Atomic-scale mechanisms on the stepwise growth of $Mo_xW_{1-x}S_2$ into hexagonal flakes

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The alloying of two-dimensional (2D) transition metal dichalcogenides (TMDs) is a practical strategy on tuning the physicochemical properties yet with negligible effect of lattice strain. Although a wide range of TMD alloys have been fabricated in recent reports, the atomic-scale mechanisms regarding their growth processes remain as open questions despite the previous achievements on stoichiometric TMDs [1]. In this work, we attempt to reveal the growth dynamics of $Mo_xW_{1-x}S_2$ flakes from solid precursor using in situ transmission electron microscopy (TEM) [2]. The systematical in situ TEM analysis and DFT calculations suggest three stepwise formation stages during the growth of $Mo_xW_{1-x}S_2$ hexagonal flakes, which are initial assembly of precursor into vertical structures, subsequent transition into horizontal structures, and final surface relaxing and faceting into hexagonal flakes. Moreover, the similarities and differences for the growth mechanisms of alloyed and stoichiometric TMDs are therefore discussed, such as the high anisotropy for the vertical structures, the thermodynamically controlled “spherization”, the surface faceting toward regular hexagonal flakes, and the high thermal stability of the alloyed flakes.

References

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