## Domain shape evolutions of MoSe<sub>2</sub>-WSe<sub>2</sub> monolayer lateral heterojunctions

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Monolayer lateral heterojunctions (HJs) consisting of two distinct transition metal dichalcogenides (TMDs) have formed a new class of atomically thin p-n junctions for applications in electronics and optoelectronics [1]. Here we report that monolayer MoSe<sub>2</sub>-WSe<sub>2</sub> lateral HJs grown by chemical vaper deposition (CVD) can lead to very distinct domain shapes in the outer WSe<sub>2</sub> caused by different termination edges of the inner MoS<sub>2</sub> (Fig.1). Depending on the distances from the precursors, the domain shape of MoSe<sub>2</sub> evolves from truncated triangle at upstream to hexagonal and eventually returns to truncated triangle at the downstream, resulting in very distinct domain shapes in the outer WSe<sub>2</sub>. Second harmonic generation microscopy reveals that the inner and the outer materials have the same crystal orientation. High-angle annular-dark-field scanning transmission electron microscopy (HAADF STEM) analysis indicates that the growth of outer WSe<sub>2</sub> is under W-rich condition, which leads to a faster outgrowth rate from the Se-zigzag (Sezz) edges of the inner MoSe<sub>2</sub>, leaving behind preferential W-zz termination edges in the outer WSe<sub>2</sub> [2]. A kinetics-driven growth model is proposed to explain the formation of forked shape edges and grain boundaries in the WSe<sub>2</sub> extended from the Se-zz edges of the inner MoSe<sub>2</sub> (Fig.2). Photoluminescence (PL) microscopy shows that the PL peak energy exhibits a nonuniform distribution, indicative of strain inhomogeneity in the outer WSe<sub>2</sub>. The strain inhomogeneity induced by growth kinetics is discussed. This work elucidates the key growth parameters for controlling the domain shapes and grain boundaries in monolayer TMD lateral HJs.

## References

- [1] M.-Y. Li et al., Science, 349 (2015), 524
- [2] S. Wang et al., Chem. Mater., 26, (2014), 6371



**Figure 1:** (a) Schematic illustration of the CVD system. (b-d) Domain shape evolutions of WSe<sub>2</sub> epitaxially grown at the edges of inner MoSe<sub>2</sub> from upstream (b) to downstream (d). The scale bar is 10 µm.



