Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Fast and Large-Area Growth of Uniform MoS_2 Monolayers on Molybdenum Foils

Guoan Tai,* *Tian Zeng*, *Jin Yu, Jianxin Zhou, Yuncheng You*, *Xufeng Wang*, *Hongrong Wu*, *Xu Sun, Tingsong Hu, and Wanlin Guo**

E-mail: taiguoan@nuaa.edu.cn and wlguo@nuaa.edu.cn

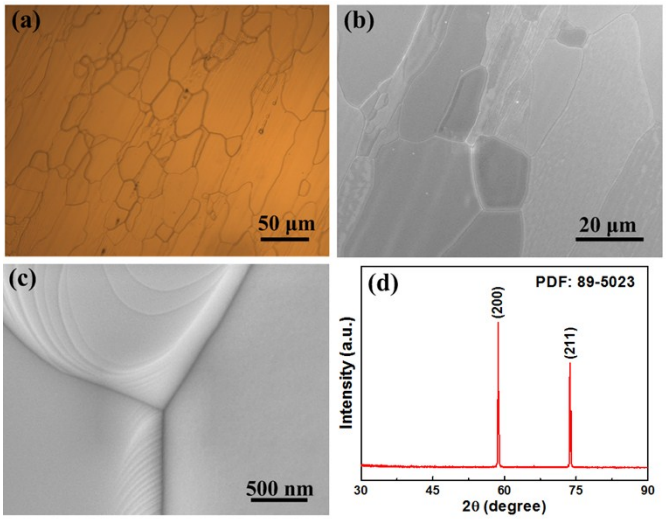

Figure S1. Structural characterization of Mo foils annealed at 1400 °C for 10 h under 50 sccm H_2 atmosphere. (a) Photograph of the annealed Mo foil. (b) Low-magnification SEM image of the Mo Foil. (c) High-magnification SEM image of the Mo foil. (d) XRD patterns of the Mo foil. The diffraction peaks can be indexed to the cubic (fcc) phase of Mo foil with lattice constants of 0.315 nm (JCPDS card: 89-5023).

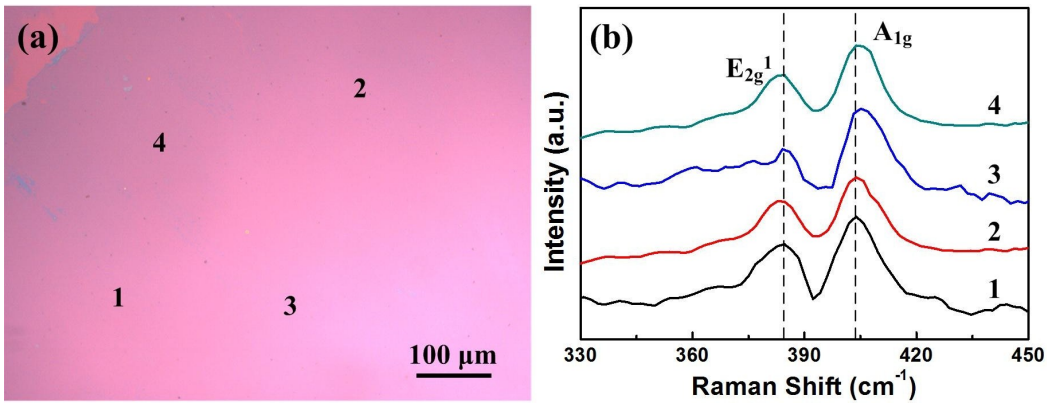

Figure S2. (a) Optical image of MoS_2 monolayers transferred onto a 285-nm SiO_2/Si substrate. (b) Raman spectra of the sample in four different regions marked as 1, 2, 3 and 4, respectively.

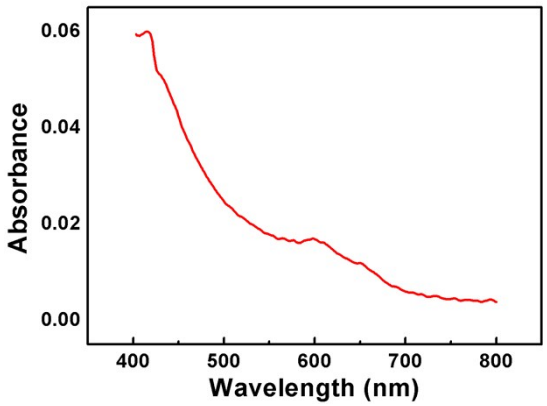

Figure S3. UV-vis absorbance spectrum of the as-prepared MoS_2 monolayer.

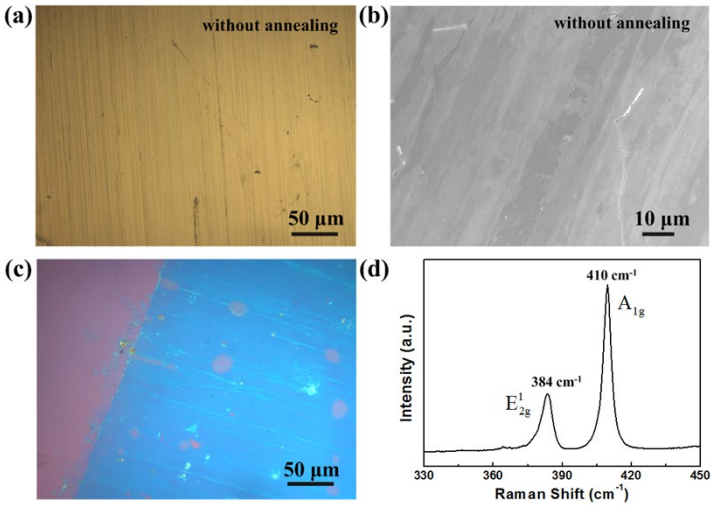

Figure S4. Structural characterization of the MoS_2 films grown by sulfurizing an unannealed Mo foil. (a) Photograph of the MoS_2 films on the unannealed Mo foil. (b) SEM image of the MoS_2 films on the unannealed Mo foil. (c) Optical image of the MoS_2 films transferred onto 285 nm SiO_2/Si substrate. (d) Corresponding Raman spectrum of the MoS_2 film transferred onto 285 nm SiO_2/Si substrate in (c).

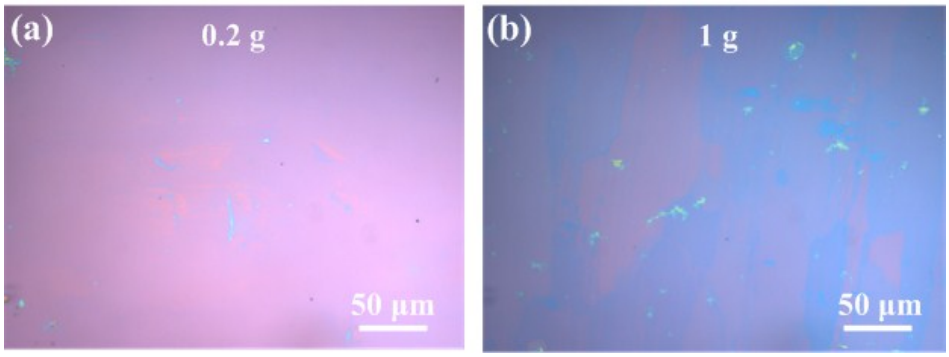

Figure S5. Optical images of MoS_2 thin films grown by sulfurizing the annealed Mo foil surfaces at 600 ^oC for 1 min with different mass of sulfur powders: (a) 0.2 and (b) 1 g.

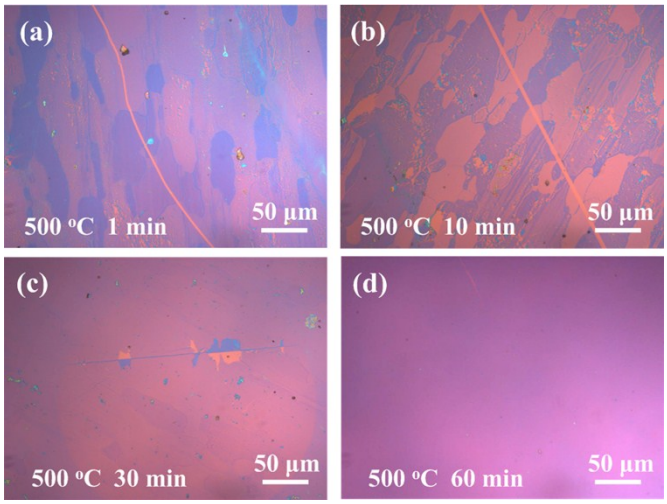

Figure S6. Optical images of MoS_2 thin films transferred onto 285 nm SiO_2/Si substrates. The films were grown by sulfurizing the annealed Mo foil surfaces at 500 °C for different reaction times: (a) 1, (b) 10, (c) 30 and (d) 60 min.

The continuous MoS_2 monolayers were formed by sulfurizing Mo foil surfaces at 500 °C for over 60 min (Figure S6d), while the monolayers could be controllably grown at 600 °C within 1 min (Figure 1e).

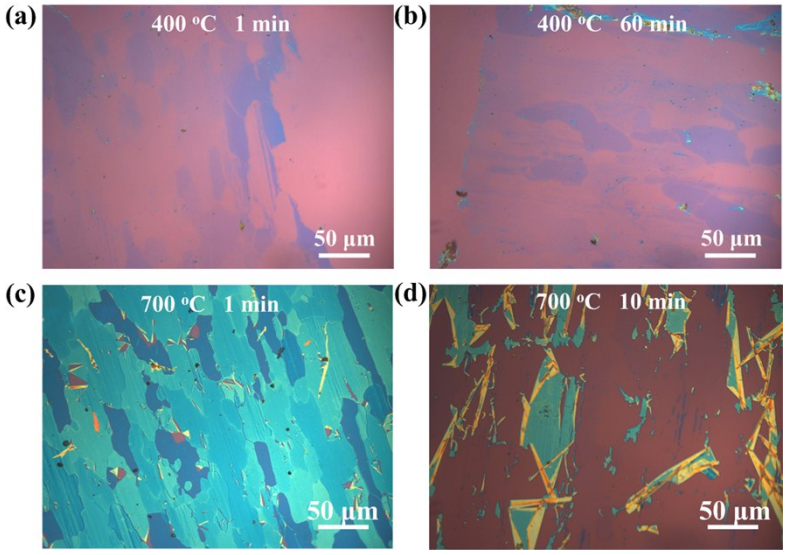

Figure S7. (a,b) Optical images of MoS_2 thin films transferred onto 285 nm SiO_2/Si at 400 °C for different reaction times: 1 and 60 min. (c,d) Optical images of multilayer MoS_2 films grown at 700 °C for different reaction times: 1 and 10 min.

Decreasing the reaction temperature down to 400 °C, discontinuous thin films were only produced (Figure S7a and b). When the temperature was more than 700 °C within 1 min, thicker films was formed (Figure S7c), and discontinuous films were observed after further prolonging the duration over 10 min (Figure S7d).

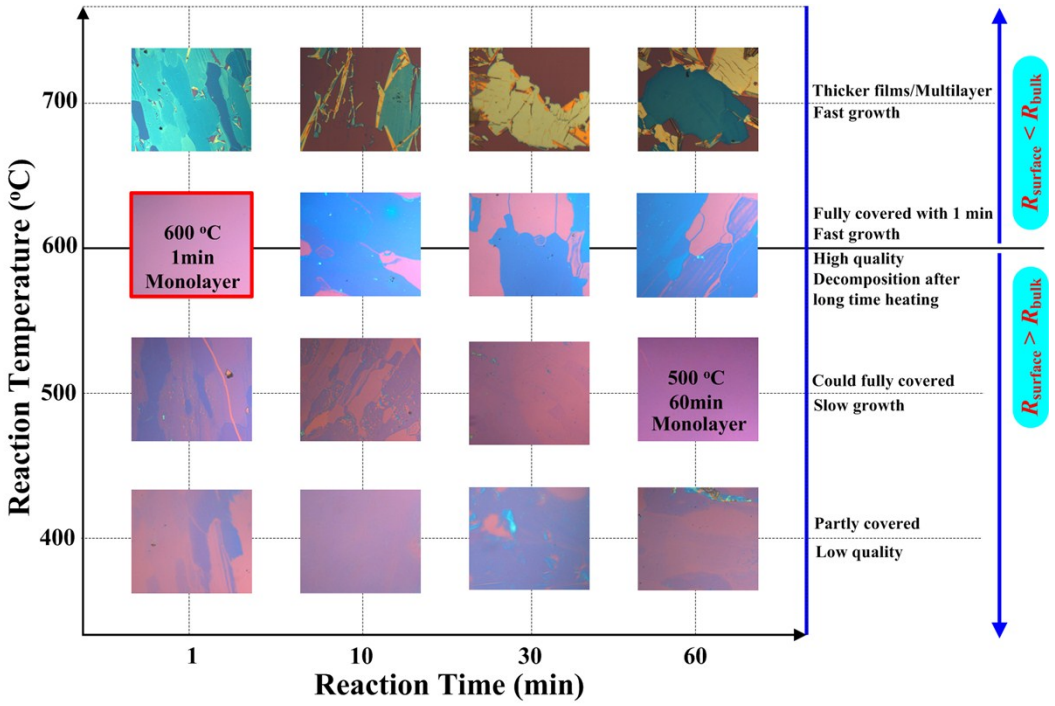

Figure S8. Dependence of growth of the MoS_2 thin films on the reaction temperature and time. $R_{surface}$ is the rate of surface diffusion, and R_{bulk} is the rate of bulk diffusion.

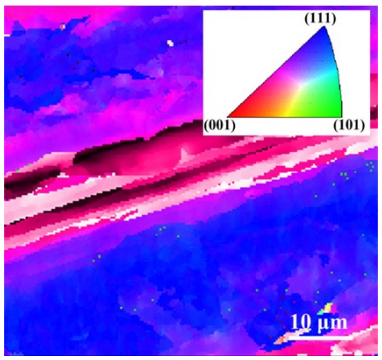

Figure S9. EBSD orientation map of a particular region on an unannealed Mo foil.

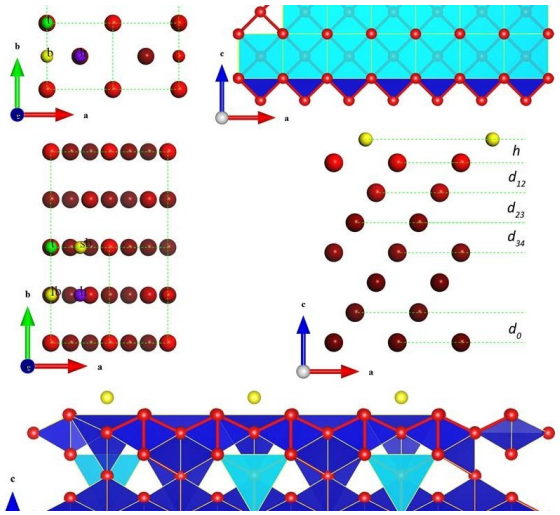

Figure S10. Theoretical model of binding energy calculation of sulfur atoms on three binding sites: Hol site (on top of a hexagon), Top site (on top of a Mo atom), and Bri site (on top of a Mo-Mo bond).

Table S1. Binding energies E_{bind} (eV) of sulfur atoms on Mo foils with different lattice surfaces at various adsorbed sites predicted by first-principles calculations.

(100)		E_{bind} (eV)	(111)		E_{bind} (eV)
0.25 ML	Top	-1.914	0.25 ML	Top	-2.636
	Bri	-2.690		L-Bri	-2.891
	Hol	-3.779		S-Bri	-2.636
0.5 ML	Top	-1.466		Hol	-2.888
	Bri	-2.281	0.5 ML	Top	-2.553
	Hol	-3.038		L-Bri	-2.875
1 ML	Top	-1.160		S-Bri	-2.553
	Bri	-1.947		Hol	-2.875
	Hol	-2.599	1 ML	Top	-1.678
				L-Bri	-2.211
				S-Bri	-1.678
				Hol	-1.939

We selected the binding energy E_{bind} at Hol site used in the text because the site has the lowest E_{bind} compared with other sites, as shown in Table S1.