Supporting information

Switching of the products by size and shape of catalytic nanoparticles during CVD growth of MoS₂ nanotubes

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1. Catalyst -- FeO nanoparticles

The TEM image of 50 nm six-horned octahedral nanoparticles is shown in Fig. S1. Other particles are shown in Fig.2 (main text).



Fig.S1 TEM image of 50 nm six-horned octahedral nanoparticles.



The catalysts were synthesized as follows:

Fig.S2 The flow chart and the conditions of the FeO particles synthesis.

Raman spectra of the three catalysts are as follows:



Fig.S3 Raman spectra of (a) 9 nm, (b) 24 nm spherical and (c) 30 nm six-horned octahedral FeO particles.

After annealing 1 min at 1000 °C, the morphologies of the nanoparticles on the SiO₂/Si substrates were as shown in Figure S4, which were characterized by Raman spectra and XRD. As Raman and XRD devices are exposed to air, FeO was transformed into another stable iron oxide (α -Fe₂O₃).





Fig.S5 Raman spectra of (a) 9 nm, (b) 24 nm spherical and (c) 30 nm six-horned octahedral FeO particles

deposited on the substrates after annealing at 1000 °C for 1 min.





six-horned octahedral FeO



Fig.S6 XRD of (a) 9 nm, (b) 24 nm spherical and (c) 30 nm six-horned octahedral FeO particles deposited on the substrates after annealing at 1000 °C for 1 min.

2. Nanowires

The CVD apparatus is shown as below:

P = 1 atm; t = 1 h



Fig.S7 Schematic drawing of the CVD growth chamber.^{30,31}



Fig.S8 SEM image after CVD with 50 nm catalyst nanoparticles.

The magnified SEM images of MoS_2 nanowires (using 30 nm catalyst) are shown in Figure S9. No particle cap could be found in the top of the nanowire, as shown in Figure S9 (a).



Fig.S9 SEM images of the (a) top and (b) bottom of MoS_2 nanowire grown on the substrate.



Fig.S10 Raman spectra of MoS₂ nanowires synthesized with 30 nm catalyst nanoparticles.



Fig.S11 (a) TEM image of MoS₂ nanowires grown with 50 nm FeO catalyst and (b) its EDS results.

3. Growth mechanism of nanowires

Calculation of MoO₃ vapor in the furnace

After the CVD, about a 10% mass loss of MoO_3 was found. Therefore, the amount of MoO_3 m_{MoO3} loaded into the reaction zones is

 $m_{MoO3\,=}\,10\%\times 0.15g=0.015g$

 $n_{MoO3} = 0.015g / 144g/mol = 10^{-4}$

The flow rate of Ar with S and MoO₃ is 800 sccm and 40 sccm, respectively. The reaction time is 60 min, and the total volume of Ar is

 $V_{Ar} = (800+40) \text{ sccm} \times 60 \text{ min} = 51200 \text{ cm}^3$

The reaction pressure of the system is 1 atmosphere. Thus the estimated partial pressure of MoO₃ is $P_{MoO3} = 10^5 \times 10^{-4} \times 22.4 \text{ L/mol} / 51.2 \text{ L} = 4 \text{ Pa}.$

Control experiment with MoO₃ only

The experiment with only flowing MoO₃ was conducted. The morphologies of the prodcuts are shown belolw.



Fig.S12 SEM images after CVD by flowing MoO_3 on substrates coated with (a) 9-nm₂ (b) 24-nm and (c) 30-nm FeO particles.

Control experiment with S only

The experiment with only flowing sulfur was also conducted. The morphology of the product is shown in Figure S13.



Fig.S13 SEM images after CVD with 9-nm FeO + S.