Atomic Structure of Vertical and In-Plane Heterostructures Formed by Two-Dimensional MoS$_2$ and ReS$_2$

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Since the advent of graphene in 2004, there has been tremendous progress in the field of two-dimensional (2D) materials. Examples include the discovery of monolayer direct bandgap semiconductors such as MoS$_2$ and WS$_2$, as well as the integration of multiple 2D materials into heterostructures in various geometries (e.g. vertical and in-plane) [1]. Briefly, vertical heterostructures are obtained by stacking different 2D materials on top of each other with only van der Waals forces present between the layers, whereas lateral heterostructures contain 2D materials that are stitched in their basal plane via covalent bonds. These vertical and in-plane heterostructures are ideal candidates to study layer-layer interactions in 2D materials, often leading to improved performance in targeted applications such as optoelectronics [2]. However, the performance of heterostructures is highly dependent on the structure and quality of the interface between the layers [3]. For example, 2D materials that are mechanically stacked on top of each other to prepare vertical heterostructures are prone to contamination at the interface, which originates from the transfer process. Moreover, control over the relative orientation of the layers is also difficult [3]. This can be mitigated by directly growing vertical heterostructures using chemical vapor deposition (CVD), a process that has better control over the interface and relative epitaxy.

Prior work has shown that the local ordering of cations in 2D W$_{1-x}$Mo$_x$S$_2$ alloys leads to anisotropic properties [4]. This study explores the conditions in which chemical ordering can occur through the formation of in-plane heterostructures in dissimilar 2D materials such as MoS$_2$ and ReS$_2$. ReS$_2$ is a great choice to introduce chemical ordering into the MoS$_2$ lattice because the two materials have different crystal structures [5]. Additionally, neighboring Re atoms tend to form covalent bonds with each other because of an extra valence electron leading to the formation of Re chains and resulting in anisotropic electronic properties such as 1D electrical conduction channels [5].

In this work, we used a two-step powder-source CVD process to grow vertical and in-plane heterostructures of 2D MoS$_2$ and ReS$_2$ on sapphire substrates [6]. The as-grown samples were imaged using aberration-corrected high-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM) to assess the interface atomic structure, defects, and epitaxy and strain between the layers. HAADF-STEM imaging was performed using an FEI Titan³ G2 at 80 kV. Figure 1a shows a low-magnification TEM image showing three freestanding triangles over a Quantifoil hole containing MoS$_2$-ReS$_2$ vertical heterostructures. A selected area diffraction pattern (SADP) obtained from the region within the green circle in Figure 1a is shown in Figure 1b. The innermost ring corresponds to the (100) and (110) planes of ReS$_2$ with a d-spacing of 6.45 Å. The second ring corresponds to the similar sets of planes of MoS$_2$ with a d-spacing of 2.73 Å. The SADP also shows the epitaxy between MoS$_2$ and ReS$_2$. An atomic resolution HAADF-STEM image of the interface between MoS$_2$ and ReS$_2$ is shown in Figure 1c, where
Re chains in ReS$_2$ are oriented along the zigzag direction of MoS$_2$. Figure 2a shows a low-magnification HAAF-STEM image of MoS$_2$ triangles stitched by ReS$_2$ that has grown between the triangles. One such triangle in the image is outlined in red. Figure 2b is an atomic-resolution HAADF-STEM image showing the in-plane heterostructure formed at the edge of the triangle and was obtained from the region marked by the blue box in Figure 2a [7].

References:

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Figure 1 MoS$_2$-ReS$_2$ vertical heterostructures: (a) low-magnification TEM image showing three vertical heterostructure triangles freestanding over a Quantifoil hole, (b) diffraction pattern obtained from the region outlined by the green circle in (a), (c) atomic-resolution HAADF-STEM image of the vertical heterostructure.

Figure 2 HAADF-STEM images of MoS$_2$-ReS$_2$ in-plane heterostructures: (a) low-magnification image of MoS$_2$ triangles (only one is outlined in red) and ReS$_2$ grown between the triangles, (b) atomic-resolution image of the in-plane heterostructure formed at the edge of the MoS$_2$ triangle outlined in red, obtained from the region marked by blue box in (a).