Atomic Study of the Grain Boundaries Involved Defect Structures in Monolayer/Bilayer Transitional Metal Dichalcogenides

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Abstract

Grain boundaries (GBs) of transitional metal dichalcogenides (TMDs, e.g. MoS_2, WS_2), including 60° GBs and small-angle tilt GBs, have considerable impacts on their chemical-physical properties. [1-3] This study focuses on the grain-boundaries-involved defect structures in MoS_2/WS_2 monolayers/bilayers by using the atomic-resolution annular dark-field scanning transmission electron microscopy (ADF-STEM). We study the high-temperature formation and dynamics of large inversion domains which are constructed from 60° GBs and have 60° orientation rotation at a local domain in monolayer MoS_2 (Figure 1). Further to this, the investigation extends to tilt-GBs in bilayer systems, showing that tilt GBs in bilayer 2D crystals of the WS_2 can be atomically sharp, where top and bottom layer GBs are located within sub-nm distances of each other (Figure 2). This study is promising to underpin the defects engineering of 2D materials in atomic level targeting at electronic properties tailoring.

References

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Figures

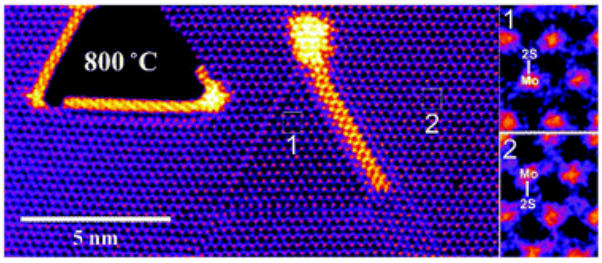

Figure 1: ADF-STEM image with colour effect showing a large-area inversion domain (ID) formed at 800 °C.

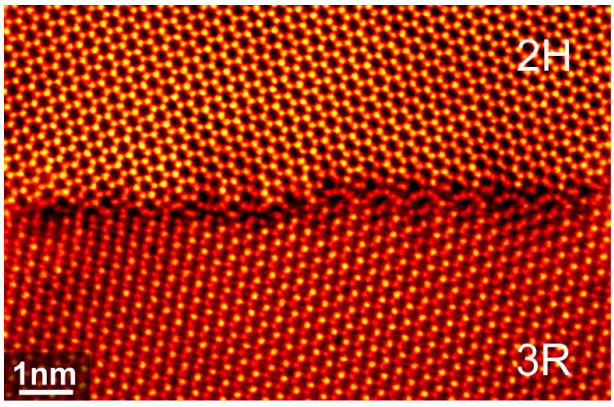

Figure 2: Atomically sharp dual grain boundary within two WS_2 bilayers with 2H and 3R stackings, separately.