

## **List of figures**

Figure 1.1(a) Structure of a hexagonal TMDC monolayer. M atoms are in black and X atoms are in yellow. (b) A hexagonal TMDC monolayer seen from above.....	3
Figure 2.1 Molybdenite.....	5
Figure 2.2 Band structure of bulk MoS <sub>2</sub> , where A and B depict the direct gap transitions, as opposed to the indirect gap transition shown by I.....	7
Figure 2.3 Bilayer structure of MoS <sub>2</sub> .....	8
Figure 2.4 Bright field image of an MoS <sub>2</sub> crystal.....	9
Figure 2.5 Time trace of drain current through a monolayer MoS <sub>2</sub> channel. The inset shows the time trace of the drain voltage.....	9
Figure 3.1(a) Raman peak intensity mapping (360 ~ 420 cm <sup>-1</sup> ), (b) PL peak intensity mapping (650 ~ 700 nm) and (c) OM image of the selected area with various MoS <sub>2</sub> layer thickness (1L, 2L and 3L). (d) Raman spectra and (e) photoluminescence of the monolayer, bilayer.....	12
Figure 3.1(a) Schematic experimental set-up. (b) The OM of the MoS <sub>2</sub> layers grown pretreated with rGO solution.(c) AFM image of a monolayer MoS <sub>2</sub> film(d) The thickness of the MoS <sub>2</sub> layer from the AFM cross-sectional profile along the line indicated in (c).....	12
Figure 2.3(a) TEM image of MoS <sub>2</sub> monolayer.(b)HR-TEM image of the marked area in figure (a) with an inset showing SAED pattern.(c)TEM image for the MoS <sub>2</sub> domain boundary at the location as indicated by the inset AFM image.(d)In-plaplane XRD result for MoS <sub>2</sub> monolayer..	13
Figure 3.4(a) Schematic illustration of the two-step thermolysis process for the synthesis of MoS <sub>2</sub> thin layers on insulating substrates. The precursor (NH <sub>4</sub> ) <sub>2</sub> MoS <sub>4</sub> was dip-coated on SiO <sub>2</sub> /Si or sapphire substrates followed by the two-step annealing process. The as-grown MoS <sub>2</sub> film can be transferred onto other arbitrary substrates. (b) Raman spectra for the bilayer and trilayer MoS <sub>2</sub> sheets grown on sapphire substrates (excitation laser: 473 nm), where the labels (Ar) and (Ar + S) represent the MoS <sub>2</sub> sheets separately prepared in pure Ar and in the mixture of Ar and sulfur during the second annealing. (c) Energies of the two characteristic Raman peaks for the micromechanically exfoliated MoS <sub>2</sub> films with various number of layers. The peak energy difference shown in the bottom graph can be used to identify the number of MoS <sub>2</sub> layers. (d) The PL intensity of the trilayer MoS <sub>2</sub> thin films prepared in (Ar + S) is stronger than those prepared in pure Ar (excitation laser 473 nm; spectra were normalized by Raman scattering peak at around 482 nm).....	15
Figure 3.5 (a) AFM image of the MoS <sub>2</sub> trilayer grown on a sapphire substrate annealed with the presence of sulfur (Ar + S). (b) High-resolution TEM image for the MoS <sub>2</sub> trilayer. The d100 is 0.27 nm, and d110 is 0.16 nm. Inset is the TEM image of MoS <sub>2</sub> film edge, where three layers of	

MoS<sub>2</sub> are identified. (c) TEM image and (d) the SAED pattern of the MoS<sub>2</sub> trilayer sample discussed in (b). (e) TEM image and (f) the SAED pattern for the MoS<sub>2</sub> grown on sapphire with Ar annealing. (g, i) TEM images and (h, j) the SAED patterns for the MoS<sub>2</sub> trilayer grown on a SiO<sub>2</sub>/Si substrate annealed with (Ar + S).....15

Figure 3.6 (a) Glancing incidence angle X-ray diffraction (GIA-XRD) and in-plane X-ray diffraction (in-plane XRD) patterns of the MoS<sub>2</sub> trilayers. (b, c) X-ray photoemission spectroscopy (XPS) measurements for the binding energies of Mo and S in the MoS<sub>2</sub> trilayers annealed with sulfur.....16

Figure 3.7(a) FESEM, (b) TEM images of sample C show curved sheet-like structure and uneven surface morphology on a large scale, and (c) EDX spectrum of sample C gives a mole ratio of S:Mo of 1.98, which is about the same value of the ratio of S:Mo for the precursors.....17

Figure 3.8 (a) XRD patterns and (b) Raman spectra of sample C#30 h, C#40 h, C#50 h, C#60 h and C#70 h, which have the same ratio of precursors as that of sample C but undergo different hydrothermal time. (c) Full width at half maximums (FWHMs), relative intensities ( $R = A_{1g}/E_{2g}^1$ ) and frequency differences ( $D = A_{1g} - E_{2g}^1$ ) of their two characteristic Raman peaks  $A_{1g}$  and  $E_{2g}^1$ .....18

Figure 3.9 Photoluminescence spectra of sample C#50 h, C#70 h and bulk MoS<sub>2</sub>. An emerging broad photoluminescence in sample C#50 h indicates the bilayer or few layers of MoS<sub>2</sub> in the synthesized nanosheets.....18

Figure 3.10 (a) FESEM, (b) TEM and (c) HRTEM images of sample C#50 h prepared by using stoichiometric S and Mo precursors through hydrothermal processing for 50 h.....19

Figure 3.11(a) A schematic illustration of the MoS<sub>2</sub> CVD system. (b) The temperature programming process used for a typical growth. (c–d) Typical growth results obtained with (c) and without (d) using PTAS as a seeding promoter. The insets in (c) are the optical image of the triangular MoS<sub>2</sub> flakes at the edge of the MoS<sub>2</sub> monolayer film, and the AFM image on the continuous MoS<sub>2</sub> monolayer film. The insets in (d) are the AFM image of the MoS<sub>2</sub> particles deposited on the surface and the corresponding height cross-section analysis. (e–f) Typical PL (e) and Raman (f) spectra of MoS<sub>2</sub> samples that were prepared with (red) and without (black) PTAS seeding promoter. The PL intensities are normalized by the intensities of the  $A_{1g}$  Raman mode. The excitation wavelength is 532.5 nm.....20

Figure 3.12 (a–i) AFM height images (except (a) which is the phase image) of MoS<sub>2</sub> domains on different regions of the growth substrate. The insets show the corresponding zoom in images. The domain sizes are marked on each of the images. Scale bar: 5  $\mu\text{m}$  (except 10  $\mu\text{m}$  in b). (j–k) Typical PL (j) and Raman (k) spectra of the triangular MoS<sub>2</sub> domains. (l–m) The mapping images of the intensity of PL (l) and  $E_{2g}$  Raman mode (m) of a triangular MoS<sub>2</sub> flake in the region J. The excitation wavelength is 532.5 nm.....21

Figure 4.1 Two-step thermolysis of ammonium thiomolybdate.....26

Figure 4.2 Reaction zones during CVD.....	27
Figure 4.3 Physiochemical steps of CVD.....	28
Figure 4.4. TGA data of MoS <sub>2</sub> nanoparticles and other mixed compounds.....	30
Figure 5.1. Typical configuration of AFM.....	34
Figure 5.2. Picture of AFM setup @DTU.....	34
Figure 5.3. Schematic setup of SEM apparatus.....	37
Figure 5.4. Picture of SEM setup @DTU.....	37
Figure 5.5. Types of electrons released during SEM imaging.....	38
Figure 5-6.Schematic of PL setup.....	41
Figure 5.7. Photographic view of PL setup @DTU.....	41
Figure 5.8. Schematic of UV- visible spectrophotometer.....	43
Figure 5.9. Photographic view of UV-Vis setup @DTU.....	44
Figure 6.1. Schematic of CVD Furnace with substrate placement prior to sulphurisation.....	45
Figure 6.2. Schematic of CVD Furnace with substrate placement during and post sulphurisation.....	46
Figure 6.3.Picture of CVD Furnace used for experimentation.....	46
Figure 6.4. Flow Chart of the entire experimental process .....	48
Figure 6.5. Block Diagram of the entire Experimental Process.....	49
Figure 6.6. Picture of the as-obtained sample.....	50
Figure 7.1. AFM image of single MoS <sub>2</sub> nanoparticulate growth indicating thickness.....	53
Figure 7.2. SEM image of nanoparticulate growth on the substrate.....	54
Figure 7.3. SEM image of island growth on the substrate.....	54
Figure 7.4. SEM image of scattered growth in a region on the substrate.....	55
Figure 7.5. SEM image of continuous growth in a region on the substrate.....	55

Figure 7.6. PL spectra of the MoS <sub>2</sub> sample no.2 .....	56
Figure 7.7. PL spectra of the MoS <sub>2</sub> sample no.4 .....	56
Figure 7.8. UV-Vis spectra of the MoS <sub>2</sub> sample no.2 .....	57
Figure 7.9. UV-Vis spectra of the MoS <sub>2</sub> sample no.4 .....	58

## **List of Abbreviations**

VLSI	Very Large Scale Integration
AFM	Atomic Force Microscopy
Ar	Argon
CVD	Chemical Vapour Deposition
Mo	Molybdenum
MoO <sub>3</sub>	Molybdenum trioxide
MoS <sub>2</sub>	Molybdenum Disulfide
PVD	Physical Vapour Deposition
SiO <sub>2</sub> /Si	Silicon Dioxide on Silicon
S	Sulphur
SCCM	Standard Cubic Centimeters per Minute
TMDC	Transition Metal Dichalcogenide Crystal
2D	Two Dimensional
SEM	Scanning Electron Microscopy
PL	Photoluminescence

## **ABSTRACT**

The search for monolayer materials to substitute silicon in electronic devices has widened in the past decade. Despite the benefits of two dimensional graphene, it has no band gap and behaves as a semi-metal. Molybdenum disulphide is a promising material as it boasts a band gap of up to 1.9eV in a monolayer form. In this project, an inexpensive method of fabricating monolayer MoS<sub>2</sub> is designed and growths on Si-substrates for future use in electronic devices will be attempted with this fabrication method.