Conclusion and Summary

Chapter 5

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The optoelectronics market is currently at 20 billion dollars per year, and is projected to rapidly expand further in the next few decades. This is driven largely by growth and advances in the sectors of solid state lighting and laser technologies. This growth was catalyzed by the introduction of high-brightness blue light emitting diodes (LEDs) with InGaN as the active layer in 1990s [1, 2]. Research in this field has thus been heavily focused on Ga-rich GaInN and AlGaN alloys, whose bandgaps cover the blue and near-ultraviolet parts of the electromagnetic spectrum. Since then, the rapid development of solid state lighting technology has revolutionized the fields of optoelectronics and optics.

A heterojunction is basically a p-n junction in a semiconductor between materials of different composition. Normal junctions are between p and n type versions of the same material. But in this case we refer to a junction formed between two group III-nitrides usually a GaN/AlN interface or a GaN/AlGaN interface. Since they are two different materials, the band structure is discontinuous from one material to the other and the band alignment across the interface is typically of type I, i.e. the bandgap of the lower bandgap material is positioned energetically within the bandgap of the wider bandgap semiconductor.

By varying the alloy composition, we can get a material with the desired bandgap. For different applications, different bandgap materials are required and this can be obtained by using group III-Nitride with different alloy compositions.

When two different atoms form a chemical bond, the difference in their electronegativities causes an effective dipole across the atomic bond. This dipole can induce a net polarization across a macroscopic layer if the symmetry of the crystal allows it. In a cubic crystal structure under no strain, the dipole moments of the atomic bonds cancel each other to produce no net polarization across the crystal. For III-V nitride semiconductors the large difference in electronegativity between the group III and group

V elements (Al=1.18, Ga=1.13, In=0.99, N=3.0) results in very strong chemical bonds in the III-Nitrides material system, and the atomic crystal arrangement is such that a net dipole moment is present even under no applied strain [3-5].

Due to the presence of strain fields in multilayer structures, and also the presence of strong polarization fields makes the band diagram complicated. Moreover the band offset can be defined properly only if we know the precise strain field. The band offsets and Fermi-level pinning at the surface are the important heterostructure device parameters.

III-V nitrides, by virtue of their wurtzite crystal structure and high degree of ionicity, exhibit a variety of material properties that are not found in zincblende III-V semiconductors, and due to their polarization effects, which recent experimental and theoretical investigations have revealed to be of great importance in the design and analysis of nitride heterostructure devices.

Now-a-days AlGaN, AlInN, InGaN alloys are attracting much attention as candidate materials for realizing deep ultraviolet (UV), light emitting diodes or laser diodes. The short wavelength lasers using these compounds have been realized as efficient light sources. These sources operating in the UV region are required for a number of applications, including long life time white lighting, sterilization and decontamination, for use in medical field and biochemical processes, for the purification of the environment, and for high density optical storage. Despite of these, they are very important for household air cleaners, automobile exhaust purifiers, UV sensing system and so on [6].

Among the findings, some works have clearly demonstrated, both theoretically and experimentally, that the mobility of the channel electrons depend strongly on the carrier concentration. However, the effects of the carrier concentration dependent mobility, as well as the diffusion part of the total current, have not yet been simultaneously taken into account.

In this work, we have presented the proposed model and performed 1-D simulation for $GaN/Al_xGa_{1-x}N$, $InN/Al_xIn_{1-x}N$and $InN/Ga_xIn_{1-x}N$ multilayer nano-heterostructures and performed simulation for strain with different material compositions using the eightband ***k.p*** method. The strain has been simulated for entire model of size 288 nm, but the significant strain has been observed only in the quantum region that lies between 100 nm and 188 nm. For all models under simulation, the strain in the quantum region is found to be tensile along both x and y directions, while compressive in nature along z-direction. The correlation between strain and bandgap for the structures has also been reported. The Results presented in the work may be beneficial for entire opto-electronic community.

We have also studied the energy band profile, potential variation, and electron–hole densities along with the space charge densities at the interfaces of GaN/AlGaN, InN/AlInN and InN/GaInN for the simulated heterostructures without external potential applied and it can be expected that the multilayer nano-heterostructure of GaN/AlGaN, InN/AlInN and InN/GaInN having interested regions in between 100 and 196 nm can be applicable for a particular device application. The energy band structure and potential distribution are found to have less variations within the active quantum region (100–188 nm) while more variations within the quantum regions (50–100 and 188–238 nm). More observable effects are observed in the space charge densities and hole densities within the active quantum regions while electron densities were found to vary in both regions. These results will lead to the new nano opto-electronic device for a particular application in the emerging areas of nanotechnology.

Our simulated results show that the values of bandgap for simulated model of $GaN/Al_xGa_{1-x}N$ multilayer nano-heterostructure decreases from 3.138 eV to 1.485 eV with increase of mole fraction of Al from 10% to 70%. Similarly, for the model of $InN/Al_xIn_{1-x}N$, the values of bandgap decreases with increase of mole fraction of Al from 10% to 70% from -0.138 eV to -3.985 eV and for the model of $InN/Ga_xIn_{1-x}N$, the values of bandgap decreases from 0.266 eV to - 1.485 eV with increase of mole fraction of Ga from 10% to 70%. These results can be observed in table 1, 2 and 3 in chapter 4 which shows, the variation of energy bandgap with Al and Ga mole fractions in $GaN/Al_xGa_{1-x}N$, $InN/Al_xIn_{1-x}N$ and $InN/Ga_xIn_{1-x}N$ multilayer nano-heterostructures respectively. Thus the

bandgap of these heterostructures can be changed by changing Al or Ga mole fraction as desired for the particular device application. This provides sufficient bandgap discontinuity to have electrical confinement of carriers in nitride heterostructures. The bandgap in $GaN/Al_xGa_{1-x}N$ decreases with increase of Al mole fraction, but remains positive, while in $InN/Al_xIn_{1-x}N$ and $InN/Ga_xIn_{1-x}N$ bandgap decreases with increase of Al and Ga mole fraction and become negative showing the increasing metallic nature.

For potential distribution, it is observed that for simulated model of $GaN/Al_xGa_{1-x}N$ multilayer nano-heterostructure in the region lying between 50 nm to 100 nm the value of potential is going on increasing with Al-composition and in active quantum region the range of potential distribution is also increasing with Al-composition, which may be due to alignment of Fermi levels of different semiconducting material to achieve the condition of equilibrium. Similar results are observed for the simulated model of $InN/Al_xIn_{1-x}N$ and $InN/Ga_xIn_{1-x}N$ multilayer nano-heterostructure. With the calculation of potential distribution, the electric field distribution can be calculated throughout the heterostructure, by knowing which the desired device can be designed.

The simulated results also show that the space charge density and hole density increases with increasing mole fraction of Al and Ga in the simulated model of $GaN/Al_xGa_{1-x}N$, $InN/Al_xIn_{1-x}N$ and $InN/Ga_xIn_{1-x}N$ multilayer nano-heterostructure. Moreover, the value of electron density is decreasing with mole fraction of Al and Ga in the simulated model of $GaN/Al_xGa_{1-x}N$, $InN/Al_xIn_{1-x}N$ and $InN/Ga_xIn_{1-x}N$ multilayer nano-heterostructure. It is because, the semiconductors taken in this work are p-type having holes as majority carriers and electrons as minority carriers, the density of electrons is, therefore, negligible in comparison to hole density and can be observed in chapter-4. It is also observed, that the hole density increases in the active quantum well region with increase in Al concentration The large internal polarization field in the heterostructure results in the formation of the electron and hole well at separate interfaces, which means the separation of the electrons and holes in space, thus the direct recombination of the electron–hole pairs is reduced and the lifetime of the light induced carriers is corresponding long. Therefore good responsivity in GaN/AlGaN, InN/AlInN, and InN/GaInN multilayer heterostructure based photoconductive detector can be expected.

Future scope of the work

In this work, we have presented the proposed model and performed 1-D simulation for GaN/$Al_xGa_{1-x}N$, InN/$Al_xIn_{1-x}N$ and InN/$Ga_xIn_{1-x}N$ multilayer nano-heterostructures for strain with different material compositions and also studied the energy band profile, potential variation, and electron–hole densities along with the space charge densities at the interfaces of GaN/AlGaN, InN/AlInN and InN/GaInN for the simulated heterostructures without external potential applied.

Although some parameters of multilayer nano-heterostructure have been discussed, but keeping in view its applications in the area of nano-optoelectronic devices such as LASER, still to be computed. The parameters that can be studied in future, being responsible for lasing action of multilayer heterostructures, are as follows:

- Quasi Fermi levels in the respective bands.
- Behavior of refractive Index change with carrier.
- Behavior of differential gain.
- Behavior of anti-guiding factor being responsible for material gain associated with the structure.
- Confinement factor associated with quantum well.
- Optical gain or material gain associated with the structure.
- Model gain.

By knowing these parameters, the multilayer nano-heterostructures based nano-opto-electronic devices could be designed which will be very useful in the optical fiber based communication systems.

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