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# Local Strain Induced Bandgap Modulation and Photoluminescence Enhancement of Multilayer Transition Metal Dichalcogenides

## Abstract

The Photocarrier relaxation between direct and indirect band gaps along the high symmetry K- $\Gamma$  line in the Brillion zone reveals interesting electronic properties of the transition metal dichalcogenides (TMDs) multilayer films.<sup>1</sup> In this study, we reported on the local strain engineering and tuning of an electronic band structure of TMDs multilayer films along the K- $\Gamma$  line by artificially creating one-dimensional wrinkle structures. Significant photoluminescence (PL) intensity enhancement in conjunction with continuously tuned optical energy gaps was recorded at the high strain regions. A direct optical band gap along K-K points and an indirect optical gap along  $\Gamma$ -K points measured from the PL spectra of multilayer samples monotonically decreased as the strain increased, while the indirect band gap along  $\Gamma$ - $\Gamma$  was unaffected owing to the same level of local strain in the range of 0%–2%. The experimental results of band gap tuning were in agreement with the density functional theory calculation results. Local strain modified the band structure in which K-conduction band valley (CBV) was aligned below the  $\Gamma$ -CBV, and this explained the observed local PL enhancement that made the material indirect via the K- $\Gamma$  transition. The study also reported experimental evidence for the funneling of photo generated excitons toward regions of a higher strain at the top of the wrinkle geometry.

Keywords: Multilayer; Local strain; PL enhancement; Band structure; Exciton funneling

## Reference

[1] Zhao, W.; Ribeiro, R. M.; Toh, M.; Carvalho, A.; Kloc, C.; Castro Neto, A. H.; Eda, *Nano Lett.* 2013, 13, 5627.

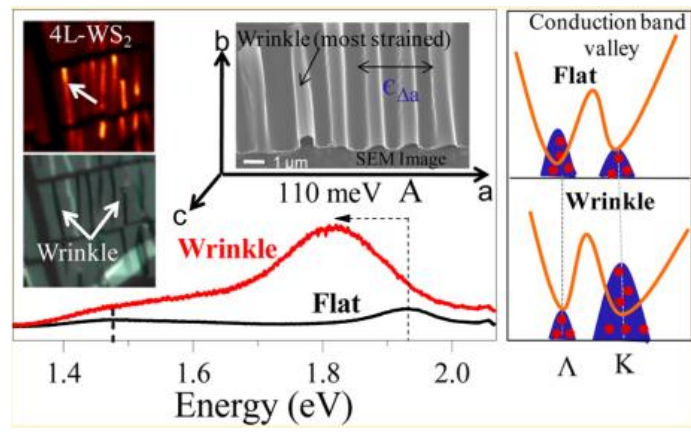


Figure: Illustration of the optical properties modulation on the wrinkle region of the 4L WS<sub>2</sub> film through PL mapping analysis. Schematic at the right showed the band structure modulation due to local strain effect.