Rapid Analysis of 2D Material Quality Using Raman Spectroscopy

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As silicon reaches its intrinsic scaling limits, emerging thin-film materials like transition metal dichalcogenides (TMDs) must adhere to the quality control standards set by decades of fine-tuning silicon. Unfortunately, current synthesis methods of TMDs by chemical vapor or atomic layer deposition (CVD or ALD) result in generally defective films, which hinder their electrical performance. In this work, we use Raman spectroscopy to study defects in MoS_2 and WSe_2 films prepared using multiple synthesis methods, including higher quality (exfoliated and CVD-grown) and more defective (e.g. sputtered or ALD) films. We optimized the tool parameters of our Raman system (532 nm laser) to obtain the best spectral resolution possible (0.3 cm^{-1}) and minimize peak fitting error. We then fit the Raman features of both TMDs using the phonon confinement (also known as RWL) model [1-4], which uses the phonon dispersion of the TMD to capture Raman peak broadening based on defect density ($n_D = 1/L_D^2$, where L_D is the defect spacing). Both MoS_2 and WSe_2 have phonon modes which are degenerate at the Γ point (momentum $k = 0$) but disperse away from it ($k \neq 0$), causing "shoulder" peaks to appear (Fig. 1a), whose intensities depend on the defectivity of the films. For WSe_2, we refer to the doubly degenerate peaks (E' and A_1') as E' for simplicity (Fig. 1b). Using the RWL model, we uncover three Raman-based metrics for the electrical quality (i.e. mobility) of MoS_2 and WSe_2: 1) the ratio between the shoulder and E' peak heights, 2) the E' peak width, and 3) the presence of the LA(M) peak. The first two criteria can distinguish between two (relatively) low-defect samples, whereas the third one appears only in more defective samples ($n_D > 2.5 \times 10^{13}$ cm^{-2}) [2]. By comparing this Raman analysis with measured electrical mobility, our Raman-based metrics allow us to predict the electrical quality of the TMDs without extensive device fabrication. We also uncover a clear difference in film quality after photolithography-based nanofabrication, suggesting that usual device fabrication [5] must be more carefully tuned in future work. In summary, we provide a comprehensive approach for evaluating the quality of TMD films from a variety of sources using simple Raman mapping, also correlating the Raman metrics with electrical data. This is an important advance which can be used to probe the electrical quality of TMDs using fast, nondestructive Raman characterization.

References

[1] K. Schauble, R. Grady, E. Pop, *Virtual MRS Spring/Fall Meeting*, Nov 2020
[2] S. Mignuzzi et al., *Physical Review B* 91 (2015) 195411
[3] W. Shi et al., *Chinese Physics Letters* 33 (2016) 057801
[4] W. Shi et al., *2D Materials* 3 (2016) 025016
[5] A. Daus, K. Schauble, E. Pop et al., *Nature Electronics* 4 (2021) 495

Figures

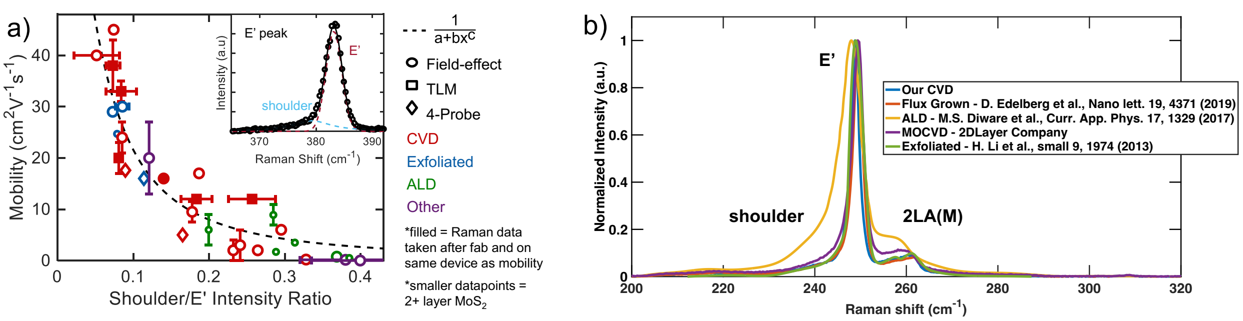

Fig. 1: a) MoS_2 mobility vs. shoulder/E' peak ratio from various sources; an inverse correlation is found. b) Raman spectra of WSe_2 obtained by various growth methods. Broader peak shoulders mark higher defect density. Our CVD sample is grown by solid-source (Se and WO_3 powder) CVD.