Defect engineering of monolayer MoS_2 by single-step CVD for tunable electronic and optoelectronic devices

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Defects in atomically thin two-dimensional (2D) materials can drive new functionalities and expand applications to multifunctional systems that are monolithically integrated. An ability to control formation of defects during the synthesis process is an important capability to create practical deployment opportunities. Molybdenum disulfide (MoS_2), a 2D semiconducting material possess intrinsic defects that can be harnessed to achieve tuneable electronic, optoelectronic, and electrochemical devices. However, achieving precise control over defect formation within monolayer MoS_2, while maintaining the structural integrity of the crystals remains a notable challenge. Here, we present a one-step, in-situ defect engineering approach for monolayer MoS_2 using a pressure dependent chemical vapour deposition (CVD) process. Monolayer MoS_2 grown in low-pressure CVD conditions (LP-MoS_2) produces sulfur vacancy (Vs) induced defect rich crystals primarily attributed to the oxygen deficient growth conditions. Conversely, in MoS2 grown in atmospheric pressure CVD conditions (AP-MoS_2), these Vs defects are passivated with oxygen present in the ambient conditions. This disparity in defect profiles profoundly impacts crucial functional properties and device performance based on as-grown MoS_2 crystals. AP-MoS_2 shows a drastically enhanced photoluminescence, which is significantly quenched in LP-MoS_2 attributed to in-gap electron donor states induced by the Vs defects. However, the n-doping induced by the Vs defects in LP-MoS_2 generates enhanced photoresponsivity and detectivity in our fabricated photodetectors compared to the AP-MoS2 based devices. Defect-rich LP-MoS_2 outperforms AP-MoS_2 as channel layers of field-effect transistors (FETs), as well as electrocatalytic material for hydrogen evolution reaction (HER). This work presents a single-step CVD approach for in-situ defect engineering in monolayer MoS_2 and presents a pathway to control defects in other 2D transition metal dichalcogenides (TMDs) materials.

References

[1] Irfan H. Abidi et. al., Advanced Functional Materials, (2024), (article just accepted)
[2] Shen, Pin-Chun, et al. " Nature Electronics 5.1 (2022): 28-36.

Figures

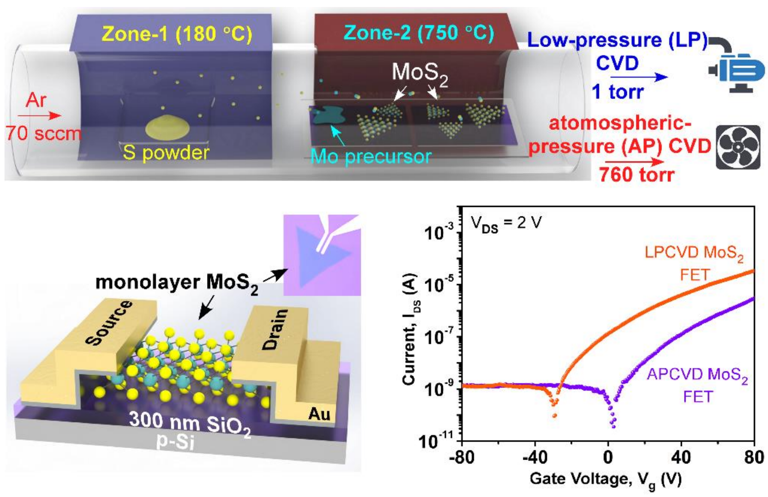

Figure 1: Schematic of CVD configuration used to modulate MoS_2 growth. Schematic and FET characteristics of AP-MoS_2 and LP-MoS_2 based devices.