Hyun Seok Lee[1,2]
Gwang Hwi An[1]
[1]Department of Physics, Chungbuk National University, Cheongju 28644, Republic of Korea.
[2]Center for Integrated Nanostructure Physics (CINAP), Institute for Basic Science (IBS), Sungkyunkwan University(SKKU),Suwon 16419, Republic of Korea.

Contact@E-mail: hsl@chungbuk.ac.kr

Formation mechanism of heterogeneous defect domains in CVD-grown hexagonal-WS_2 monolayers

Two-dimensional transition-metal dichalcogenides (TMDs) with versatile material library have been spotlighted for numerous unexplored research fields, thanks to various potential applications. Synthesized monolayer TMDs by a chemical vapor deposition (CVD) method inevitably contain intricate defects such as vacancys.[1] Monolayer WS_2 grown by CVD typically have a triangular or hexagonal shape depending on growth conditions. Hexagonal WS_2 flakes consist of alternating heterogeneous defect domains; S vacancy (SV) and W vacancy (WV) domains in a single monolayer crystal. Electron mobility and photoluminesence properties of the WV-rich domain with deep-trap states were lower by one order of magnitude than those of the SV-rich domain with shallow-donor states.[2, 3] However, a prevailing growth mechanism is not elucidated on the basis of experimental evidences, although we had proposed a possible mechanism based on the precoursor accumulation model [2]. Here, we discuss various experimental evidences to support our propoased model for the formation mechanism of the heterogeneous defect domain. As the flake shape evolves from triangle to hexagonal shape as a growth time increases, the remnant W-precursors not having reacted with S atoms accumulate near the triangular facet edges, resulting in SV domain formation (S deficient). In contrast, at the corners of the triangular flake, the blind zone without the accumulation process results in a relatively low concentration of the W-source, resulting in the WV domain formation (W deficient). Eventually, as the facets grow further, each domain along the truncated facets that evolve from the three corners develops and a hexagonal shape with alternating heterogenious defect domains is formed along six facet directions. This selective accumulation behavior of remnant W-precursors at the SV-facets is evidenced by atomic force microscopy image and micro-photoluminescence/Raman mapping image for each evolution step of flake shape depending on growth time. Our results pave a way to understant a defect domain formation mechansm in CVD-grown TMD monolayers.

References

[1] Z. Cai et al., Chem. Rev.118(2018)6091
[2] H. Y. Jeong et al., Adv. Mater. 29(2017)1605043
[3] H. Ly et al., ACS Nano 11(2017) 7534

Figures

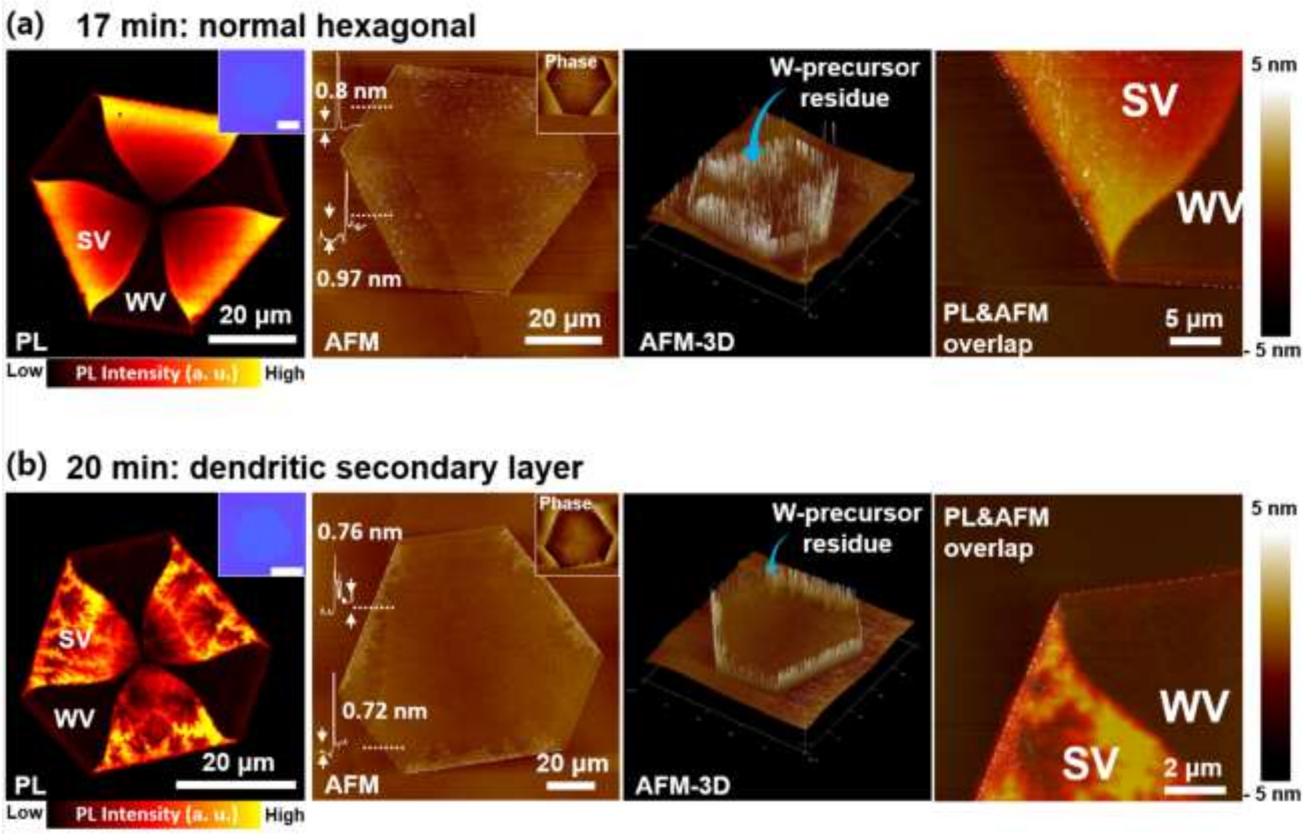

Figure 1: AFM topography images for elucidating selective accumulation of remnant W-precursor at SV domain facet. (a) short growth time for normal hexagonal WS_2 and(b) long growth time for dendritic secondary layer formation on hexagonal WS_2.

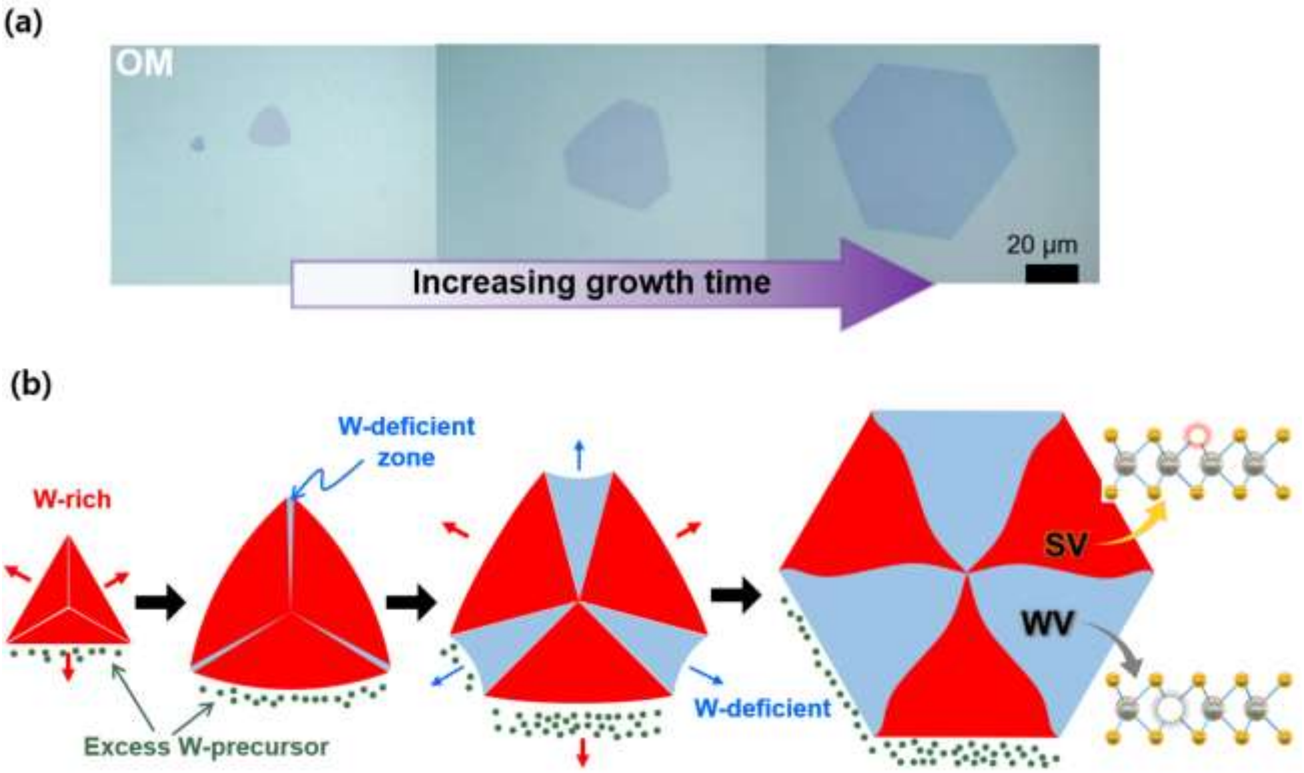

Figure 2: (a) Optical micrograph images for evolution of hexagonal WS_2 depending on a growth time. (b) schematics depicting a formation mechanism of heterogeneous defect domain based on experimental evidences.