Correlation between defect occupation and threshold voltage in a MoS_2-FET

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Metal-organic chemical vapour deposition (MOCVD) is a highly promising approach for synthesising transition metal dichalcogenide (TMDC) monolayers on a wafer scale. However, MOCVD-grown monolayers (ML) still have high defect densities that cause in-gap states and thus unwanted background doping. Moreover, TMDC-substrate interaction is currently discussed as an important doping mechanism, where defect states apparently also play a key role [1]. Thus, to understand and optimize the functionality of field effect transistors (FETs) based on TMDCs it is crucial to understand the impact of in-gap states and their occupation on doping and consequently on the threshold voltage of TMDC FETs.
Here, we employ gate-controlled, temperature-dependent photoluminescence (PL) spectroscopy [1,2] to reveal the correlation between defect occupation and threshold voltages in a molybdenum disulfide (MoS_2) monolayer field-effect transistor (FET). 1.2 monolayers (ML) of MoS_2 were deposited on a 2-inch, c-plane sapphire substrate using an industry-standard, 200 mm CVD reactor with $Mo(CO)_6$ and H_2S precursors. At low temperatures, the PL spectrum of the MoS_2 monolayer is dominated by a distinct defect emission, stemming from excitons bound to in-gap defect states. Transferring MoS_2 to Si/SiO_2 and fabricating a MoS_2 field effect transistor (FET) allows to control the population of the in-gap states in the TMDC monolayer by shifting the Fermi energy (E_F) with the back gate voltage. A strong bound exciton emission is observed if E_F is below the in-gap states. Increasing E_F above the in-gap state energy leads to a population of the in-gap states, which results in a significant intensity drop of the bound exciton emission. Interestingly, we found a distinct correlation between the gate voltage required to suppress the defect emission, i.e., to populate the defect states, and the threshold voltage in the FET, both systematically changing with temperature (Fig. 1). This correlation demonstrates that the occupation of in-gap states as monitored by PL spectroscopy is a key factor that determines the threshold voltage in TMDC based FETs.

References

[1] Zhu et al., The Journal of Physical Chemistry C, 129, 8294–8302 (2025)
[2] Nuytten et al., Materials Science in Semiconductor Processing, 193, 109489 (2025)

Figures

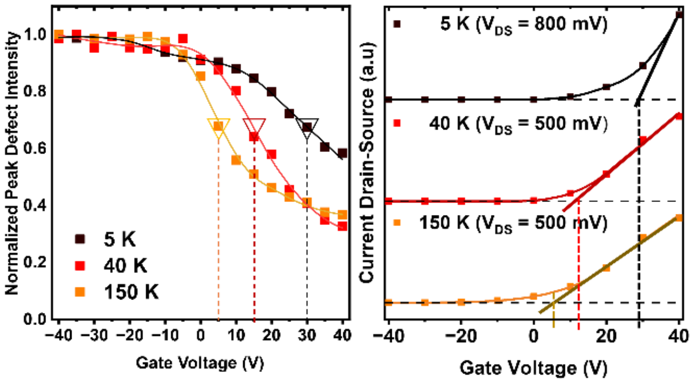

Figure 1: Left: Gate-dependent defect PL intensity for different temperatures. Right: Transfer characteristics of the MoS_2-FET for different temperatures.