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Observation of a Quasi-ordered Structure in Monolayer $W_xMo_{(1-x)}S_2$ Alloys

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Two-dimensional (2D) transition metal dichalcogenides (TMDs), such as MoS_2 and WS_2, have been widely studied (*1–3*) and proposed as promising materials for applications in catalysis and electronics. They are not only efficient catalysts for the hydrogen evolution reactions (HER) (*4*, *5*), but also promising materials for applications in electronics and optoelectronics owing to their direct-band gap character. Alloying can be used to further tune the physical, electronic and chemical properties of 2D TMDs (*6–8*). As an example, 2D $MoS_{2(1-x)}$ Se_{2x} shows enhanced catalytic activity for HER when compared to pristine MoS_2 and $MoSe_2$ (*6*). While there has been a tremendous progress in the synthesis and optoelectronic characterization of 2D crystal alloys, little has been done to understand their atomic-scale alloy structure. This understanding is important since the local atomic and chemical structure can considerably impact the catalytic and electronic properties of TMDs.

Here we show the atomic structure and chemistry of $W_xMo_{1-x}S_2$ monolayers using aberration-corrected annular dark field (ADF) scanning transmission electron microscopy (STEM). Triangular $W_xMo_{1-x}S_2$ alloys were grown on Si/SiO_2 substrates using powder vaporization at 800°C (*9*). The synthesized $W_xMo_{1-x}S_2$ monolayers have triangular shape with an average lateral size of ~10 micrometers, as can be seen in Figure 1(a-b). ADF-STEM imaging was performed using a FEI Titan^3 60-300 S/TEM at 80 kV, at Penn State. Figure 1(c-d) demonstrates an atomic resolution ADF-STEM image and the corresponding Bandpass-filtered image taken from the center of the triangle, slightly closer to the edge 1 (marked as blue). One can observe the striping patterns of W and Mo atoms along the edge 1 at the center of the triangle, where the Mo and W concentrations are almost equal. The two metal species form homo-nuclear chains along the edges of the triangular $W_xMo_{1-x}S_2$ alloys. To verify the formation of the W and Mo stripes along the edges, we have imaged the atomic registry of three different regions at the center of the triangle along each edge and have calculated three pair correlation coefficients in each region (as described in Ref.(*10, 11*)). Comparing the calculated pair correlation coefficients in three zigzag directions, this study shows a preferred formation of strips along the edges for each region.
This study further explores the origin for the formation of the stripes using density functional theory (DFT) calculations. The atomic-scale striated structures observed in this work may lead to anisotropic properties in monolayer TMDs at the macroscale, which might be beneficial for some applications, such as thermal management.

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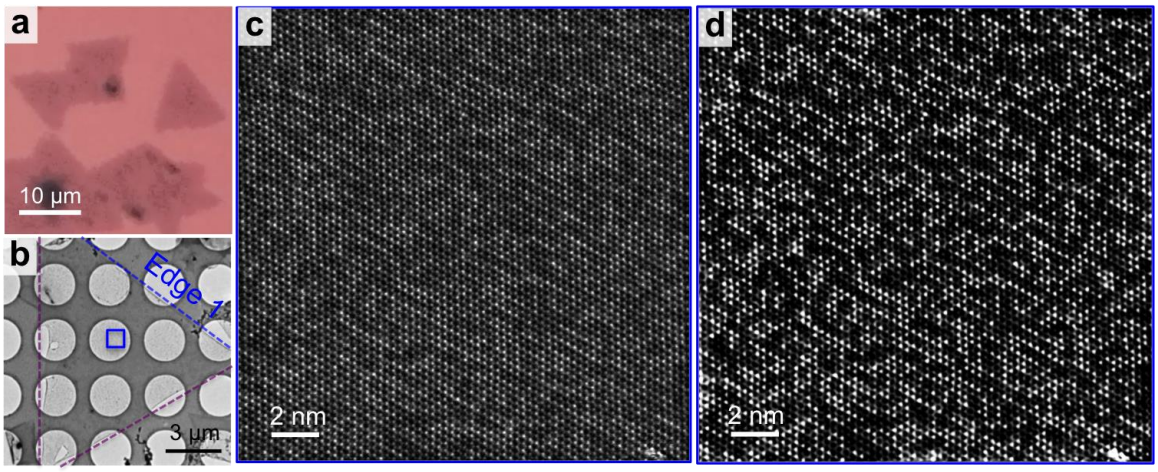

Figure 1. (a) Optical image of monolayer $W_xMo_{1-x}S_2$ crystals grown on a Si/SiO_2 substrate. (b) TEM image of a monolayer $W_xMo_{1-x}S_2$ crystal transferred to a TEM grid. (c) Atomic-resolution ADF-STEM image and (d) the corresponding Bandpass-filtered image acquired from the region marked by a blue square in (b). The imaged region is chosen slightly closer to the edge 1 (blue). The filtering is performed for a better visualization of the W stripes.

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