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List of Abbreviations

AEF	Analytical enhancement factor
AFM	Atomic force microscopy
CM	Chemical enhancement
CVD	Chemical vapor deposition
CBM	Conduction band minima
CuPc	Copper phthalocyanine
CV	Crystal Violet
DI	Distilled water
EM	Electromagnetic enhancement
eV	Electron volt
LWD	Long working distance
MW	Mega watt
MB	Methylene blue
MO	Methyl orange
MEMS	Microelectrochemical system
MoS ₂	Molybdenum disulphide
NA	Numerical aperture
1D	One dimensional
OTR	Optothermal Raman
ppm	Parts per million
PL	Photoluminescence
PVD	Physical vapor deposition
R6G	Rhodamine 6G

RT	Room temperature
SEM	Scanning electron microscope
SThM	Scanning thermal microscope
SAED	Selected area electron diffraction
Si	Silicon
SiO ₂	Silicon dioxide
Ag	Silver
SERS	Surface enhanced Raman spectroscopy
SPR	Surface plasmon resonance
TEC	Thermal expansion coefficient
TDTR	Time domain thermo reflectance
TEM	Transmission electron microscopy
TMD	Transition metal dichalcogenide
2D	Two dimensional
UV	Ultraviolet
VBM	Valence band maxima
VFL	Vertically oriented few-layer
Vis	Visible
XRD	X-ray diffraction

List of Symbols

α	Absorption coefficient
ω	Angular frequency
E_g	Bandgap
k_b	Boltzmann's constant
E_c	Conduction band
I-V	Current voltage
ρ	Density of material
q	Electronic charge
E_F	Fermi energy
χ_P	First order power coefficient
χ_T	First order temperature coefficient
η	Ideality factor
S	Illuminated area
P_{inc}	Incident light intensity
g	Interfacial thermal conductance
P	Laser power
μ	Mobility
I_{Ph}	Photocurrent
R	Photoresponsivity
h	Planck's constant
C_p	Specific heat capacity
T	Temperature
k	Thermal conductivity

k_s	Thermal conductivity of supported film
R_m	Thermal resistance
E_v	Valence band
V	Voltage
W	Watt
λ	Wavelength

Preface

Molybdenum disulfide (MoS₂) is a layered transition metal dichalcogenide, which shows tunable bandgap and good thermal transport behaviour along with high absorption coefficient and mechanically flexible nature. These features of MoS₂ make it suitable for use in next generation electronic and optoelectronic devices. This thesis entitled **“CVD Grown Thermal Conducting 2D-MoS₂ Nanostructures for Photodetection and SERS Applications”** is focused on the synthesis of thermal conducting and semiconducting MoS₂ nanostructures via chemical vapour deposition (CVD) technique and their photodetection and Surface-Enhanced Raman Scattering (SERS) applications. We have prepared three different morphologies of MoS₂ nanostructures- horizontally grown interconnected network of few-layer MoS₂ over Si substrate, horizontally grown triangular bi-layer MoS₂ over SiO₂/Si substrate and vertically oriented few-layer (VFL) MoS₂ over Si substrate. We have characterized prepared MoS₂ films by optical microscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and atomic force microscopy (AFM) techniques. To confirm the phase and the semiconducting nature of prepared MoS₂, X-ray diffraction (XRD) and Raman spectroscopy techniques have been performed. The semiconducting nature of prepared MoS₂ nanostructures have been confirmed via Photoluminescence (PL) spectroscopy. In the present work, thermal transport behaviour of triangular bi-layer MoS₂ and VFL-MoS₂ has been investigated using optothermal Raman technique. We have calculated the thermal conductivity (k_s) of $\sim 42 \pm 8 \text{ W m}^{-1} \text{ K}^{-1}$ and interfacial thermal conductance (g) of $\sim 1.264 \pm 0.128 \text{ MW m}^{-2} \text{ K}^{-1}$ for triangular bi-layer MoS₂ supported over SiO₂/Si substrate. Higher thermal conductivity of $\sim 100 \pm 14 \text{ W m}^{-1} \text{ K}^{-1}$ has been found for VFL-MoS₂ nanostructure, which can be associated with reduced

phonon-defect scattering due to fewer defects and minimal strain in grown VFL-MoS₂ nanostructure. Further, thermal sensitive quantum confinement phenomenon has been observed in above samples by performing temperature dependent PL study, which provides the information about the tunable nature of their bandgap suitable for optoelectronics application.

Based on the thermal conducting and semiconducting nature of prepared MoS₂ nanostructures, we have used these films for photodetection and SERS applications. The CVD grown MoS₂ nanostructures are n-type in nature and hence they form p-n heterojunction with p-type Si substrate. We have successfully demonstrated the photodetection application of interconnected few-layer MoS₂/Si heterojunction and VFL-MoS₂/Si heterojunction. We have observed the photoresponsivity of $\sim 0.1413 \text{ A W}^{-1}$ for few-layer MoS₂/Si heterojunction under white light illumination (0.15 mW cm^{-2}) at -2 V bias. Higher photoresponsivity of $\sim 7.37 \text{ A W}^{-1}$ has been obtained for VFL-MoS₂/Si heterojunction under green light illumination (0.15 mW cm^{-2}) at -2 V bias, which can be attributed to the strong light absorption, intralayer carrier transport speed, and effective charge separation. Further, SERS application of prepared MoS₂ nanostructures has been investigated to detect organic pollutants- Rhodamine 6G (R6G) and Methyl orange (MO). We have successfully detected R6G dye using all the prepared MoS₂ nanostructures, while MO dye was detected using VFL-MoS₂ nanostructure. The highest detection limit (10^{-10} M concentration for both the dyes) has been observed for VFL-MoS₂ nanosheets over Si as SERS substrate. This high detection limit can be attributed to the enhanced light trapping and effective dye adsorption due to vertical morphology and vibronic-coupling-enabled charge transfer between MoS₂ and organic dyes.

The present thesis has been organized into seven chapters. The consecutive chapters are organized as follows-

Chapter 1 gives a brief introduction to 2D MoS₂ nanostructure along with an overview of the current literature on thermal conductivity measurement, photodetection and SERS applications of MoS₂ nanostructure.

Chapter 2 describes the synthesis process of three different morphologies of MoS₂ nanostructures. A concise overview of the characterization instruments like XRD, SEM, TEM, Raman, PL and AFM, is provided for structural and morphological studies of MoS₂. This chapter also describes the current voltage measurement process and the preparation method of SERS substrate.

Chapter 3 discusses the temperature and power-dependent Raman studies of horizontally grown triangular bi-layer MoS₂ nanosheets over SiO₂/Si substrate and vertically oriented few-layer (VFL) MoS₂ nanosheets over Si substrate. Thermal conductivity calculation using Optothermal Raman technique has been described in detail.

Chapter 4 discusses the thermal sensitive quantum confinement behaviour of triangular bi-layer MoS₂ and VFL-MoS₂ nanostructures. Tunability of bandgap with temperature has been discussed using appropriate models.

Chapter 5 describes the photodetection application of horizontally grown interconnected network of few-layer MoS₂ and VFL-MoS₂ over Si substrate using p-n junction mode under visible light illumination. Different optoelectronic parameters have been obtained and photodetection mechanism has been discussed in this chapter.

Chapter 6 discusses the SERS detection of R6G and MO molecules using prepared different MoS₂ nanostructures. The mechanisms like molecular resonance, excitonic resonance and vibronic coupling enable charge transfer have been discussed in detail.

Chapter 7 thesis work has been summarized and the scope for the future work related to this field has been discussed.