

List of Figures

Figures	Title	Page
1.1	Wurtzite hcp structure of GaN comprising tetrahedral coordination of Ga and N atoms with lattice constant a and c	3
1.2	Stick and ball representation of Ga face and N face wurtzite crystal structure	4
1.3	Spontaneous polarization in GaN and AlGa _N materials grown in [0001] direction.	5
1.4	The orientation of the piezoelectric and spontaneous polarization in wurtzite AlGa _N /GaN and InGa _N /GaN heterostructures with Ga- and N-face polarity with tensile and compressive strain	7
1.5	Bandgap vs. lattice constants of III-Ns and other semiconductors.	9
1.6	Energy band diagram for the narrow (GaN) and wide bandgap (AlGa _N) materials with (a) Band offsets before the formation of heterojunction (b) Band bending after heterojunction formation	9
1.7	Epitaxial structure of AlGa _N /GaN HEMT.	11
1.8	Device schematic of AlGa _N /GaN HEMT	14
1.9	Energy band diagram of the AlGa _N /GaN HEMT with 2DEG under different operating conditions: (a) cut-off ($V_{GS} < V_T$) (b) linear ($V_D < (V_{GS} - V_T)$) (c) saturation ($V_D > (V_{GS} - V_T)$)	15
1.10	Generalized block diagram of the heavy metal ion sensor	17
1.11	Classification of heavy metal ion sensors	22
2.1	A generalized Sentaurus TCAD process flow utilized in this Thesis.	32
2.2	(a) The epitaxial structure of the designed AlGa _N /GaN HEMT (b) Enlarged view of designed structure indicating top layers of the device, (c) Optimal meshing of the designed AlGa _N /GaN HEMT. (The X and Y-axis are in μm scale) (d) Schematic cross-section view of Designed AlGa _N /GaN HEMT	33
2.3	Experimental (star symbol) and Simulated (dashed line) Drain current vs. Gate voltage (I_D - V_G) characteristics of HEMT at $V_D=10\text{V}$ along with Transconductance (g_m) with experimental (purple circle symbol) and simulated curve (dash-dot line) at $V_D=10\text{V}$ and 300K.	42
2.4	Band diagram of the top layers of AlGa _N /GaN HEMT and electron density at 2DEG interface	42
2.5	(a) Observation of piezoelectric polarization at the top layers of the designed AlGa _N /GaN HEMT (b) 2DEG electron density at AlGa _N /GaN heterojunction at $V_{DS}=10\text{ V}$ and $V_{GS}=0\text{ V}$	43
2.6	Variation of Drain current (I_D) and Drain voltage (V_D) for the HEMT with and without consideration of self-heating effects along with experimental results. A star symbol shows experimental results; dashed lines indicate simulated results with self-heating effects, and dotted lines show simulated results without self-heating effects.	44
2.7	(a) Effects of self-heating at the 2DEG channel at $V_{GS}=2\text{ V}$, $V_{DS}=10\text{ V}$, and 20 V from source to drain of the HEMT structure. (b) increment of lattice heat between drain and gate region at $V_{GS}=2\text{ V}$, and $V_{DS}=10\text{ V}$ and (c) $V_{GS}=2\text{ V}$, and $V_{DS}=20\text{ V}$ (x and y-axis are in μm range).	45
2.8	Potential and layer representation for solid/electrolyte interface modeling	46
3.1	Schematic of the thermal evaporation system	52
3.2	Thermal evaporation system at Microfabrication lab, IIT Jodhpur	53
3.3	Schematic representation of the RF sputtering system	53
3.4	Illustration of the RF sputtering process	54
3.5	Photograph of the sputtering system at microfabrication lab, IIT Jodhpur	55
3.6	Illustration of Spin coating process	55
3.7	Photograph of the spin coating system, installed at IIT Jodhpur	56
3.8	Image of MJB-4 mask aligner system at microfabrication lab, IIT Jodhpur.	57
3.9	A pictorial illustration of exposure and development process using positive photoresist.	57
3.10	Schematic description etching process.	58
3.11	schematic illustration of X-ray diffraction	59
3.12	Explanation of Bragg's law for X-ray diffraction.	59
3.13	X-ray diffraction system (D8 Advance, Bruker) at IIT Jodhpur	60
3.14	Schematic setup of Atomic Force Microscopy (AFM)	61
3.15	Pictorial view of Atomic Force Microscopy (AFM)	61

	Page	
3.16	Schematic illustration and working of FESEM	62
3.17	Experimental system for FESEM (Source: MRC, MNIT, Jaipur)	63
3.18	Schematic representation of the working and instrumentation part of the TEM system	63
3.19	Working of Raman spectroscopy	64
3.20	Schematic representation of Atomic Absorption Spectroscopy	65
3.21	Atomic Absorption Spectroscopy System for elemental analysis of solutions (Source: MRC, MNIT Jaipur)	65
3.22	(a) Schematic representation of ICP-MS (b) ICP-MS System for detection of ionic concentration (Source: CRF, IIT Delhi)	66
3.23	Probe station with Keithley-4200 SCS for electrical characterization at IIT Jodhpur.	66
4.1	Epitaxial structure of AlGaIn/GaN HEMT grown by MOCVD.	68
4.2	Cross-sectional TEM of the AlGaIn/GaN HEMT structure	69
4.3	HRXRD of the epilayer of the AlGaIn/GaN HEMT structure	69
4.4	AFM morphology of the surface of the AlGaIn/GaN HEMT wafer	70
4.5	Process flow for AlGaIn/GaN HEMT sensor fabrication.	70
4.6	Schematic illustration of (a) deposition of Al/Cr/Au metals over HEMT sample by thermal evaporation (b) patterning of the metals for source and drain contact formation using photolithography	71
4.7	(a) Schematic illustration of Si ₃ N ₄ patterning on AlGaIn/GaN HEMT (b) Gate patterning on AlGaIn GaN HEMT (c), (d) Images of fabricated devices by following the fabrication process steps	73
4.8	Device mounting on PCB and contact extension for Sensing application	74
4.9	Schematic of TLM structure	74
4.10	Explanatory graph for TLM calculation	75
4.11	Optical microscopic image of the fabricated TLM structure	75
4.12	(a) I-V characteristics at different contact spacing and (b) Observed resistance of the AlGaIn/GaN HEMT TLM structure with respect to the spacing of two successive contacts	76
4.13	Drain current vs. Gate voltage (I_D-V_G) characteristics of the processed HEMT for sensing application at $V_{DS}=5$ V along with the Transconductance (g_m) curve. Logarithmic transfer characteristics of HEMT is shown in the inset.	77
4.14	Drain current vs. Drain voltage (I_D-V_D) characteristics of the as process AlGaIn/GaN HEMT for sensing application from $V_{GS} = -1.5$ V to $V_{GS} = 1$ V	77
5.1	Functionalization process of MPA and GSH on Au gate contact of AlGaIn/GaN HEMT	81
5.2	The layered structure of the AlGaIn/GaN HEMT sensor with the functionalized gate by 3-Mercaptopropionic acid (MPA) and Glutathione (GSH) for the detection of Cd ²⁺ ions.	82
5.3	Real-time electrical response of AlGaIn/GaN HEMT sensor with different Cd ²⁺ ion concentrations at $V_{DS} = +0.5$ V.	82
5.4	I_D-V_D characteristics of the device where its gate was exposed to a 10-ppm Cd ²⁺ ion concentration and Cd ²⁺ ion free solutions, respectively	83
5.5	Calibration curve and the response of the device w.r.t. Cd ²⁺ ion concentration (inset: response at the lower concentration of Cd ²⁺)	84
5.6	Response time of the sensor at 1 ppb Cd ²⁺ concentration	84
5.7	Selectivity observation of the sensor (a) Comparison of the response of the Cd ²⁺ ions with different heavy metal ions. Here, M is the heavy metal (Cd, Cr, Cu, Hg, Ni, Pb, Zn), and n is no. of charges on metal ions (n= 1, 2, 3). (b) Selectivity histogram of the developed sensor with Cd ²⁺ and other metal ions by normalized current calculation.	85
5.8	Influence of the pH on the response of the sensor at 10ppm Cd ²⁺ ion concentration.	86
5.9	Response and recovery of the Cd ²⁺ ion sensor.	86
5.10	Repeatability behavior of the Cd ²⁺ ion sensor.	87
5.11	Reproducibility of the developed Cd ²⁺ ion sensor.	87
5.12	Mechanism of MPA-GSH functionalized Au gated AlGaIn/GaN HEMT sensor for Cd ²⁺ ion detection	88
6.1	Functionalization process of DMTD on the gate region of AlGaIn/GaN HEMT.	93
6.2	Real time response of AlGaIn/ GaN HEMT sensor for Pb ²⁺ ion concentrations ranging from blank solution to 10 ppm concentration ($V_{DS} = +0.5$ V)	93
6.3	Calibration (fitting) curve and the sensor's response versus applied Pb ²⁺ ion concentration (inset: response at a lower concentration).	94
6.4	Effects of pH on I_{DS} of the sensor in 1 ppm concentration of Pb ²⁺ ions.	95

	<i>Page</i>	
6.5	Response and recovery of Pb ²⁺ ion AlGaIn/ GaN HEMT sensor	96
6.6	Repeatability analysis of the sensor	96
6.7	Proposed mechanism of DMTD functionalized AlGaIn/GaN HEMT sensor for Pb ²⁺ ion detection.	98
7.1	The hydrothermal synthesis process of MoS ₂ using MoO ₃ , CH ₄ N ₂ S, and NaOH	101
7.2	SEM images of (a) MoS ₂ flower-like structures, (b) magnified view of MoS ₂ flower-like structures.	103
7.3	XRD pattern of the flower-like MoS ₂	103
7.4	Raman Spectrum of as-deposited MoS ₂	104
7.5	(a) FESEM (b) cross-sectional FESEM of the MoS ₂ functionalized Au-gated AlGaIn/GaN HEMT.	104
7.6	(a) AFM images and (b) Raman spectra of MoS ₂ functionalized surface of AlGaIn/GaN HEMT	105
7.7	I _{DS} -V _{DS} characteristics of the device after different steps of functionalization and sensing	105
7.8	Real time Hg ²⁺ ion sensing on MoS ₂ functionalized AlGaIn/ GaN HEMT.	106
7.9	Sensor response and calibration curve for Hg ²⁺ ion detection using MoS ₂ functionalized AlGaIn/ GaN HEMT (inset: sensor response at lower concentration)	107
7.10	(a) Relative sensing response of the sensor for various heavy metal and Hg ²⁺ ions from 0.01 ppt to 10 ppm concentration (b) Response ratio of the sensor for Hg ²⁺ ions and other interfering heavy metal ions for selectivity analysis.	108
7.11	Response and recovery of the developed sensor	109
7.12	Repeatability of the developed Sensor	109
7.13	Reproducibility of the MoS ₂ functionalized AlGaIn/ GaN HEMT sensor.	110
7.14	Sensing mechanism of MoS ₂ functionalized AlGaIn/ GaN HEMT for Hg ²⁺ ion detection (a) HEMT with MoS ₂ functionalization (b) Hg-S complex formation on the gate region of HEMT at low concentration of Hg ²⁺ ions (c) electrostatic interaction between Hg ²⁺ ions and MoS ₂ layer at high concentration of Hg ²⁺ ions.	111

