Kinetics of wafer-scale epitaxial growth of MoS_2 on sapphire

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Monolayers of transition metal dichalcogenides (TMDs) such as MoS_2 could potentially revolutionize a range of electronic and optoelectronic applications; however, there is a lack of understanding regarding the basis fundamentals of their growth. Metal organic chemical vapor deposition (MOCVD) with its gaseous precursors allows for tight control and modulation of parameters such as gas phase composition and growth time. MoS_2 films grown on sapphire substrates are epitaxial with minimal strain.

In this work, we discuss the wafer-scale growth of MoS_2 monolayers on sapphire via MOCVD. The films were grown on 2" c-plane sapphire wafers in a horizontal cold-wall reactor at 900-1000 °C using H_2S and $Mo(CO)_6$ as precursors with a nominal chalcogen to metal ratio of 20,000 with H_2 as the carrier gas. Atomic force microscopy and scanning electron microscopy were used to measure the surface coverage and domain density. Additionally, the coverage dependance of Raman, photoluminescence, and absorption spectra along with the in-plane X-ray diffraction patterns will be shown and discussed.

We were able to obtain fully coalesced epitaxial MoS_2 films within only 12 minutes of growth. Within 30 s, the film fully nucleates on the substrate, achieving domain densities of 1-2*10^3 μm^{-2}, which remains relatively constant for the rest of the growth. Then, the domains laterally grow out linearly at a rate of about 150 nm^2/min until they being to merge. After 3 minutes of growth, 65% of the sapphire is covered. However, the growth rate subsequently decreases due to reduced adsorption on the MoS_2. After the film fully coalesces, bi- and multilayer structures begin to grow that eventually evolve into pyramids and spirals at sufficiently long growth times.

To adjust the domain density of the sample, we grew MoS_2 films at different temperatures. Reducing the growth temperature increased the domain density, while for longer growths, bi- and multilayer coverage was minimized when grown at 950 °C. Additionally, pre-annealing the sapphire under a H_2 and H_2S mixture limits nucleation to along the step edges in the substrate and is likely due to sulfur passivation of the sapphire.

Our results help probe the effects of surface chemistry and growth conditions on the MOCVD growth of MoS_2, thereby enabling a deeper understanding of the fundamental kinetics of the system. This knowledge will be applicable to other TMDs as well as other deposition techniques.