Supplementary to
Wafer-scale MoS$_2$ with water-vapor assisted showerhead MOCVD

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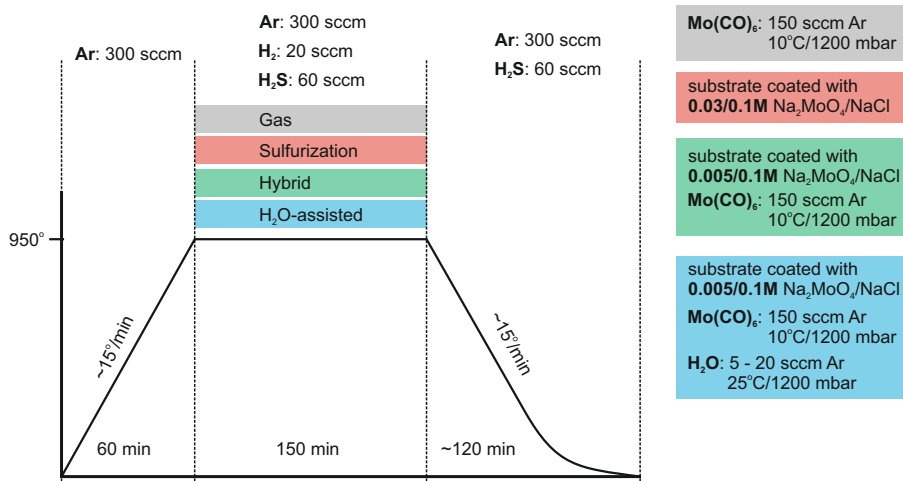
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Fig. 1 The process flow of each investigated growth method. All growth were done at the 830 mbar pressure and at ambient flow of 300 sccm Ar during heating, 300 sccm Ar, 20 sccm H_2 and 60 sccm H_2S during growth step and 300 sccm Ar with 60 sccm H_2S during cooling.
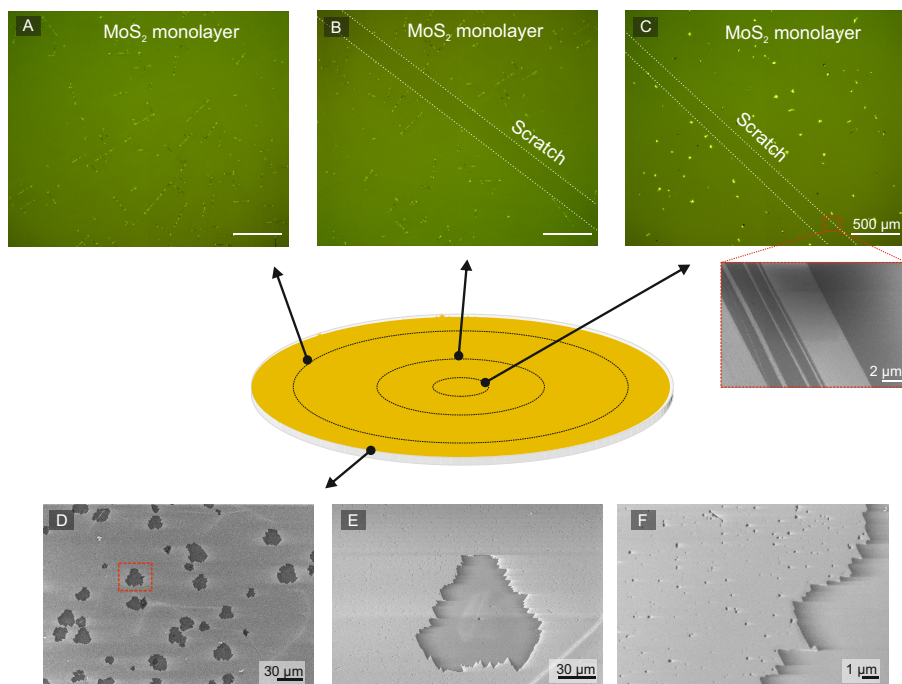
Fig. 2 Sets of optical (A-C) and scanning electron microscope (SEM) (D-F) images taken from marked. arbitrary wafer locations of the material synthesized with H_2O-assisted growth method. Majority of the substrate area is covered with monolayer film occasionally showing secondary layer contrast (white spots on panels A-C). Inset on panel C shows a SEM image of the scratch edge. Single crystals can be found by the edge of the substrate and are shown on panel D. Panels E and F depict the incremental magnification of the single crystal MoS_2 flake.
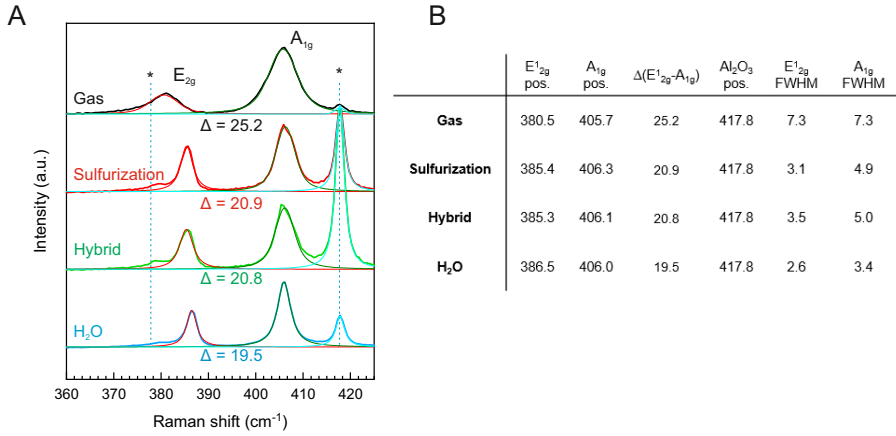
A

B

	E^1_{2g} pos.	A_{1g} pos.	$\Delta(E^1_{2g}\text{-}A_{1g})$	Al_2O_3 pos.	E^1_{2g} FWHM	A_{1g} FWHM
Gas	380.5	405.7	25.2	417.8	7.3	7.3
Sulfurization	385.4	406.3	20.9	417.8	3.1	4.9
Hybrid	385.3	406.1	20.8	417.8	3.5	5.0
H_2O	386.5	406.0	19.5	417.8	2.6	3.4

Fig. 3 A detailed look at typical MoS_2 Raman peaks taken at monolayer locations of MoS_2 synthesized with gas-phase (black), sulfurization (red), hybrid (green) and H_2O assisted (blue) method (A) with detailed peak positions. Positions marked with ∗ represent sapphire substrate Raman peaks. (B) Comparison of MoS_2 properties and their significant improvement for water-assisted growth method.
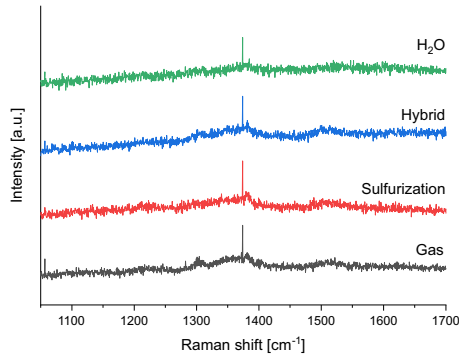

Fig. 4 Raman spectra of all growth methods show no or trace presence of carbon peaks occurring at 1340 cm^{-1} and 1580 cm^{-1}. This measurement indicates no detectable carbon deposition on MoS_2.
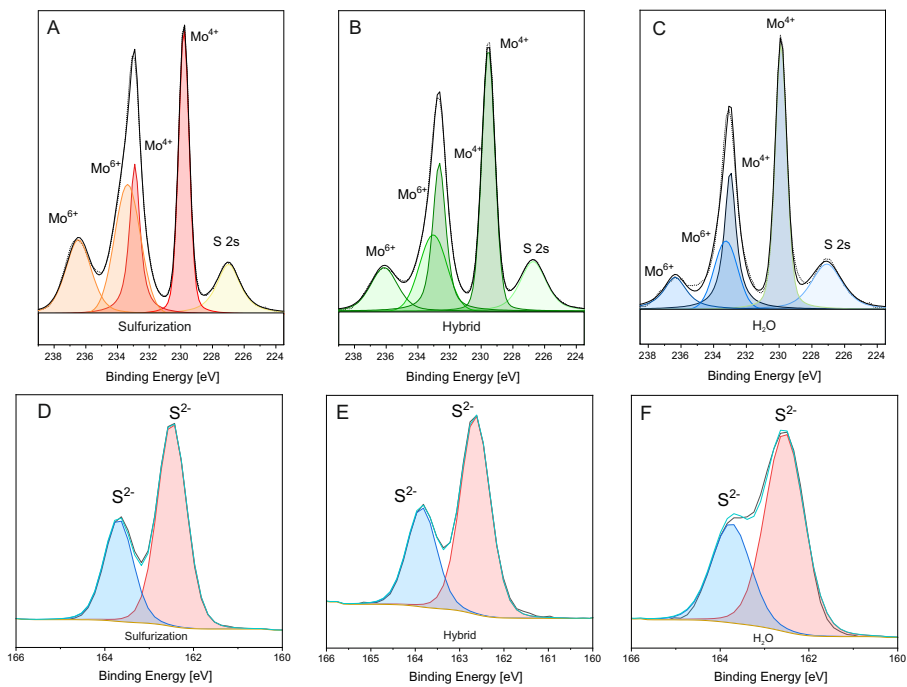
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Fig. 5 Analysis of Mo 3d XPS peaks and its intensities for sulfurization (A), hybrid (B) and H_2O (C) growth methods corroborates a decrease in residual molybdenum oxides. S 2p peaks of monolayer MoS_2 synthesized with sulfurization (E), hybrid (F) and H_2O assisted (G) growth methods.

Sample	MoOx %	MoS2 %	Mo : S	Na %
Sulfurization	54.99 ±2.4	45.00 ±2.4	2.22 ±0.1	11.58 ±0.7
Hybrid	31.32 ±7.4	68.675 ±7.4	6.17 ±1.1	0.43 ±0.4
H$_2$O	37.58 ±0.9	62.41 ±0.9	3.38 ±0.5	0.42 ±0.4

Table 1 Average atomic ratios taken from 3 substrates synthesized with each, consecutive growth method along with oxide and sodium content.
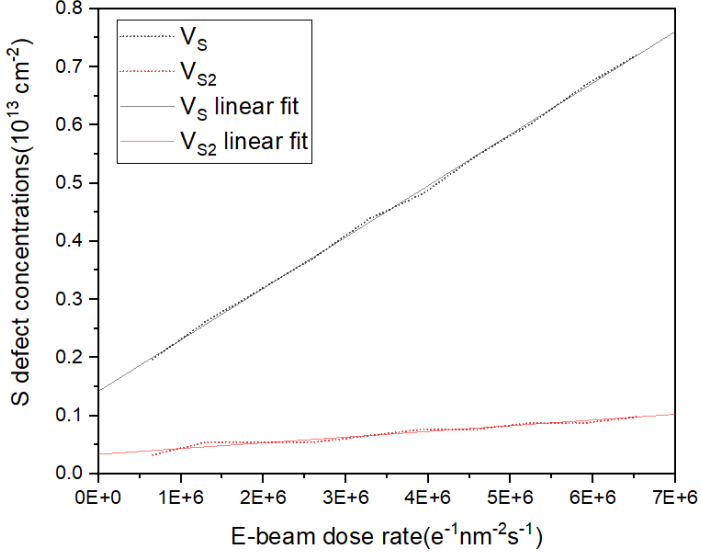

Fig. 6 The general defect density was calculated using a E-beam dose rate test and remains at 1.4×10^{13} single sulfur (V_S) vacancies per cm^2 and 0.3×10^{13} double sulfur defects (V_{S2}) per cm^2.