Supplementary Information

Substrate Lattice-Guided Seed Formation Controls the Orientation of 2D Transition Metal Dichalcogenides

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Mo Concentration profile

We evaporated MoO_3 and S separately at the conditions same as the typical growth and the energy dispersive X-ray analysis (EDX) was adopted to measure the concentration of Mo species at the locations with various distances from the MoO_3 source. Since MoO_3 can be deposited on sapphire substrates, we observe that the density of the precipitates decreases with the increasing distance (Table S1). We use the Mo peak intensity (reference to the Al and O peaks of the substrate) to obtain relative Mo concentration as shown in Figure S1.

The determination of S concentration along the reaction tube using the same method is challenging since S is volatile and they can only be deposited at the cold areas rather than the hot reaction zone. However, we anticipate that S is homogeneous based on the following experimental observations; (1) the position of the sulfur source is at least 30 cm far from the MoO_3 source but the S vapors still can reach the whole substrate which means that the decay of the S concentration should not be obvious with the distance. (2) We can always find yellow colored S deposits on the wall of the quartz tube at the downstream side, indicating that the S vapors can reach the whole regions in the tube. Therefore, our experiment is in S-rich condition (relative to MoO_3) condition and S concentration can be considered as constant along the reaction zone.

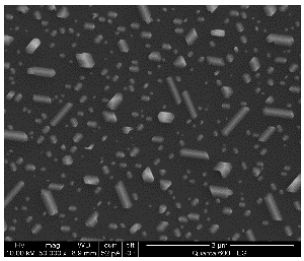
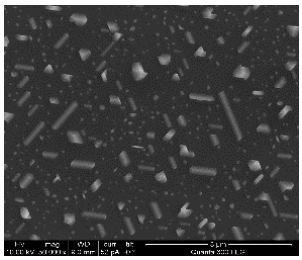
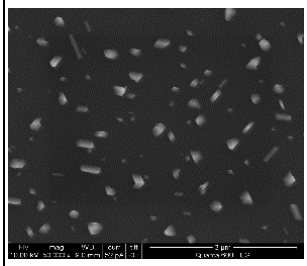
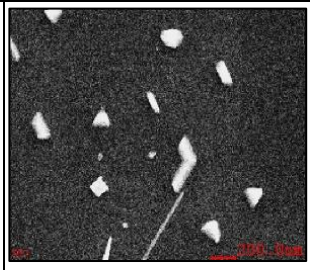
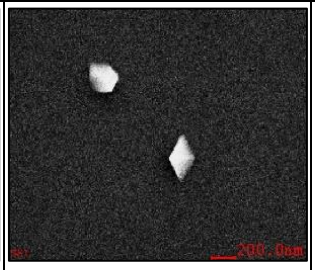
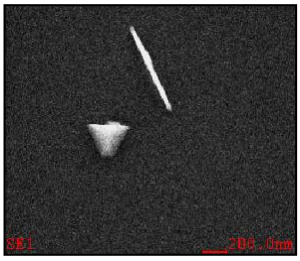
Mo	Distance	2 cm	3 cm	4 cm
	Wt%	05.50	05.19	02.37
				
	Distance	7 cm	8 cm	9 cm
	Wt%	01.68	01.54	01.23
				

Table S1. The SEM images and weight percent (wt%) of Mo at different distances from MoO_3 source. The percentage of Mo with respect to detected elements (Al, O, and Mo).

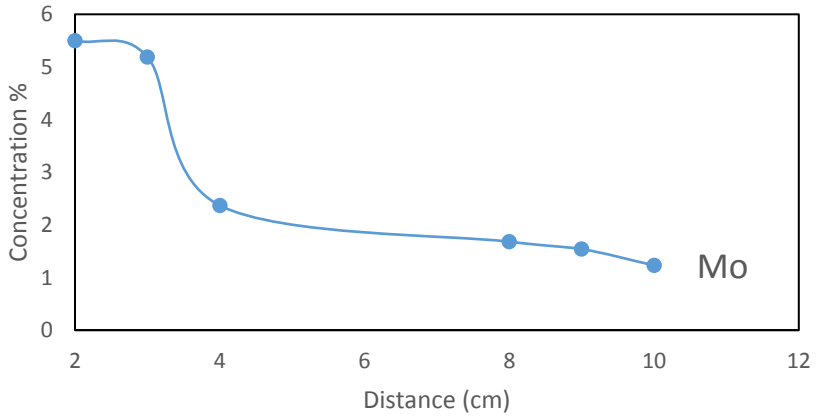


Figure S1. The concentration of Mo at different distances from MoO_3 source based on EDX data in Table S1.

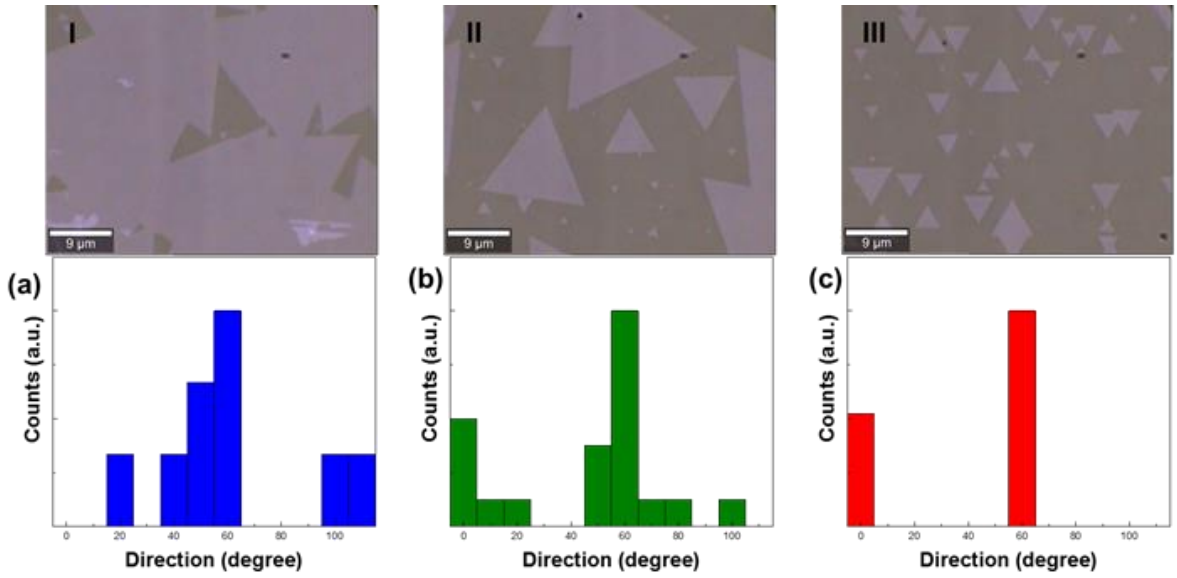


Figure S2. Optical microscopy (OM) images and statistical orientation analysis for the as-grown MoS_2 flakes at different locations (a) location I, (b) location II, and (c) location III.

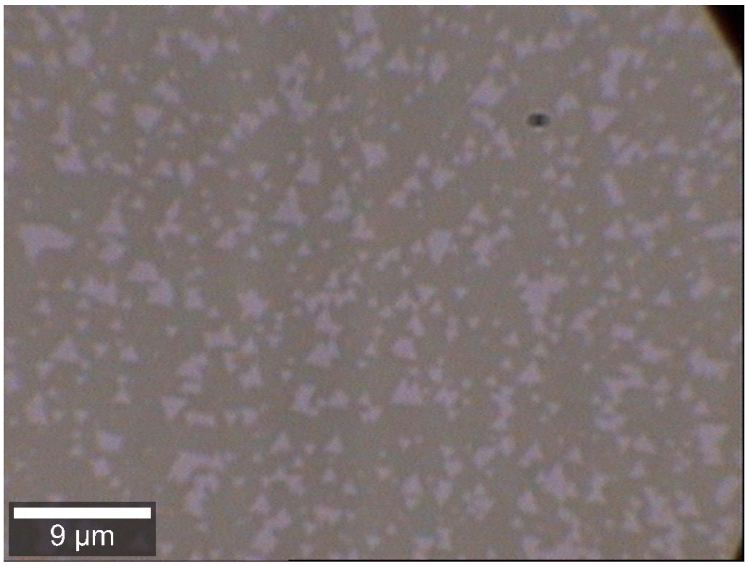


Figure S3. Extending the period of seed formation at 750°C results in tiny monolayers with the lateral dimension less than 1 μm.

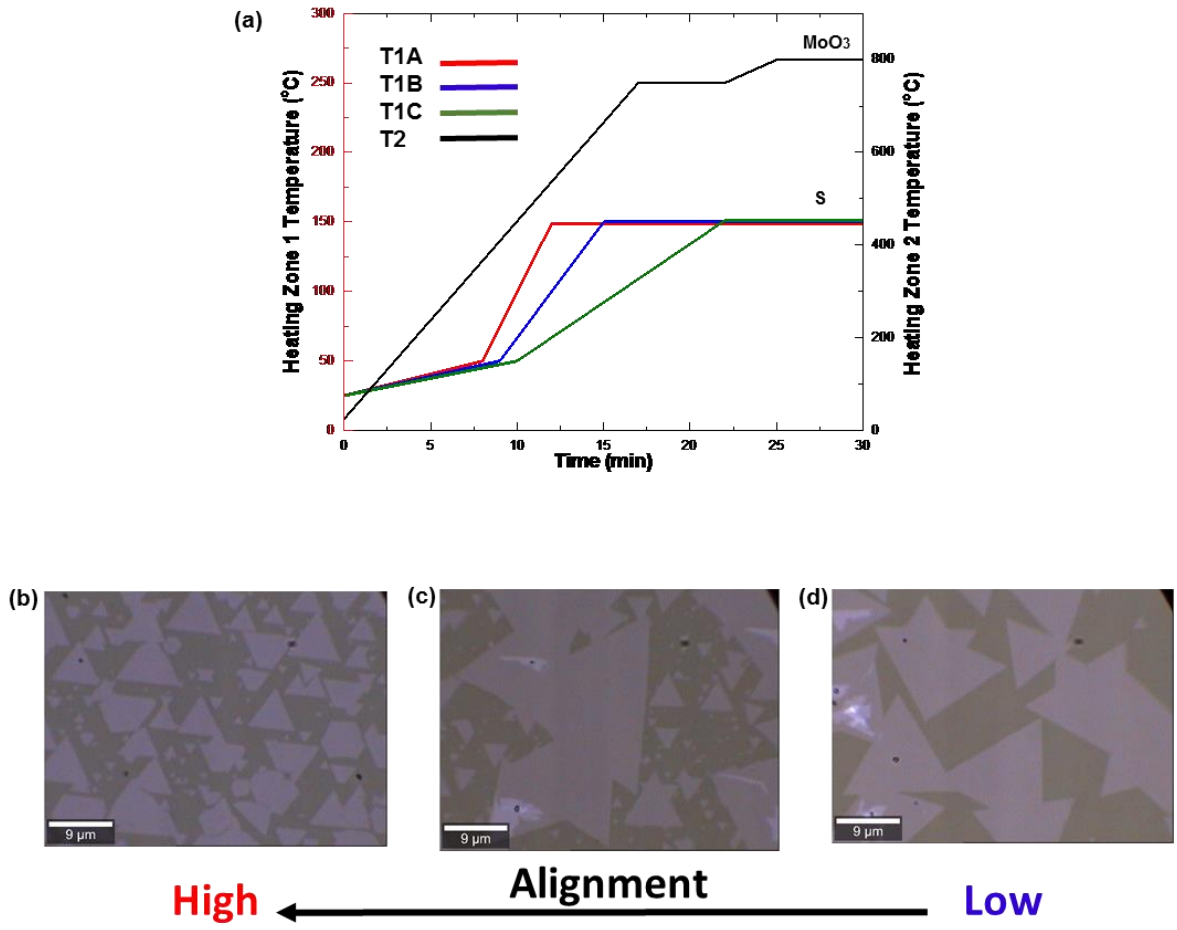


Figure S4. (a) The heating profiles for S powders (T1) and MoO_3 (T_{1A}, T_{1B} and T_{1C}). **(b, c and d)** The optical microscopy images of the as-grown MoS_2 flakes using T_{1A}, T_{1B} and T_{1C} heating profiles respectively.

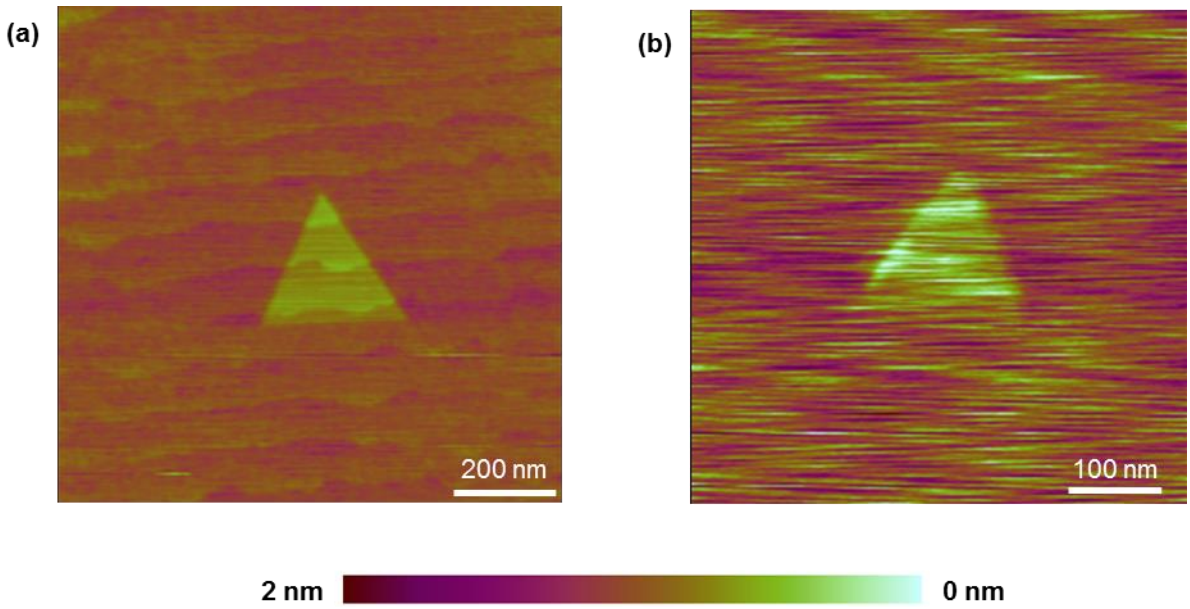


Figure S5. AFM characterizations of the seeds at the end of seed formation stage. **(a and b)** AFM image of the MoS_2 seeds at the upstream region.

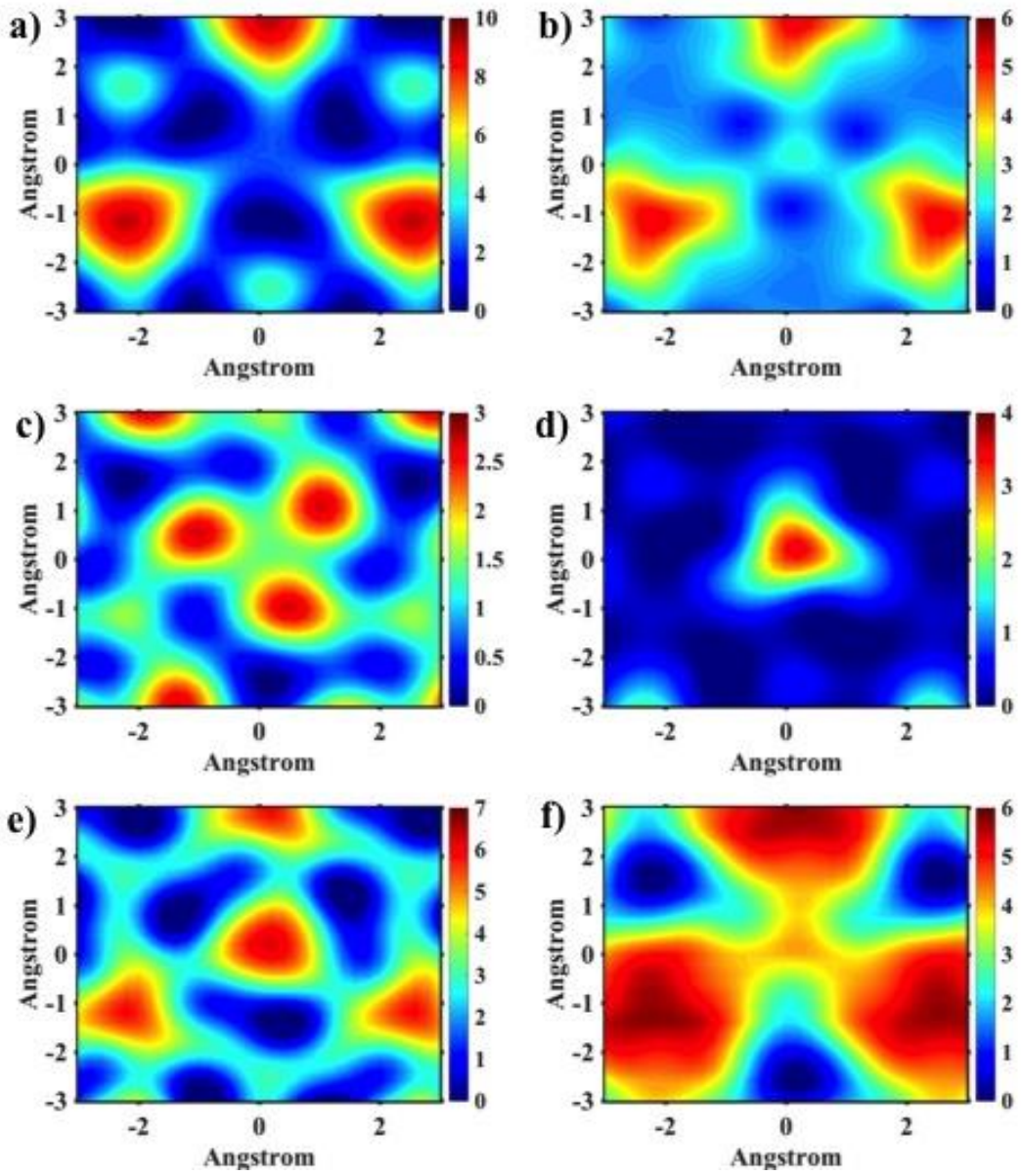


Figure S6. Scanned potential energy surface as a function of the relative position between the MoS_2 seed and a sapphire substrate. **(a)** The relative angle is fixed as 10 degree; **(b)** the relative angle is fixed as 20 degree; **(c)** the relative angle is fixed as 30 degree; **(d)** the relative angle is fixed as 40 degree; **(e)** the relative angle is fixed as 50 degree; **(f)** the relative angle is fixed as 60 degree. Considering the symmetric feature of our prototypical model, we only demonstrate the results within 60 degrees.