In Situ Characterization of 2D Materials Growth in MOCVD

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In recent years the field of 2D materials has developed rapidly, with a surge in interest due, in part, to breakthroughs in fabrication processes such as mechanical exfoliation, which, in 2004, allowed for the creation of the first 2D material: graphene. Since then, research into other methods, such as metalorganic chemical vapour deposition (MOCVD), has been ongoing with the goal of finding reliable ways to create 2D-monolayers at the wafer scale. Achieving this would enable a more reproducible means of exploiting the 2D materials' properties and provide a path towards commercialization [1].



Fig. 1: During the growth of a single monolayer, the small size of WS_2 islands allow some parts of the substrate to be exposed to the *in-situ* light illumination, indicating the important role of coverage in the analysis of reflectance measurements.

The new interest in 2D materials is also sparked by their intriguing properties which have potential applications across multiple fields such as optics, electronics, and energy storage, contributing to advancements in technologies ranging from flexible electronic devices to highly efficient solar cells. Their unique characteristics, including high conductivity, exceptional mechanical strength, and remarkable optical properties, make them highly sought after for a wide range of applications. For instance, in the realm of optoelectronics, 2D transition-metal dichalcogenides (TMDs) such as WS₂ and MoS₂ are being explored for their potential in creating photodetectors, light-emitting diodes and lasers [2] enabled by their direct optical bandgaps which are achieved in the monolayer limit and which are not available in the corresponding bulk crystals [3]. Defects in TMDs are also very interesting as potential sources of single-photon emission, with applications in quantum information.

Our current research aims to characterize the growth and optical properties of WS_2 monolayers that have been grown using an AIXTRON CCS 3x2" commercial MOCVD system. Using a Laytec EpiTT reflectance instrument located inside the MOCVD system, we were able to perform *in situ* normal-incidence reflectance characterization simultaneously at wavelengths of 405, 633 and 905 nm. We have found that the virtual interface method[4], typically used to obtain growth rates and optical constants for thicker materials, cannot be applied accurately to 2D materials. Instead, we propose a new model utilizing coverage, and through the analysis of experimental data, we determine that the coverage is not linear over time. This non-linearity is attributed to underlying physical phenomena that happen during the growth including nucleation, ripening, and coalescence.

References

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Fig. 2: Illustration of the coverage contribution of each type of stack to the total reflectance.