

Supporting Information

Chemical Vapor Deposition of MoS₂ Layers from Mo-S-C-O-H System: Thermodynamic Modeling and Validation

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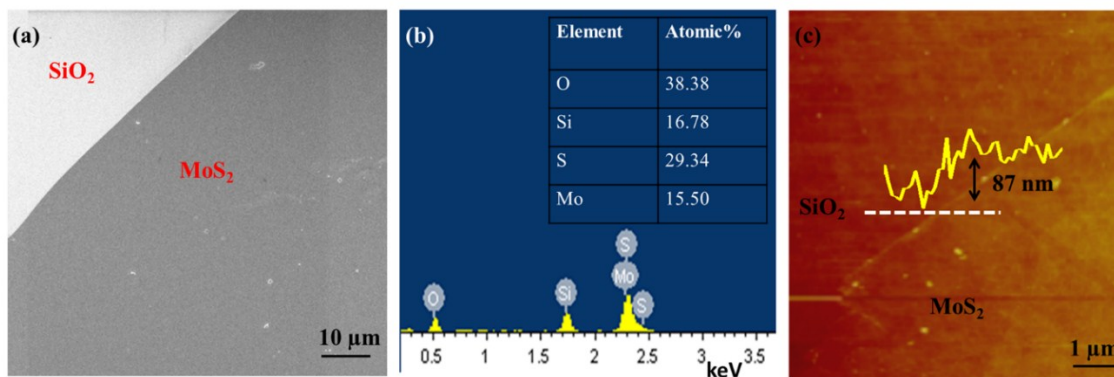


Figure S1(a). SEM image of MoS₂ film grown for 10 minutes on SiO₂. (b) EDS analysis of the film. (c) AFM image of the MoS₂ film.

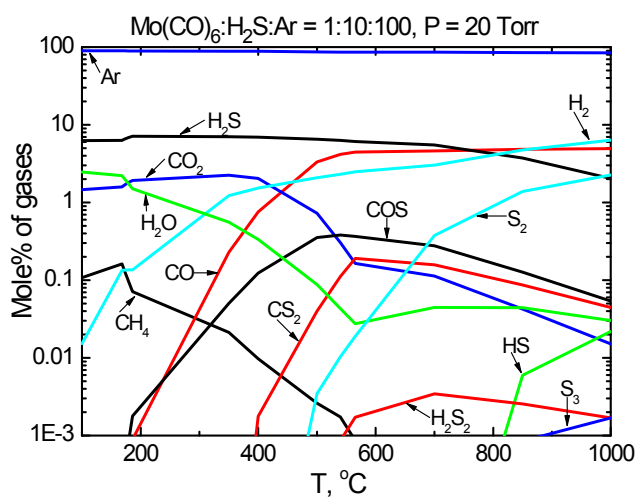


Figure S2. Mole% of gaseous phases formed in Ar ambient at 20 Torr.

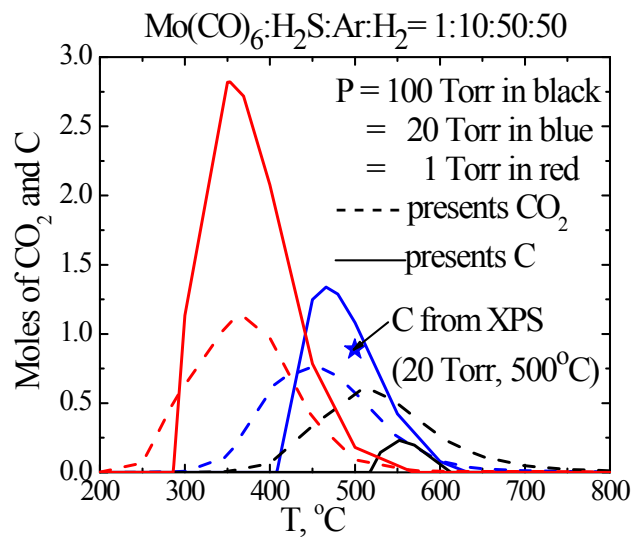


Figure S3. Composition of C and CO_2 formed in $\text{Ar}:\text{H}_2=50:50$ at different P.

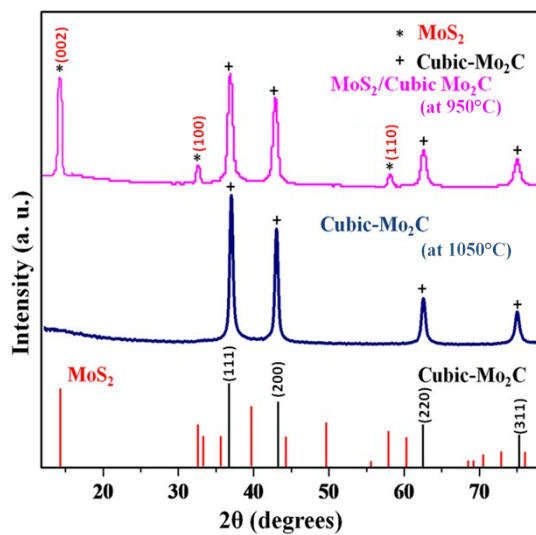


Figure S4. XRD validating theoretical prediction of $\text{Mo}_2\text{C}-\text{MoS}_2$ and pure Mo_2C films at 950°C and 1050°C respectively, for high flow rate of H_2 (1000 sccm) at 600 Torr.

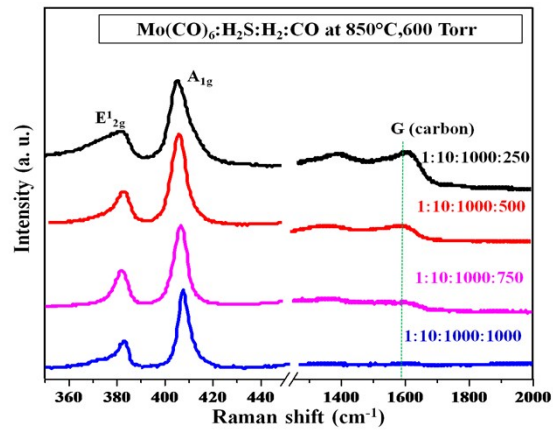


Figure S5. Raman spectra for $h=1000$ sccm to estimate C content in the MoS₂-C films at $T = 850^{\circ}\text{C}$ and $P = 600$ Torr.

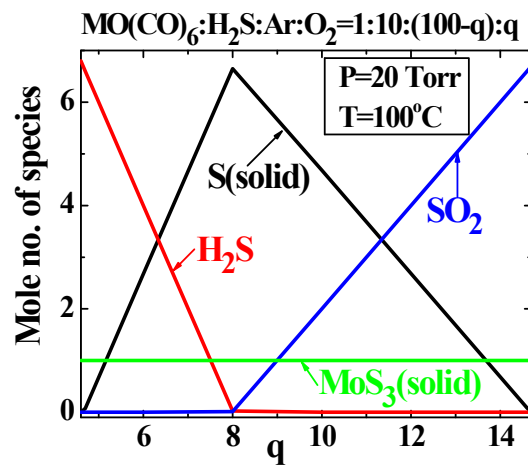


Figure S6. Gaseous and solid (S and MoS₃) species with O₂ leak in Ar ambient.

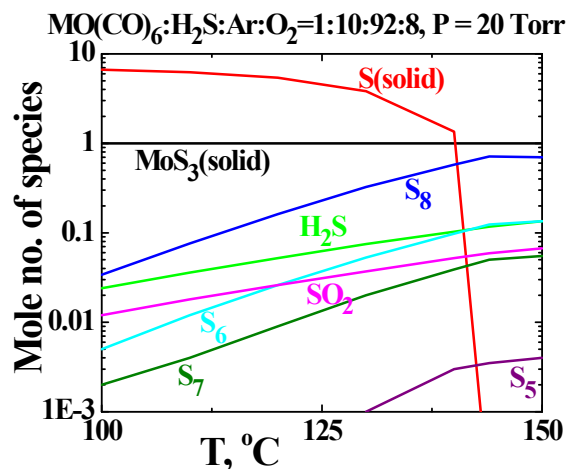


Figure S7. Gaseous and solid species with O_2 leak in the system at different T.

Table S1. Range of CVD conditions used.

Precursor	Mo(CO)_6 powder (99.99% purity, Sigma Aldrich)
Precursor vapor flow rate	7 to 1 sccm
Reacting gas	H_2S (99.5% from Bhoruka)
Reacting gas flow rate	1 to 10 sccm (Electronic mass flow controllers from MKS Instruments used for regulating gas flow)
Carrier gas	Ar, H_2 , and Ar/ H_2 mixture
Carrier gas flow rate	100 to 1000 sccm
Total reactor pressure P_{tot}	20 to 700 Torr (maintained using a bellows-sealed throttle valve connected at the mouth of a rotary vane pump, and read by a capacitance manometer)
Substrate temperature T_{sub}	350°C to 1050°C
Sublimator temperature	100°C to 130°C
Substrates used	300 nm thermally grown SiO_2 on Si, c-plane sapphire, and fused quartz
Duration of Deposition runs	40 seconds to 10 minutes

Table S2. Compositional data deduced from XPS spectra.

MoS₂	Element	Atomic percentage
20 Torr, 350C	Mo 3d	1
	S 2s	2.18
	C 1s	4.07
600 Torr, 500C	Mo 3d	1
	S 2s	2.34
	C 1s	1.98
20 Torr, 500C	Mo 3d	1
	S 2s	2.10
	C 1s	0.98
20 Torr, 500C	Mo 3d	1
	S 2s	2.34
	C 1s	0.8