High-Resolution S/TEM Imaging and Cathodoluminescence of 2D TMD Heterostructures

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The significant technological implications of two-dimensional (2D) transition metal dichalcogenides (TMDs) stem from their appealing properties, such as the transition from an indirect to a direct band gap when reduced to a monolayer [1]. The integration of multiple 2D TMDs into heterostructures, both in vertical and in-plane configurations, has greatly advanced the development of these materials for specific applications in optoelectronics [2]. However, the electronic and optical performance of these heterostructures heavily relies on the interfaces formed between the constituent TMDs [3]. The interface structure and, consequently, the performance of the heterostructures can be significantly affected by defects and strain at the interface, originating from the lattice mismatch between the two 2D materials [4]. Nevertheless, this presents an opportunity to manipulate the interface characteristics by carefully selecting TMDs and synthesis methods to tailor the properties of the resulting heterostructures. Our investigation employs scanning/transmission electron microscopy (S/TEM) imaging, cathodoluminescence (CL), and Electron Energy Loss Spectroscopy (EELS) spectroscopy to analyze the atomic structure, defects, epitaxy, and strain at the interfaces of various TMD 2D crystals in both vertical and in-plane heterostructures. In this study, we explore vdW epitaxy in vertical and in-plane heterostructures and investigate their nano-optical response.

Investigation of vdW epitaxy in vertical heterostructures were carried out in ReS\textsubscript{2}/MoS\textsubscript{2} system, synthesized using a two-step chemical vapor deposition (CVD) process. Additionally, density functional theory (DFT) calculations were employed in tandem with S/TEM characterization to investigate the nature of structural relaxations at the interface. The presence of vdW epitaxy in the vertical heterostructure was confirmed by the large selected-area diffraction. This work shows the top layer of ReS\textsubscript{2} experiencing strain while adjusting to epitaxy with underlying MoS\textsubscript{2} layer.

We also investigate the atomic structure and nano-optical response in the in-plane heterostructures of MoSe\textsubscript{2}/WSe\textsubscript{2}, both having a hexagonal structure using cathodoluminescence (CL) in combination with EELS and STEM. This study is conducted in MoSe\textsubscript{2} quantum dots embedded in WSe\textsubscript{2} matrix, showing excitons leading to light emission and observation of energy shift as a function of the quantum dot size.
References:

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