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Comprehensive S/TEM Study of Interfaces in CVD Grown Vertical and In-plane Heterostructures of Two-Dimensional MoS_2 and ReS_2

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Two-dimensional (2D) transition metal dichalcogenides (TMDs) are technologically consequential materials owing to their attractive properties such as indirect to direct band gap transition upon thinning to a monolayer [1]. Integration of multiple 2D TMDs into heterostructures in various geometries (vertical and in-plane) has accelerated the development of these materials into targeted applications in optoelectronics [2]. However, the performance of these heterostructures is highly dependent on the interfaces formed between constituent TMDs [3]. For example, defects and strain at the interface, originating from the lattice mismatch between the two 2D materials, can significantly affect the interface structure and consequently the heterostructure performance [4]. At the same time, this provides an opportunity to control the interface characteristics by careful selection of TMDs and synthesis methods to tune the properties of resulting heterostructures.

Most of the studies on heterostructures so far focused on those formed by isotropic TMDs such as MoS_2, WS_2, WSe_2 and $MoSe_2$. Whereas, reports on heterostructures formed between an isotropic and an anisotropic TMDs are sparse. In this study, ReS_2 was chosen to form an interface with MoS_2 because those two materials have different crystal structures. ReS_2 has an anisotropic structure, as opposed to isotropic MoS_2 [5]. Such anisotropy in the system can introduce modulations in the atomic and interfacial structure that is derived from strain and lattice mismatch. Moreover, MoS_2-ReS_2 heterostructures are expected to exhibit type I band alignment, strong interlayer interaction and demonstrate excellent photoresponse properties [6]. Therefore, it is imperative to synthesize MoS_2-ReS_2 heterostructures with well-defined interfaces and to understand their atomic structure.

Here, we used a two-step CVD process to synthesize vertical and in-plane MoS_2-ReS_2 heterostructures wherein, MoS_2 is grown on c-plane sapphire during the first step and ReS_2 is subsequently grown on MoS_2/sapphire in the second step. The as grown heterostructures are transferred to Cu quantifoil holey carbon grids for studying their microstructure. We employed scanning/transmission electron microscopy (S/TEM) techniques to investigate the interface atomic structure, defects, epitaxy and strain between the MoS_2 and ReS_2 layers. Figure 1a shows a low magnification TEM image of MoS_2-ReS_2 vertical heterostructure. Selected area diffraction pattern (SADP) obtained from the area outlined by the dashed circle in Figure 1a is presented in Figure 1b. SADP highlights that ReS_2 aligns epitaxially with MoS_2 as evident by the matching orientation of diffraction spots. Figure 1c is an atomic resolution high-angle annual dark-field (HAADF)-STEM image of a vertical heterostructure showing monolayer ReS_2 grown on top of monolayer MoS_2. FFT pattern obtained from the atomic resolution image, as shown in Figure 1d, further confirms the epitaxy between MoS_2 and ReS_2 at atomic length scale. Figure 2a is a low magnification TEM image illustrating how ReS_2 grows in the gap between MoS_2 triangles during the second step of the synthesis procedure leading to the formation of in-plane heterostructure. An atomic resolution HAADF-STEM image taken from the edge of a MoS_2 triangle confirms the formation of in-plane heterostructure, as presented in Figure 2b. The presentation will include more in-depth analysis on various features observed in the heterostructures along with results from other TEM characterization techniques [7].

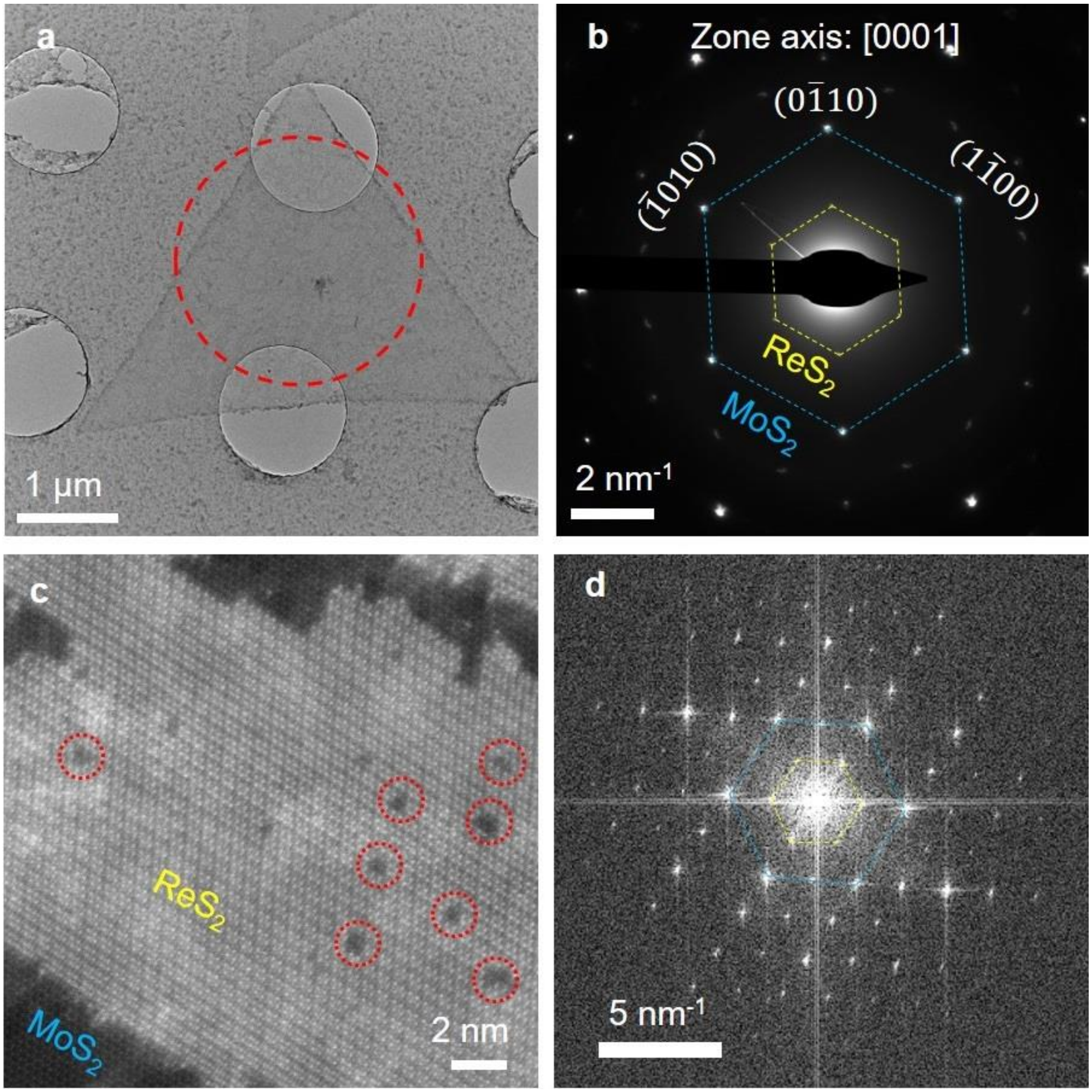

Figure 1. MoS2-ReS2 vertical heterostructures: (a) Low magnification TEM image of MoS2/ReS2 vertical heterostructure, (b) selected area DP obtained from the area outlined by the dashed circle in (a), (c) atomic resolution HAADF-STEM image of the vertical heterostructure showing the underlying monolayer MoS2 with a monolayer ReS2 crystal grown on top and (d) binned FFT pattern obtained from (c) highlighting the epitaxy between MoS2 an ReS2.

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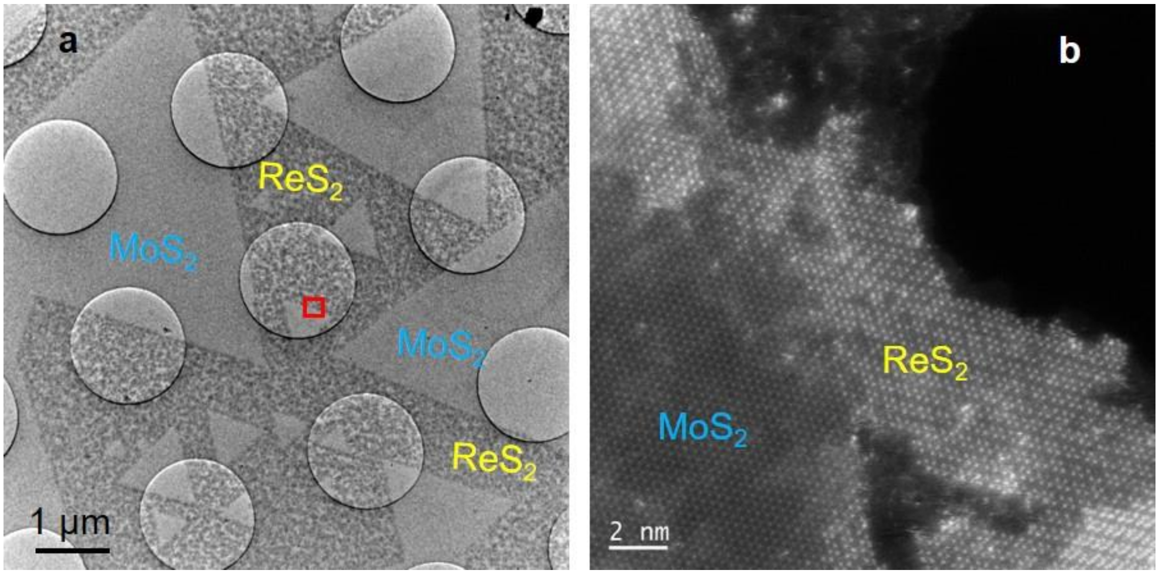

Figure 2. MoS2-ReS2 in-plane heterostructures: (a) Low-magnification TEM image showing MoS2 triangles with ReS2 grown between the triangles thus filling the space and (b) atomic-resolution HAADF-STEM image of in-plane heterostructure formed at the edge of a MoS2 triangle, obtained from the region marked by the red box in (a).

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