Epitaxial Growth and Characterization of MoS_2 by Metalorganic Chemical Vapor Deposition (MOCVD) for Next Generation Devices

Shalini Kumari[1,2], Chen Chen[2], Nicholas Trainor[1,2], Andrew R. Graves[2], Thomas V. McKnight[1,2], Meghan E. Leger[1,2], and J. M. Redwing[1,2]

[1]Department of Materials Science and Engineering, [2]2D Crystal Consortium – Materials Innovation Platform, The Pennsylvania State University, University Park, PA, 16802.

Abstract:
2D Transition Metal Dichalcogenides (TMDs), particularly monolayer molybdenum disulfide (MoS_2), hold immense promise for next-generation device applications due to their unique electronic and optical properties. Metalorganic chemical vapor deposition (MOCVD) emerges as a key technique for epitaxial TMD monolayer growth, enabling the use of high substrate temperatures (900-1000^{o}C) and precise control over precursor flow rates with chalcogen/metal ratios (10^3-10^5). In addition, the flow rate of precursors can be modulated during growth to enhance the surface diffusion of metal-containing species and control the lateral growth rate of TMD domains. Recently, we have focused on the epitaxial growth of MoS_2 on 2” c-plane sapphire and 1cm*1cm nitride substrates and studied how the critical growth parameters e.g. temperature, pressure, precursor flow, substrate surface chemistry, substrate orientation and substrate miscut angle impact the film growth and their optical and electrical properties.

Coalesced MoS_2 monolayers were grown on 2” diameter c-plane sapphire and 1 * 1 cm^2 nitrides substrates in a cold-wall horizontal MOCVD reactor with an inductively heated graphite susceptor with gas-foil wafer rotation. Molybdenum hexacarbonyl ($M(CO)_6$) was used as the metal precursor while hydrogen sulfide (H_2S) was the chalcogen source with H_2 as the carrier gas at 50 Torr reactor pressure. The single step (only lateral growth) growth process were utilized to achieve coalescence followed by post growth annealing in H_2S to 300 °C to inhibit the decomposition of the obtained MoS_2 films. Surface morphology, epitaxial crystallinity, and optical properties of the grown TMDs were systematically characterized by AFM, FESEM, RHEED, Raman, Photoluminescence, UV-VIS-IR absorption spectrum, in-situ Ellipsometry, and In-plane XRD. Characterization results show interesting effects of temperature, pressure, precursor flow, substrate surface chemistry, orientation and miscut angle of the sapphire substrates on the film growth and their optical and electrical properties. The epitaxial orientation of the TMD is found to be strongly dependent on the pre-growth annealing ambient (H_2 vs H_2S/H_2Se) and the growth temperature which can be tuned to minimize inversion domains and high angle grain boundaries which negatively impact field-effect mobility. These endeavors facilitate a profound comprehension of the fundamental mechanisms of monolayer MoS_2 growth, thereby paving the way for the advancement of next-generation electrical and optoelectronic devices.