Atomically of MoS₂ thin layers via a two step thermal evaporation - exfoliation method

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Electronic Supplementary Information

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ESI.1 AFM Images

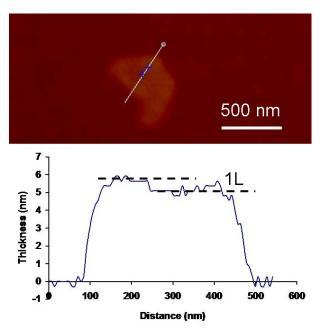


Fig. S1 A flake made of 8 layers. A one layer step on the top of the 8th layer can be resolved.

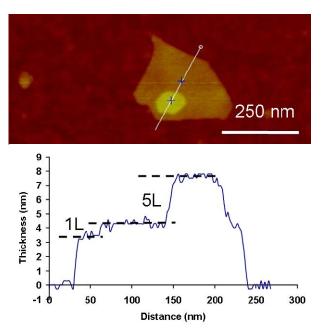


Fig. S2 A flake made of 6 layers. A single step and a 5 layer sheet on the top of this can also be observed

ESI.2 Proposed Reaction Mechanisms

At the lower temperatures of 775 °C, MoO_3 has been reduced to MoO_2 as the evaporated sulphur interacts with oxygen atoms of MoO_3 to produce SO_2 , which is extracted as a gaseous by-product. At the higher temperature of 830 °C a mixture of MoS_2 and MoO_3 is obtained as the sulphur replaces the oxygen in MoO_2 . This leads to the decrease in the percentage of gaseous sulphur which makes the annealing atmosphere less of a reduction environment. The replaced oxygen ions at higher temperatures along with the lack of sulphur allow a fraction of MoO_2 to re-oxidize back to MoO_3 . Similar interactions have been reported by Ressler et al.³⁰ in a study of the formation of sub Mo oxides from MoO_3 in a reducing (H₂) environment. The proposed reaction mechanisms at 830 °C provide an overview of the composition of the end-product in relation to the initial ratio of reactents.

Proposed reaction mechanism at 775 °C:

 $2MoO_3 + S \rightarrow 2MoO_2 + SO_2$

Proposed reaction mechanism at 830 °C:

 $MoO_2 + 3S \rightarrow MoS_2 + SO_2$

 $3MoO_2 + 2S \rightarrow MoS_2 + 2MoO_3$