Wafer-scale epitaxial MOCVD of transition metal dichalcogenides at 2DCC - featuring *in-situ* spectroscopic ellipsometry

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Abstract:

The epitaxial growth of wafer-scale transition metal dichalcogenides (TMDs) by metal-organic chemical vapor deposition (MOCVD) offers a promising route for integrating atomically thin semiconductors into next-generation electronic, optoelectronic, and quantum devices. However, achieving large-area, uniform monolayers with controlled defect density, stoichiometry, and crystallographic orientation remains challenging due to the complex interplay of precursor kinetics, substrate interactions, and growth thermodynamics.

At 2DCC, we employ metal-organic chemical vapor deposition (MOCVD) to synthesize wafer-scale epitaxial WSe_2 on 50 mm diameter c-plane sapphire substrates using a controlled "nucleation-ripening-lateral" growth approach. By systematically tuning growth parameters—such as nucleation temperature and lateral growth duration—we investigate the dynamics of film evolution in the nucleation-coalescence regime.

The resulting films are characterized using atomic force microscopy (AFM) to assess morphology (lateral coverage, coalescence), while Raman spectroscopy, photoluminescence (PL) spectroscopy, X-ray photoelectron spectroscopy (XPS), and in-plane X-ray diffraction (XRD) are employed to evaluate composition (stoichiometry, phase), crystallographic orientation, and optical properties. Our findings reveal a 1T-to-2H phase transition, with the 1T phase fraction decreasing from 58% in as-nucleated films (0 min lateral growth) to negligible levels after 7 min of lateral growth. Notably, Raman, PL, XPS, and AFM analyses demonstrate high consistency across the wafer, from the wafer center to 20 mm off-center, confirming excellent uniformity. Additionally, we are developing in-situ spectroscopic ellipsometry (SE) as a real-time, non-destructive tool to monitor growth mechanisms and dynamically optimize parameters by tracking optical properties. The integration of MOCVD with *in-situ* SE holds promise as a universal platform for yield control in synthesizing other 2D materials (e.g., $MoSe_2$, WS_2) and their heterostructures. Future directions include machine-learning-assisted SE analysis for predictive growth optimization.

Keywords: MOCVD, transition metal dichalcogenides (TMDs), wafer-scale epitaxy, *in-situ* spectroscopic ellipsometry, real-time monitoring.