TABLE OF FIGURE

Chapter 1: Introduction		Page No
Figure 1	The energy band diagram of n-P type two semiconductors (to form a heterojunction) (a) Before contact, (b) After contact.	4
Figure 2	N-p heterojunction - (a) Before contact, (b) After contact.	5
Figure 3	Formation of heterojunction.	6
Figure 4	Energy band diagram for two p-P type (isotype) semiconductors - (a) Before contact, (b) After contact.	7
Figure 5	Energy band diagram for N-n type (isotype) semiconductors - (a) Before contact, (b) After contact.	7
Figure 6	Energy band diagram for compositionally graded semiconductor.	8
Figure 7	Possible types of band alignments at a heterojunction interface (type I, type II and type III alignments).	9
Figure 8	Energy band diagrams for a metal-semiconductor (n-type) contact.	11
Figure 9	Energy band diagrams for a metal-semiconductor (p-type) contact.	12
Figure 10	Double heterostructure.	13
Figure 11	Simplified band diagram of double heterostructure showing carrier confinement.	13

Figure 12	Conduction band structure of heterojunction between	13
	AlGaN/GaN.	
Figure 13	Multilayer heterostructure.	14
Figure 14	(a) Strain free wurtzite unit cell and (b) graphite-like semi metallic phase unit cell under large compressive in-plane strain.	16
Chapter	2: Theoretical Detail	
Figure 1	The typical band structure of semiconductors.	33
Figure 2	Direct and indirect semiconductors.	34
Figure 3	Effect of strain at Γ point on III-V semiconductor band structures.	49
Chapter :	3: Modeling and Simulation	
Figure 1	Band structure for Wurtzite GaN.	57
Figure 2	Detailed electronic Band Structure of GaN.	58
Figure 3	Lattice structure of GaN.	58
Figure 4	Detailed electronic Band Structure of InN.	60
Figure 5	Band structure for Wurtzite AlN.	62
Figure 6	Detailed electronic Band Structure of AlN.	62
Figure 7	Detailed electronic Band Structure of $Al_xGa_{1-x}N$ for $x=0.2$.	64

Figure 8	Detailed electronic Band Structure of $Al_xIn_{1-x}N$ for $x=0.2$.	65
Figure 9	Detailed electronic Band Structure of $Ga_xIn_{1-x}N$ for $x=0.2$.	66
Figure 10	Simulated model of multilayer nano-heterostructure.	68
Chapter 4	: Result and Discussion	
Figure 1	A comparison of bonds between closed packed planes for the crystal structures.	88
Figure 2	Geometry of unstrained unit cell of III-V semiconductors with the primitive translation vectors \mathbf{a}_i and the set $(\hat{\mathbf{e}}_x, \hat{\mathbf{e}}_y, \hat{\mathbf{e}}_z)$ of Cartesian unit vectors. a_r and c_r denote the unstrained lattice constants.	89
Figure 3	Variation in Strain for GaN/Al _x Ga _{1-x} N multilayer nanoheterostructure with different Al-concentration.	92
Figure 4	3-D view of strain for $GaN/Al_{0.20}Ga_{0.80}N$ multilayer nanoheterostructure.	93
Figure 5	Variation in strain for InN/AlInN multilayer nanoheterostructure with different Al-concentration.	95
Figure 6	Variation in strain for InN/GaInN multilayer nanoheterostructure with different Ga-concentration.	96
Figure 7	Strain variation with composition for GaN/AlGaN multilayer nano-heterostructure.	97
Figure 8	Strain variation with composition for InN/AlInN multilayer nano-heterostructure.	97

Figure 9	Strain variation with composition for InN/GaInN multilayer nano-heterostructure.	98
Figure 10	Calculated strain in AlInN as a function of Al-composition	98
Figure 11	Energy band profile for simulated model of multilayer nanoheterostructure of $GaN/Al_xGa_{1-x}N$ for Al-10%.	102
Figure 12	Energy band profile for simulated model of multilayer nanoheterostructure of $GaN/Al_xGa_{1-x}N$ for Al-30%.	102
Figure 13	Energy band profile for simulated model of multilayer nanoheterostructure of GaN/Al _x Ga _{1-x} N for Al-50%.	103
Figure 14	Energy band profile for simulated model of multilayer nanoheterostructure of GaN/Al _x Ga _{1-x} N for Al-70%.	103
Figure 15	Energy bandgap variation with Al-concentration for $GaN/Al_xGa_{1-x}N \ multilayer \ nano-heterostructure.$	104
Figure 16	Potential distribution for different Al-concentration for simulated model of nano-heterostructure of $GaN/Al_xGa_{1-x}N$.	106
Figure 17	Space charge densities for different Al-concentration for simulated model of nano-heterostructure of $GaN/Al_xGa_{1-x}N$.	107
Figure 18	One-dimensional electron densities for different Alconcentration for simulated model of nano-heterostructure of $GaN/Al_xGa_{1-x}N$.	108
Figure 19	One-dimensional hole densities for different Al-concentration for simulated model of nano-heterostructure of $GaN/Al_xGa_{1-x}N$.	109
Figure 20	Energy band profile for simulated model of multilayer nano-	112

heterostructure of $InN/Al_xIn_{1-x}N$ for Al-10%.

Figure 21	Energy band profile for simulated model of multilayer nanoheterostructure of $InN/Al_xIn_{1-x}N$ for Al-30%.	112
Figure 22	Energy band profile for simulated model of multilayer nanoheterostructure of $InN/Al_xIn_{1-x}N$ for Al-50%.	113
Figure 23	Energy band profile for simulated model of multilayer nanoheterostructure of InN/Al _x In _{1-x} N for Al-70%.	113
Figure 24	Energy bandgap variation with Al-concentration for $InN/Al_xIn_{1-x}N \ multilayer \ nano-heterostructure.$	114
Figure 25	Potential distribution for different Al-concentration for simulated model of nano-heterostructure of $InN/Al_xIn_{1-x}N$.	116
Figure 26	One-dimensional space charge density for different Alconcentration for simulated model of nano-heterostructure of $InN/Al_xIn_{1-x}N$.	117
Figure 27	One-dimensional electron density for different Al-concentration for simulated model of nano-heterostructure of $InN/Al_xIn_{1-x}N$.	118
Figure 28	One-dimensional hole density for different Al-concentration for simulated model of nano-heterostructure of $InN/Al_xIn_{1-x}N$.	119
Figure 29	Energy band profile for simulated model of multilayer nanoheterostructure of InN/Ga _x In _{1-x} N for Ga-10%.	120
Figure 30	Energy band profile for simulated model of multilayer nanoheterostructure of $InN/Ga_xIn_{1-x}N$ for $Ga-30\%$.	121
Figure 31	Energy band profile for simulated model of multilayer nanoheterostructure of InN/Ga _x In _{1-x} N for Ga-50%.	121

Figure 32	Energy band profile for simulated model of multilayer nanoheterostructure of InN/Ga _x In _{1-x} N for Ga-70%.	122
Figure 33	Energy bandgap variation with Ga-concentration for InN/Ga _x In _{1-x} N multilayer nano-heterostructure.	123
Figure 34	Potential distribution for different Ga-concentrations for simulated model of nano-heterostructure of $InN/Ga_xIn_{1-x}N$.	124
Figure 35	One-dimensional space charge density for different Gaconcentration for simulated model of nano-heterostructure of $InN/Ga_xIn_{1-x}N$.	125
Figure 36	One-dimensional electron density for different Gaconcentration for simulated model of nano-heterostructure of $InNGal_xIn_{1-x}N$.	126
Figure 37	One-dimensional hole density for different Ga-concentration for simulated model of nano-heterostructure of InN/Ga _x In _{1-x} N.	127