Novel Insights into the Homo-/Heteroepitaxy of van der Waals Materials

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Quantification of defects in synthetic van der Waals (vdW) materials remains to date rather challenging hence underreported. In this work, a methodology for the defect quantification of 2D materials is systematically developed. The homo- and heteroepitaxy of Transition Metal Dichalcogenides (TMD) and Topological Insulators (TI) on various 2D vdW virtual substrates is in-depth researched (Figure 1a). The epitaxy experiments are performed using the Plasma-Assisted Molecular Beam Epitaxy (PA-MBE) approach [1, 2]. The presented studies attain insights into the fundamentals of vdW epitaxy, particularly essential for device applications that require multilayer stacking of 2D compounds. The homoepitaxy of WSe_2 [3] is probed using Atomic Force Microscopy (AFM) (Figure 1b) and reveals the presence of characteristic triangular-shaped WSe_2 crystals. Surprisingly, this homoepitaxy is characterized by a 6-fold in-plane rotational periodicity while defect-free epitaxy requires having a 3-fold in-plane periodicity. The latter, due to the lack of inversion symmetry of the TMD/TI compound. Consequently, this discrepancy originates from the formation of stacking faults as characterized by plan-view Transmission Electron Microscopy measurements (Figure 1c). Stacking faults in TMD occur when crystals are stacked in various sequences such as the 3R vs 2H phases. Based on the nucleation density (~5.0E+10 cm^{-2}) and the relative occurrence of the stacking phases (60 % vs 40 %), the density of 60° Grain Boundaries (GB) is simulated (Figure 1d). This, enables to define a lower limit of the defect density which is quantified as high as ~2.6E+10 cm^{-2}. Remarkably, the homoepitaxy of Bi_2Se_3 (Figure 1e) does not suffer from this inability to control the bilayer stacking phase and can therefore be grown with a significantly higher crystalline quality. This could potentially be explained by the different crystal structure nature of the TI vs TMD and/or a possible stronger interlayer coupling. Additionally, the performed heteroepitaxies have revealed the role of lattice mismatch and surface energy on diffusivity and nucleation density, and hence on defect density. This work therefore highlights essential fundamental insights into both the homo- and heteroepitaxy of various vdW materials.

References

[1] El Kazzi et al., Journal of Applied Physics, 123(13) (2018) 135702
[2] Mortelmans et al., Nanotechnology, 30(46) (2019) 465601
[3] Mortelmans et al., 2D Materials, (2020) DOI: https://doi.org/10.1088/2053-1583/ab70ec

Figures

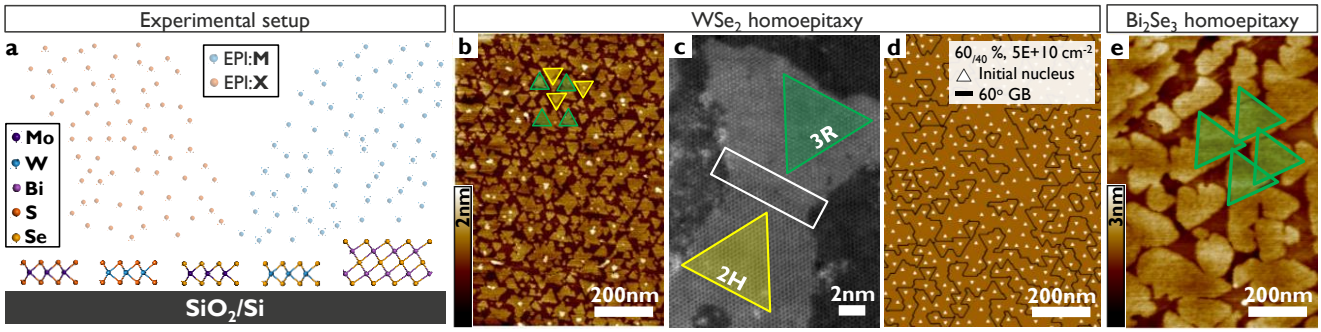

Figure 1: a) Schematic representation of the experimental PA-MBE setup. b) AFM image of the WSe_2 homoepitaxy. c) The formation process of 60° grain boundaries. d) Simulated defect density based on nucleation density and stacking control. e) AFM image of the Bi_2Se_3 homoepitaxy for comparison.