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3D/2D heterostructure: epitaxial growth of WSe₂ on GaP(111)_B

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Among the semiconducting Transition Metals Dichalcogenides (TMDs), WSe₂ appears particularly interesting due to large spin-orbit coupling and spin-splitting in the K valley [1] as well as a high carrier mobility. MBE has demonstrated valuable results for the growth of WSe₂ and related heterostructures, especially on 2D-substrates, because of the natural van der Waals interface between the epi-layer and the substrate surface. On the other hand, new generation of heterojunction have emerged, using 3D substrate as demonstrated by Pierucci et al. [2] with the MBE growth of monolayer thick and highly oriented WSe₂ film on top of GaAs(111)_B after a proper surface passivation treatment. Since rather high growth temperatures promote a better crystallographic quality of TMD layers, GaP represents an interesting alternative to GaAs considering its similar crystallographic structure and its higher thermal stability.

In this work, we demonstrate the epitaxial growth of few layers WSe₂ on GaP(111)_B by MBE, emphasizing the role of the growth temperature and of a subsequent annealing of the grown layers under a selenium flux on the polytype formed and on its structural and morphological properties. We point out the formation of the metastable 1T' phase at low growth temperature (T_G), evidenced by intermediate streaks in the RHEED pattern close to a 2×2 reconstruction (Fig. 1a), as well as the 3R phase observed with angle resolved photoemission spectroscopy [3] and transmission electron microscopy (Fig. 1c). On the other hand, a higher T_G favours a 3D growth evidenced by dots along the RHEED vertical streaks (Fig. 1b). We underscore the importance of a Se-annealing treatment in order to promote the semiconducting 2H phase formation and to improve the surface morphology (Fig. 1a & b). Optimal WSe₂ 2H bilayer and trilayer grown between 450°C and 500°C, annealed at 650°C, exhibit a flawless interface with a clear van der Waals gap (Fig. 1d). In this case, grazing incident X-Ray diffraction reveals a 1.1° in-plane disorientation (Fig. 2a) and a mean grain size of ~30 nm, supported by scanning tunnelling microscopy images (Fig. 2b). Photoemission measurements highlight the systematic p-type doping of the epi-layer, and a staggered band alignment with a slight variation of the band offset depending on the initial substrate doping type.

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[1] Z. Zhu et al., *Phys. Rev. B* **84** 153402 (2011)

[2] D. Pierucci *et al.*, *Nanoscale* **14** 5859-68 (2022).

[3] A. Mahmoudi *et al.*, *ACS Nano* **17** 21307-16 (2023).

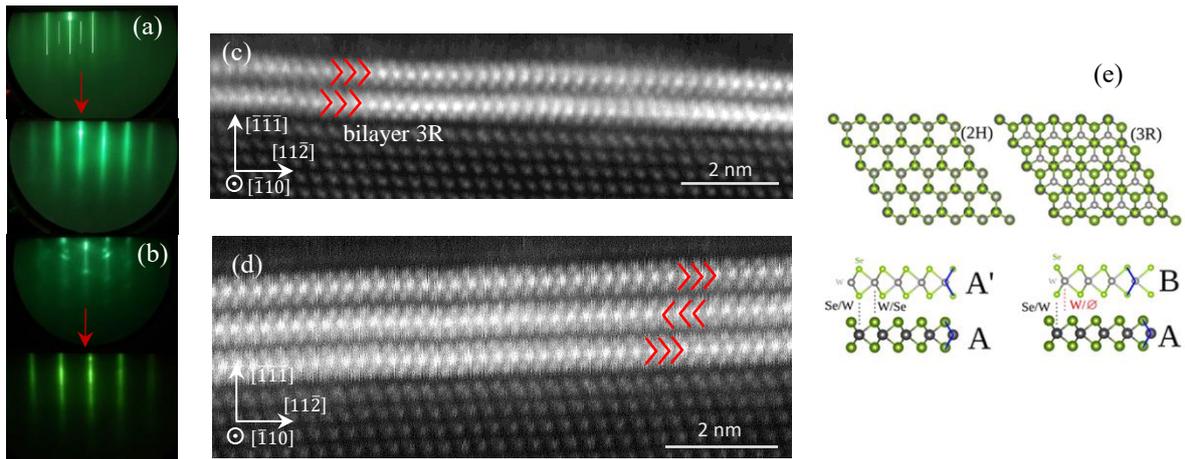


Figure 1: RHEED patterns before and after a Se-annealing step for a bilayer growth at (a) 250°C and (b) 450°C. STEM-HAADF images of (c) a bilayer grown at 250°C and (d) an annealed trilayer grown at 450°C with (e) the schematic representation of bilayer WSe₂: top and lateral views of 2H and 3R stacking sequences, extracted from Mahmoudi et al. [3].

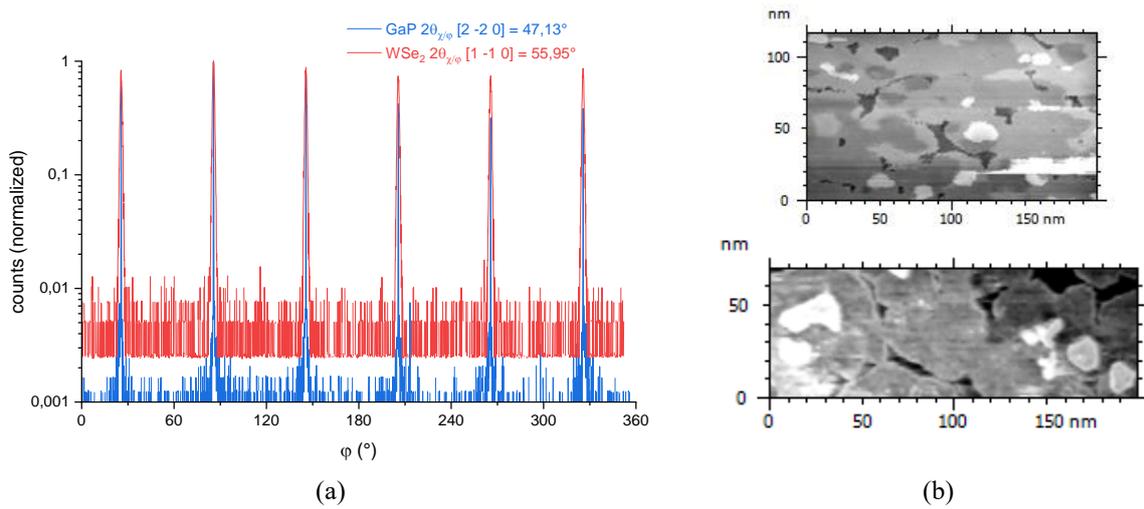


Figure 2: (a) 360° GaP [2-20] and WSe₂ [1-10] azimuthal ϕ spectra measured by grazing incident X-ray diffraction for a WSe₂ bilayer grown at 450°C and Se-annealed. (b) STM images recorded at different locations on the surface of an annealed WSe₂ bilayer grown at 450°C.