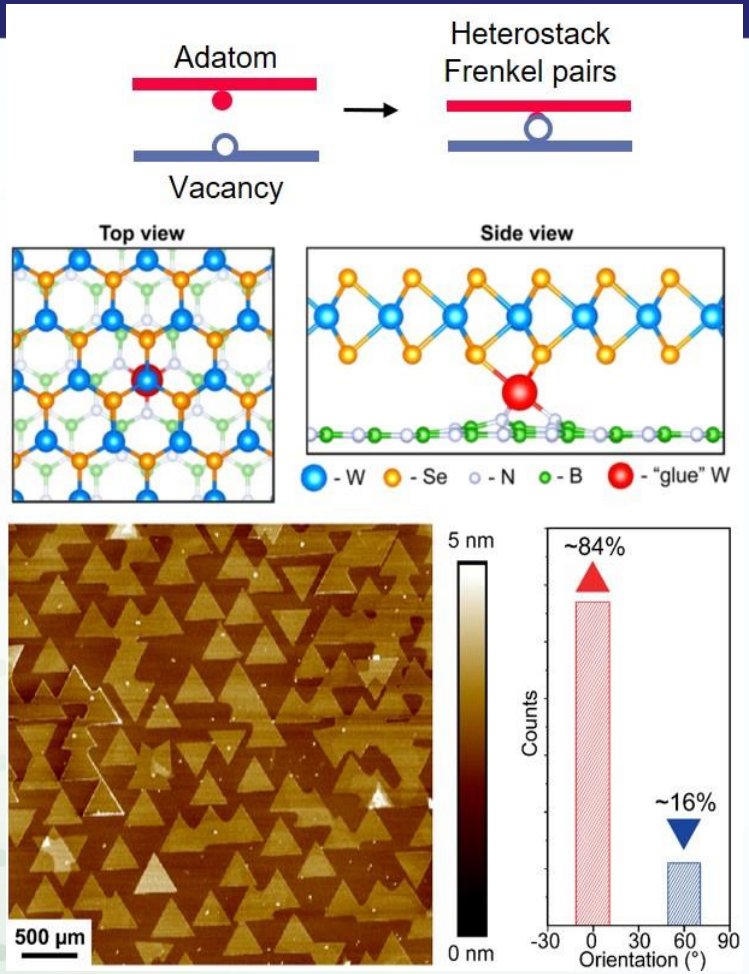
A graphene lattice remains the same under a rotation of 180º. This special symmetry is lost in monolayer transition metal dichalcogenides (TMDs), e.g. every horizontal Mo-S bond would end up as S-Mo bonds. While this lack of inversion symmetry brings out fascinating properties such as spin-coupled valley degrees of freedom, it also means that when two grains related by 180º rotation merge, the two lattices cannot smoothly stitch together, leaving an unavoidable scar – an inversion domain boundary (IDB) – that degrades transport properties.

In two recent 2DCC publications, joint experimental and theory efforts identified a general method to achieve orientational selectivity, originating from a localized defect pair that amplifies the energetic distinction between the two orientations. For monolayer MoS_2 or WSe_2 grown on hexagonal boron nitride (hBN), the defect pair is a generalization of a so-called Frenkel pair – a interstitial-vacancy pair shared between adjacent layers of a 2D heterostack. MoS_2 and WSe_2 domains initiated from such defects exhibit an orientation uniformity of over 80%, leading to suppression IDBs upon coalescence, as confirmed by aberration-corrected scanning/transmission electron microscopy. Fully coalesced 2D chalcogenide monolayer films synthesized using this approach demonstrated superior optical and electrical properties compared to films grown on sapphire under similar conditions. The results motivate further efforts focused on the development of single crystal hBN substrates and epilayers for synthesis of wafer-scale single crystal TMD films.



Published in ACS Nano 12, 2241 (2019) and Phys Rev. B 99, 155430 (2019)

DMR DIVISION OF MATERIALS RESEARCH
DIRECTORATE FOR MATHEMATICAL AND PHYSICAL SCIENCES

Also supported by DMR-1420620, TG-DMR170050, EFRI-1433378, EFRI-1542707, AFOSR 17RT0244, and ARO W911NF-17-1-0324

2DCC-MIP