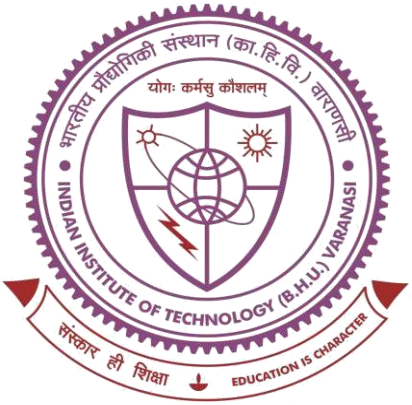
Layer, Morphology and Substrate Dependent Anisotropic, Thermal and SERS Studies of CVD Grown 2H-MoS_2



Thesis submitted in partial fulfilment

for the Award of

Doctor of Philosophy

By

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It is certified that the work contained in the thesis titled ***"Layer, Morphology and Substrate Dependent Anisotropic, Thermal and SERS Studies of CVD Grown 2H-MoS_2"*** by **Ankita Singh** has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

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I, *"Ankita Singh"*, certify that the work embodied in this thesis is my own bonafide work carried out by me under the supervision of *"Dr. Ashish Kumar Mishra"* from *"July 2018"* to *"February 2024"*, at the *"School of Materials Science and Technology"*, Indian Institute of Technology (BHU), Varanasi, India. The matter embodied in this thesis has not been submitted for the award of any other degree/diploma. I declare that I have faithfully acknowledged and given credits to the research workers wherever their works have been cited in my work in this thesis. I further declare that I have not willfully copied any other's work, paragraphs, text, data, results, *etc.*, reported in journals, books, magazines, reports dissertations, thesis, *etc.*, or available at websites and have not included them in this thesis and have not cited as my own work.

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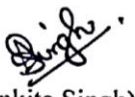

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(Ankita Singh)

Dedicated to my beloved parents

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List of Abbreviation

AFM	Atomic force microscopy
ARPRS	Angle resolved polarized Raman spectroscopy
BSE	Backscattered electrons
BZ	Brillouin zone
CB	Conduction band
CM	Chemical enhancement
CT	Charge transfer
CVD	Chemical vapor deposition
DFT	Density functional theory
DFPT	Density functional perturbation theory.
DOS	Density of states
DP	Deformation potential
EF	Enhancement factor
EM	Electromagnetic enhancement
eV	Electron volt
FI	Fröhlich interaction
FTO	Fluorine-doped tin oxide
FWHM	Full width at half-maximum
HOMO	Highest occupied molecular orbitals
ILC	Interlayer coupling
LSPR	Localized surface plasmon resonance
LUMO	Lowest unoccupied molecular orbitals
LWD	Long working distance
MBE	Molecular beam epitaxy
MOCVD	Metal-organic chemical vapor deposition

MoS_2	Molybdenum disulfide
MFC	Mass flow controller
MW	Mega watt
N.A.	Numerical aperture
OTR	Optothermal Raman
PL	Photoluminescence
PECVD	Plasma-assisted chemical vapor deposition
PICT	Photo-induced charge transfer
PVD	Physical vapor deposition
RT	Room temperature
Si	Silicon
SiO_2	Silicon dioxide
sccm	Standard cubic centimeter per minute
SERS	Surface enhanced Raman spectroscopy
SE	Secondary electrons
SEM	Scanning electron microscopy
SOC	Spin orbit coupling
2D	Two dimensional
TDTR	Time-domain thermos-reflectance
TMDs	Transition metal dichalcogenides
VB	Valence band

List of Symbols

α	Absorption coefficient
N_A	Avogadro constant
$(\Delta\omega)_{anh}$	Anharmonic phonon-phonon interaction
k_B	Boltzmann's constant.
$\langle\hbar\omega\rangle$	Average phonon energy involved in the electron-phonon interaction
ω_0	Extrapolated peak position of phonon modes at 0 K
n	Degeneracy
$E_g(0)$	Energy of A exciton at 0 K
$E_g(T)$	Energy of A exciton at temperature T
χ_P	First-order power-dependent coefficient
χ_T	First order temperature coefficient
γ	Grüneisen parameter
g	Interfacial thermal conductance
α_a	In-plane thermal expansion coefficient
α_c	Out of-plane thermal expansion coefficient
$\hat{g}_i$	Polarization of the incident laser light
$\hat{g}_s$	Polarization of the scattered laser light
I_o	PL intensity at 0 K
S	Strength of the electron-phonon coupling
E_{SO}	Spin orbit coupling energy
$I_{PL}(T)$	Temperature-dependent PL intensity
$k_{rad}(T)$	Temperature-dependent radiative recombination rates
$k_{nonrad}(T)$	Temperature-dependent nonradiative recombination rates
k_s	Thermal conductivity
α_T	Thermal expansion coefficient
$(\Delta\omega)_{latt}$	Thermal expansion of the lattice
R_m	Thermal resistance
β	Varshni coefficients related to the electron-phonon interaction.
λ	Wavelength