Mechanistic Insights into the Salt-Assisted CVD Growth of MoS_2

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Abstract

MoS_2, a member of the transition-metal dichalcogenide (TMD) family, has attracted considerable interest due to its unique structure and exceptional physical and chemical properties. It exhibits a thickness-dependent bandgap, transitioning from an indirect bandgap of ~1.2 eV in the bulk to a direct bandgap of ~1.85 eV in the monolayer, making it highly attractive for applications in optoelectronics, nanoelectronics, spintronics, valleytronics, and catalysis [1]. Although conventional CVD is typically performed at high temperatures, salt-assisted CVD enables low-temperature and large-area synthesis [2]. However, a comprehensive understanding of the underlying growth mechanism remains lacking. Current interpretations of salt-assisted CVD propose two primary pathways: the formation of volatile metal oxy-halide intermediates that enhance precursor transport [2], and the formation of alkali metal molybdate phases that act as reactive intermediates and seeding layers during nucleation [3]. While both mechanisms have been individually reported, their relative importance at lower temperatures remains unclear. Here, we investigate the interplay between these pathways to understand their roles in enabling low-temperature growth. The formation of intermediate species, including sodium molybdates and molybdenum oxychlorides, plays a central role in this process. Sodium molybdate phases were confirmed by ex-situ XRD, Raman spectroscopy, and EDS analysis. In contrast, volatile molybdenum oxychlorides cannot be directly detected by solid-state techniques; thermogravimetric analysis coupled with annealing revealed a ~15% weight loss attributed to the evaporation of Mo-O-Cl species. This mechanistic insight is crucial for rational control of nucleation, defect density, and film uniformity, enabling reproducible and scalable low-temperature MoS_2 synthesis for flexible and CMOS-compatible device applications.

References

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Figures

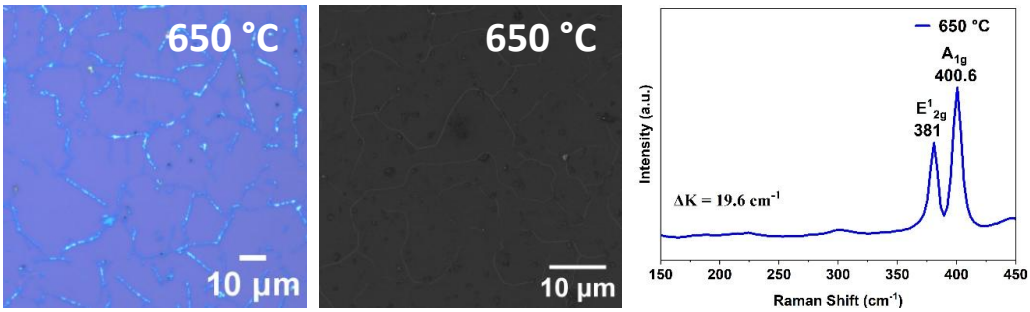

Figure 1: Optical image, SEM image, and Raman spectra of monolayer MoS_2 grown at 650 °C