Towards Quantifying Defect Density in Molybdenum Disulfide (MoS_2) via Optical Emission Spectroscopy

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Monolayer molybdenum disulfide (MoS_2) absorbs and emits light via a direct optical bandgap, making it a promising material for many optoelectronic applications. While metal-organic chemical vapor deposition (MOCVD) is a scalable method for producing monolayer MoS_2, the optical emission of material produced in this manner is lower compared to the mechanical exfoliated MoS_2 due to high defect density. In this study, uniform monolayer MoS_2 films were grown on a 2-inch sapphire substrate. Optical characterization reveals that thermal annealing at temperatures up to 340 °C in the atmosphere enhances the optical emission of MoS_2 grown in N_2, increasing PL intensity by a factor of three, while changing from dominant Trion emission to a more neutral exciton one. We propose that during the annealing sulfur vacancies are passivated by oxygen atoms. This reduces the number of excess electrons, leading to lower background n-doping and reduced nonradiative Auger losses [1]. Low temperature (5.5 K) PL measurements support the hypothesis of defect annealing: Deep defect emission dominates the spectrum for the as-grown sample, while annealing leads to near bandgap emission. These empirical observations lay a foundation for scalable techniques for quantifying defect concentration of MOCVD-grown MoS_2 based on the "observed" optical emission changes. A Bayesian model will incorporate prior information about defects in MOCVD MoS_2 and a likelihood function that accounts for defect distribution and associated uncertainties, yielding posterior probabilities of defect occurrence. Overall, this study investigates the post-growth treatment of MoS_2 and presents a scalable approach to improving its optical emission and defect quantification, advancing its potential for optoelectronic applications.

Reference

[1] Nan et al., ACS nano, 6 (2014) 5738-5745

Figures

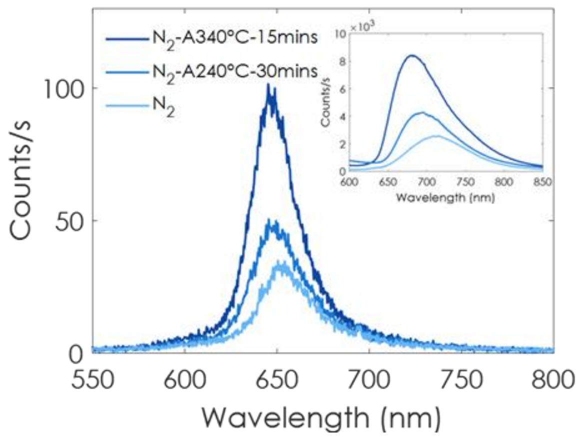

Figure 1: Room-temperature PL spectra of MoS_2 samples treated at 240°C and 340°C in the atmosphere. The inset shows PL spectra of N_2-grown MoS_2 under the same thermal treatments, measured at 5.5K.