

Supplementary materials

Epitaxial configuration of unidirectionally-aligned MoS₂ monolayer on sapphire

Akihiro Ohtake^{,†}, Jun Nara[†], and Yoshiki Sakuma[†]*

[†]National Institute for Materials Science (NIMS), Tsukuba 305-0044, Japan

Corresponding Author: OHTAKE.Akihiro@nims.go.jp

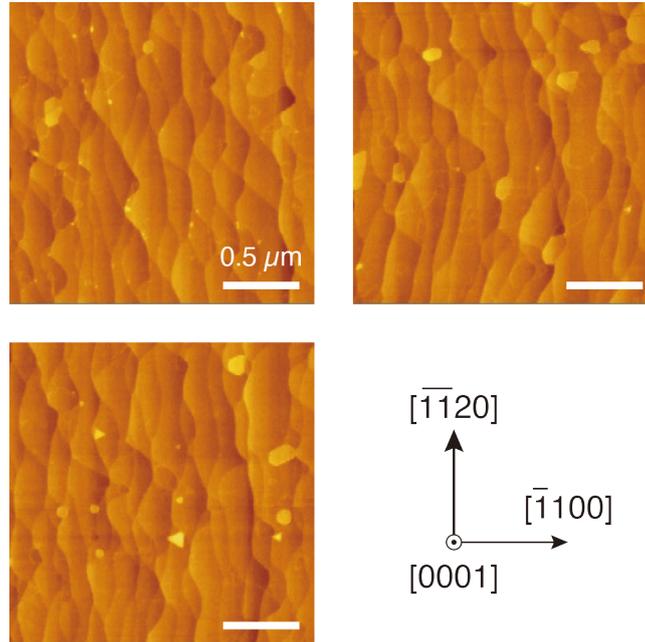


Figure S1. Representative AFM images measured from randomly selected areas of the ML-MoS₂ sample grown on the sapphire (0001) substrate at 975°C for 60 min. The image dimensions are 2 x 2 μm². It is clearly seen that the MoS₂ ML is continuous and that the nucleation of second-layer MoS₂ islands is very limited.

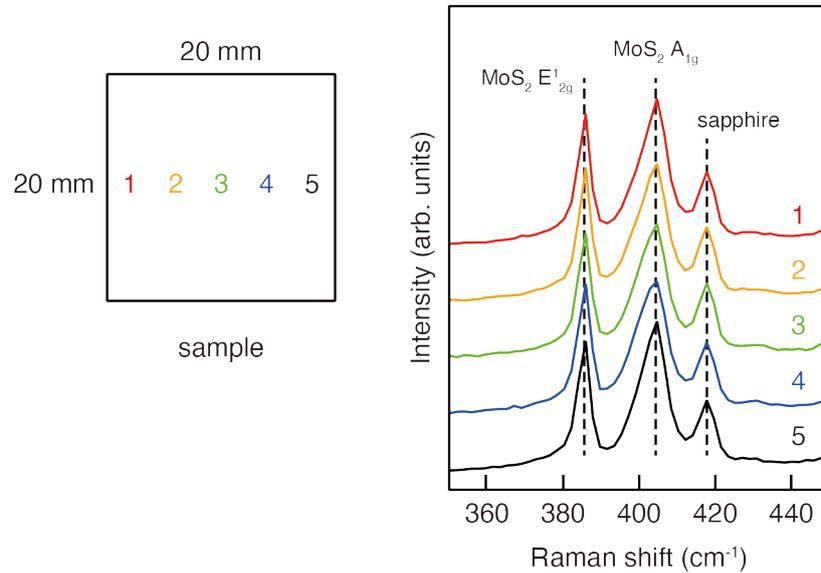


Figure S2. Raman spectra taken from five locations across the ML-MoS₂ sample grown on the sapphire (0001) substrate at 975°C for 60 min. The difference in peak positions for the E_{12g} and A_{1g} modes are less than 19 cm⁻¹, which provides evidence for the 1 ML-thick MoS₂ film [1].

[1] C. Lee, H. Yan, L.E. Brus, T.F. Heinz, J. Hone, and S. Ryu, Anomalous Lattice Vibrations of Single- and Few-Layer MoS₂, ACS Nano, 4, 2695-2700 (2010).

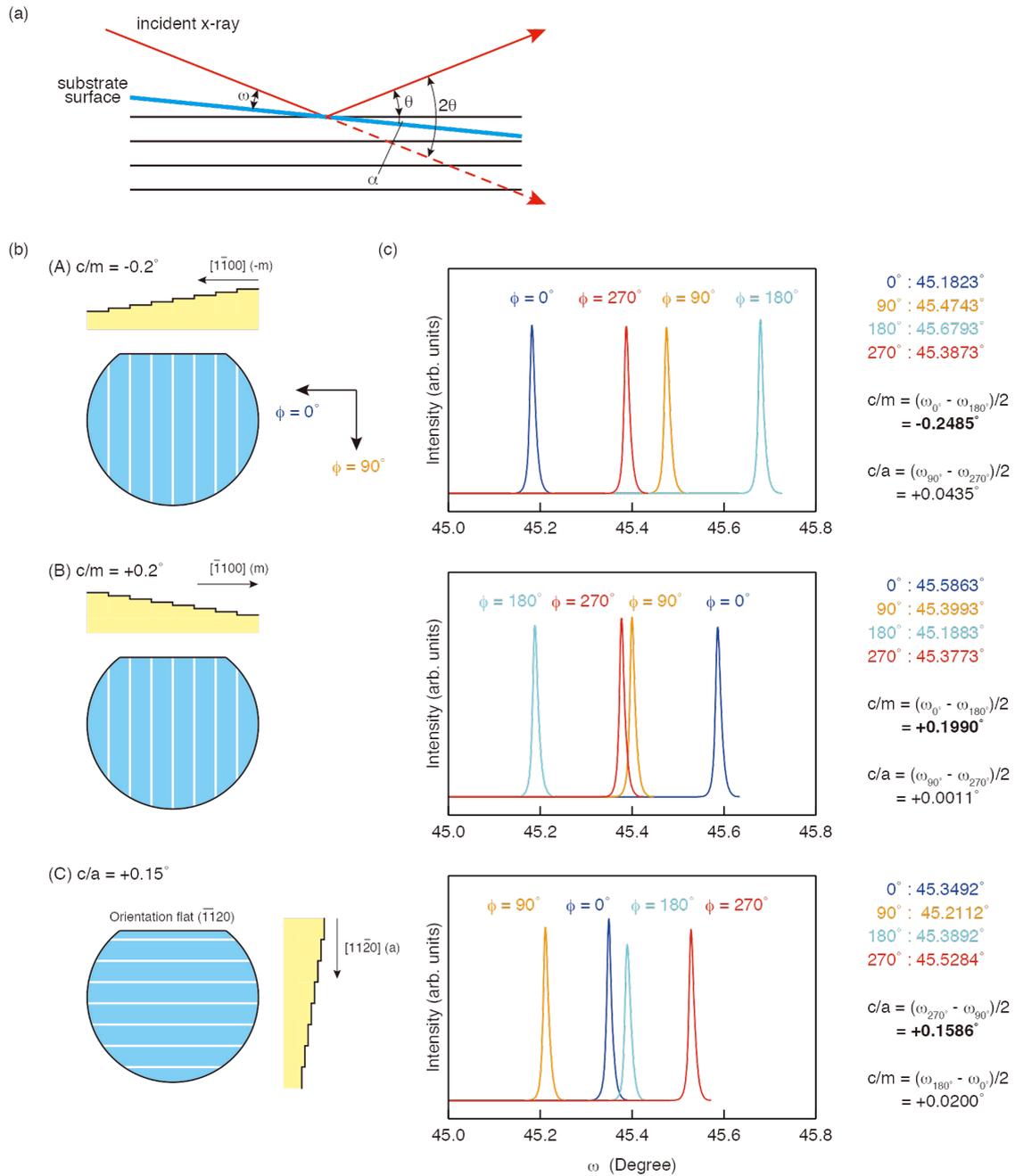


Figure S3. (a) Schematic drawing of the setup for XRD rocking curve measurements. (b) Schematic illustrations of sapphire substrate with miscut angles of $\sim 0.2^\circ$ along the $[1\bar{1}00]$ (A), $[\bar{1}100]$ (B) and $[11\bar{2}0]$ (C) directions. (c) Measured XRD rocking curves. The actual miscut angles are $c/m = -0.2485^\circ$ (a), $c/m = +0.199^\circ$ (b), and $c/a = +0.1586^\circ$ (c). The incidental miscut angles for the orthogonal directions are negligible; 0.0435° (a), 0.0011° (b), and 0.0200° (c).

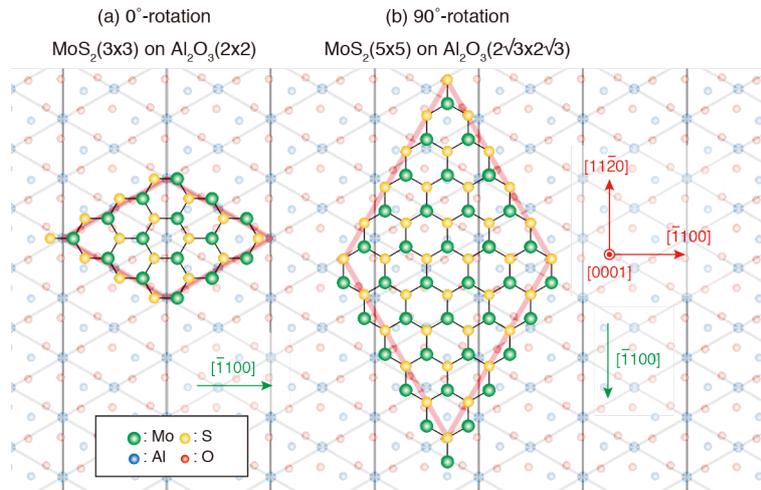


Figure S4. Schematic illustrations of 0° and 90° domains of ML-MoS₂ on the sapphire substrate. In the 0° domain, the MoS₂(3×3) supercell is lattice-matched with the Al₂O₃(2×2) cell (lattice mismatch = -0.42 %). In the 90° domain, MoS₂(5×5) cell is nearly lattice-matched to Al₂O₃(2√3×2√3)-R30° cell (lattice mismatch = -4.18 %).