Self-organized 2H | 3R lateral boundaries in bilayer WSe_2 grown by chemical vapor deposition

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The transition metal dichalcogenides (TMDs) family exhibits a variety of polytypes in the bilayer (2ML) form, with the most known being the rhombohedral AB bilayer (non-centrosymmetric, 3R-like) and the hexagonal AA' bilayer (centrosymmetric, 2H) [1]. The 3R bilayer structure of TMDs is particularly notable for supporting a permanent ferroelectric polarization, attributed to its reduced symmetry [2]. In this study, we investigate self-organized 2H | 3R boundaries in mixed-phase 2ML WSe_2 crystals grown by chemical vapor deposition (CVD) [3], as shown in Fig.1(a). We utilize micro-Raman and second harmonic generation (SHG) techniques to differentiate and assign the different polytype domains, see Fig.1(b-c). Additionally, we find that transmission electron microscopy (TEM) provides useful complementary information for polytypes identification [4]. Finally, in Fig.1(d), we use dark field (DF)-TEM to resolve a characteristic sawtooth structure at the 2H | 3R boundary whose proposed atomic reconstruction can be related to twin boundaries in other TMDs [5].

References

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Figures

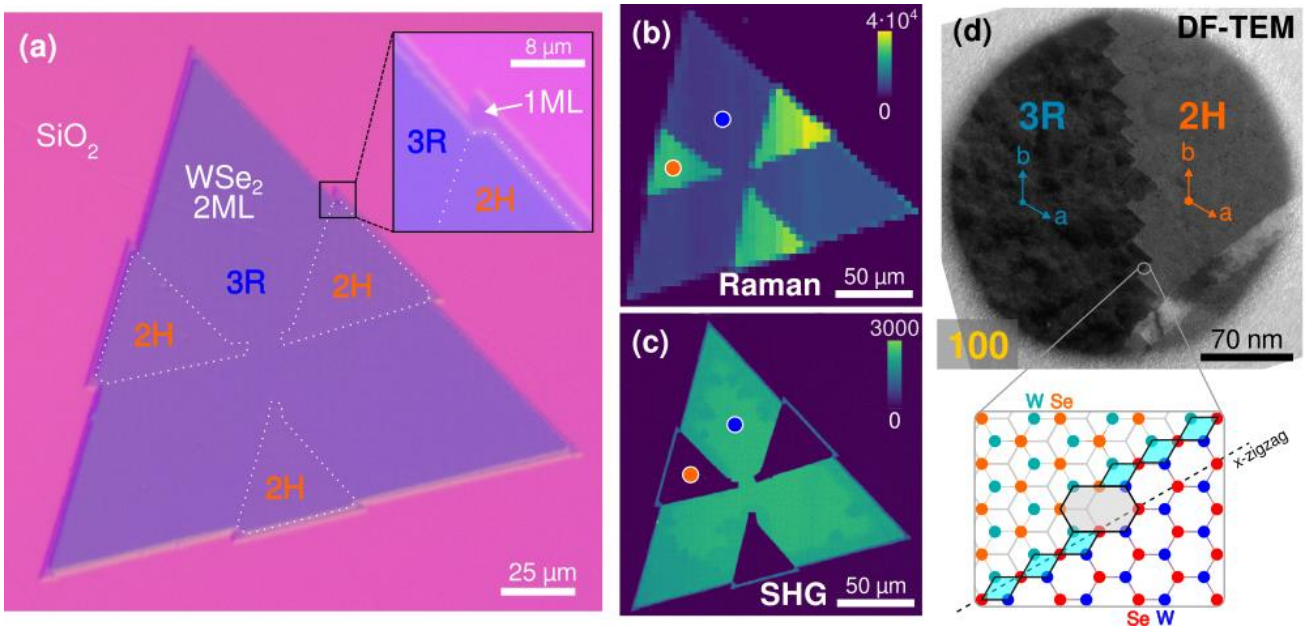

Figure 1: (a) Monocrystal WSe_2 with near complete 2ML coverage and hint of different stacking order: 3R main region and 2H inclusions. (b) Room-temperature integrated Raman intensity map on the A_{1g} mode. (c) Room-temperature SHG intensity map. (d) Dark field TEM image of the real space 2H | 3R lateral boundary, obtained by selecting the 100 reflection, with proposed atomic reconstruction of phase boundary.