Doping effect numerical comparison of band gap energy and active region range for GaN and GaAs based semiconductor

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Abstract. This work reports the effect of doping concentration on the energy-band structure of semiconductor materials. The research focuses on the resultant values of bandgap energy and its depletion region (length/area), based on the initial concentrations of doping which are the donors and acceptors. The energy-band diagram is simulated by initializing the various materials’ properties of Gallium Nitride (GaN) and Gallium Arsenide (GaAs), and solving the Poisson’s equation derived from Maxwell’s equation. The equation is solved by applying the finite difference method (FDM) and using the Newton-Raphson method. Both of these materials are compared with different doping concentrations ($1x10^{13}-1x10^{17}$ cm$^{-3}$). Taking the GaAs properties as the controlled variable, the band structure is validated with literature findings. The measured band gap energy of GaN changes from 1.52eV to 7.6689eV, and GaAs, from 1.1330eV to 5.6431eV. It increases with the proportion to the doping concentration increments. However, when obtaining both of the spatial active regions for GaN and GaAs, it reduce from $(1.9990\mu m-0.0790\mu m)\times1\mu m^2$ and from $(1.9990\mu m-0.0890\mu m)\times1\mu m^2$ respectively. The findings show the effect of doping concentration on the semiconductor energy-band structure. Thus, the numerical system is expected to be used as the determination of the internal quantum efficiency, and the output spectrum of light-emitting diode (LED) chip.

1. Introduction

As the modernized semiconductor developments such as light-emitting diodes (LED), solar cells, and laser diodes are globally demanding, realizing the physics behind the epitaxial technologies that are precise in its configuration, chemical composition, and doping properties, is importantly-beneficial. To aid in the understanding of the mechanism of these devices, certain computational modelings have been developed [1]–[3]. Recently, there are several methods that focus on the thermoelectric properties, the effective mass of carries, piezo-polarization effects, heterostructure configuration, etc. are being considered to the semiconductor’s mechanism [4]–[7]. Generally, most of the dynamical mechanism of the carriers are connectively explained via its energy band structure (EBS) or deductively conclude by its efficiency calculation, [7], [8].

Yet, the effects of doping which are the donors and acceptors carrier of the semiconductor, to the overview of EBS are still required thorough explanation involving semiclassical calculation. Recently, K. P. Misra et.al. and A.M. Robert et.al., presented new interesting modelings to consider for the bandgap energy (BE) comprehension [5], [9]. BE can be calculated based on EBS. Similarly, the
depletion region (DR) is one of the variables that can be deduced from the overview of EBS as well. Nevertheless, their correlations with the doping concentrations are vague. Thus, in this ongoing research, we are motivated to focus on both of these properties. The description of the numerical simulation is explained by introducing the modeling and approximations used to understand the main inquired variables, the BE, and the DR.

2. Numerical Model and Simulation Parameters

2.1. Drift-Diffusion Model and Approximations.
Understanding the overview of the dynamical mechanism inside a semiconductor would be possible by constructing and comprehending the EBS. To construct the EBS, the well-known modeling, the Drift-Diffusion model (DDM) is used. Generally, the complete (currently) DDM requires 3 fundamental equations related to the semiconductor electricity principals which are the current equations, continuity equations, and Poisson’s equation. Where the 2 former equations are applied to the latter Poisson’s equation, and then solved by making use of the finite difference method (FDM) and Newton-Raphson method. The DDM has been widely used as previous literatures for analysing and solving problem in semiconductor field [1], [10], [11].

The DDM is initiated by approximating the semiconductor to a homogenous media, imposing conditions at the boundary of the epi-layer with 0 and built-in (electric barrier) potential at the start of n-type and at the end of p-type of the semiconductor. The most important approach that is taken in is that the model is reduced to a 1-D model and considering that the carriers evolve homogenously at each specific nodal point on the x-axis through the p-n region. The illustration of Fig. 1(a) shows the epi-layer starts from the initial point in the n-type and ends with the final point in the p-type of the semiconductor. Fig. 1(b) is cut from a single nodal point of the p-n region along the x-axis, where the homogeneity is imposed across this surface area.

![Diagram](image)

**Figure 1.** Schematic diagram of the P-N region where (a) 3D view of the region and (b) is the area of a single nodal point along the x-axis.

2.2. Main Inquired Variables.
The EBS is based on the valence and conduction band of the semiconductor where both of the bands are derived from DDM. Taking the length along the semiconductor x-axis as the domain for the bands, they are formulated as the following

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\[ E_v(x) = k_B T \ln \left( \frac{p(x)}{N_v} \right) + q \varphi_p(x) \]  
\[ E_c(x) = q \varphi_n(x) - k_B T \ln \left( \frac{n(x)}{N_c} \right) \]  

Where \( E_v \) and \( E_c \) are the valence and conduction band respectively, \( p \) and \( n \) the holes and electrons concentration, \( \varphi_p \) and \( \varphi_n \) are the quasi-Fermi levels, \( k_B \) is the Boltzmann’s constant, \( q \) is the single carrier charge, \( T \) is the absolute temperature, and \( N_v \) and \( N_c \) are the effective density of states (DOS).

From here, one can directly calculate the bandgap energy, \( E_g \). Since the homogeneity is conserved, the mean value of the calculated bandgap is representing the whole semiconductor. The two bands are correlated via the expression

\[ E_c = E_v + E_g \]  

The depletion region (active region) of the semiconductor is the space where the recombination between the carries occurs. The region is determined in the integral form

\[ R = \int_{S_1}^{S_2} dV \]  

\[ \left| \frac{d}{dV}(E_c(V), E_v(V)) \right| \geq \delta \]  

, where \( S_1 \) and \( S_2 \) must satisfy

\[ |E_v((S_1, S_2) \pm \Delta S)| \geq \delta; |E_c((S_1, S_2) \pm \Delta S)| \geq \delta \]  

\( \delta \) is the minimum energy of recombination that occurred in a semiconductor, \( V \) is the volume of the p-n region, and \( S_1 \) and \( S_2 \) are the nodal points closest to the boundary of where the recombination occurs, \( \Delta S \) is the length between 2 consecutive nodal points on the surface. Based on the visualization in Fig. 1, the surface areas normal to the x-axis are equally constant. This led to a simpler way to determine the region via the following form

\[ A \int_{x_1}^{x_2} dx \]  

\( A \) is the surface area of the p-n region normal to the x-axis. \( x_1 \) and \( x_2 \) are the nodal points closest to the end of p and n region respectively where it must satisfy a similar condition just like \( S_1 \) and \( S_2 \), with \( x_1 \) and \( x_2 \).

In Table 1, the parameters that are involved, are tabulated. The simulation was conducted in the GNU Octave environment. The simulation is subjected to calculate the bandgap energy and active region, based on different values of doping concentration, \( N_a \) the acceptor concentration, and \( N_d \) the donor concentration which is explained in the next section. The results of two different materials, GaN and GaAs are compared in the next section as well. Where initially, the validation was done by the comparison of GaAs’s EBS in [10] (Appendix B).
Table 1 Simulation parameters for GaN and GaAs at \( T = 300K \)

| Properties                                      | GaAs [Ref] | GaN[Ref] | Units       |
|------------------------------------------------|------------|-----------|-------------|
| Intrinsic carrier concentration, \( n_i \)     | 1.74e6[p]  | 1.9e-10[s]| cm\(^{-3}\) |
| Effective DOS in Conduction Band, \( N_c \)     | 4.4e17[p]  | 2.3e18[s] | cm\(^{-3}\) |
| Effective DOS in Valence Band, \( N_v \)       | 9.4e18[p]  | 1.8e19[s] | cm\(^{-3}\) |
| Electron Mobility, \( \mu_e \)                 | 4000[ph]   | 1800[s]   | cm\(^2\)/(Vs) |
| Hole Mobility, \( \mu_h \)                     | 400[ph]    | 30[s]     | cm\(^2\)/(Vs) |
| Non radiative time constant, \( \tau_n \)      | 10e-12[ph] | 1e-8[s]   | s            |
| Relative dielectric constant, \( \epsilon \)   | 13.18[ph]  | 8.9[s]    |              |
| N-type surface area\(^1\)                      | 1.0        | 1.0       | \( \mu \) m |
| P-type surface area\(^1\)                      | 1.0        | 1.0       | \( \mu \) m |
| Thickness                                       | 1.0        | 1.0       | \( \mu \) m |

DOS – Density of states
\(^1\)Surface area is normal to the x-axis

3. EBS, bandgap energy, and depletion region

The value of doping concentration, \( N_a \) and \( N_d \), of the simulation are varied. For EBS construction, 5 values of doping concentration were chosen. But for the bandgap energy and depletion region calculations, 8 values were chosen. The value of both acceptor and donor concentrations are equally changed. While maintaining the clear trend of the graph in each figure in this section, they are reduced from their original size (Appendix A). Detailed explanations are provided in the next subsections.

3.1. Energy band structure

The EBS of both GaN and GaAs are constructed based on 5 different values of doping concentration, changed according to the colour from red \((N_a, N_d = 1 \times 10^{13}\text{cm}^{-3})\), yellow \((N_a, N_d = 1 \times 10^{14}\text{cm}^{-3})\), green \((N_a, N_d = 1 \times 10^{15}\text{cm}^{-3})\), blue \((N_a, N_d = 1 \times 10^{16}\text{cm}^{-3})\) and black \((N_a, N_d = 1 \times 10^{17}\text{cm}^{-3})\) in increasing order. All of the lines with more than 0 energy are the conduction bands, while the rest are the valence bands.
Comparing figure 2(a) and 2(b), it shows that both of them have a similar trend where visually, the red- and yellow-colored bands do not show significant depletion region. Green-, blue-, and black-colored bands have their depletion region clearly to be seen with black as the most significant among them. Another noticeable difference is, the conduction and valence bands in (a) are generally close to each other, with the largest difference of ~3.5eV, compared to the difference of conduction and valence bands value in (b), the largest difference is ~5.0eV. This shows that GaN has higher difference compared to GaAs, which is true according to findings of GaAs (1.42eV) that are lower than GaN (3.42eV) [12], [13].

The next 2 subsections discuss in detail regarding the BE and DR that changes with 8 different values of doping concentration. Where the increment of doping concentration is set to be halved (multiple of 5) of the increment for EBS construction (multiple of 10).

3.2. Bandgap energy

![Figure 3. The band energy against the doping concentration where (a) is GaAs and (b) is GaN.](image)

The BE values of each different doping concentration are calculated based on the average difference, between the valence and conduction band on each nodal point. The data extracted from Figure 3 are tabulated in Table 2.

| Doping Concentration (cm\(^{-3}\)) | GaAs \(E_g\) (eV) | GaN \(E_g\) (eV) |
|-----------------------------------|------------------|------------------|
| 1e13                              | 1.1330           | 1.5215           |
| 5e13                              | 1.7692           | 2.3989           |
| 1e14                              | 2.4083           | 3.2765           |
| 5e14                              | 3.0524           | 4.1546           |
| 1e15                              | 3.7015           | 5.0336           |
| 5e15                              | 4.3503           | 5.9124           |
| 1e16                              | 4.9974           | 6.7908           |
| 5e16                              | 5.6431           | 7.6689           |

The changes in GaAs (red) BE are much less drastic than in GaN (blue) though, at the lowest doping concentration, the bandgap energies are close to each other. At low doping concentrations, both of the bandgap energies show a drastic increase when the doping concentrations increase as well, but at the higher values of doping concentrations, the changes are smaller. The trend of both graphs in (a) and (b) shows that the changes of bandgap energies lead to their saturation values.
The increment of BE due to the increment of doping concentrations is due to the increment of total carries in the semiconductor. This is due to the changes in average electric potential inside the p-n region. The saturation occurs as the presence of unnecessary extra carriers for recombination that leads to current overflow. Yet, based on Figure 3 and Table 2, different material of intrinsic semiconductor will have a different saturation point where this is true comparing to the original BE values of GaN and GaAs [12], [13]. Nevertheless, a more thorough fundamental physical investigation is required for these behaviors to be well-understood.

3.3. Depletion Region

![Depletion Region Diagram](image)

**Figure 4.** The depletion region against doping concentration where (a) is GaN and (b) is GaAs

The calculation of the DR is based on different concentration values. As it was explained in Section 2, the DR is the space where the recombination of carriers occurs which is why it can also be called the active region. The thickness (x-axis) of p-n region is equal to 1μm (p-region) + 1μm (n-region). Figure 4(a) and (b) show that both GaN (blue) and GaAs (red) have a similar trend where at low-level doping concentration, the region covers most of the p-n region. As the doping concentrations are increased, the DR decreases rapidly and saturated with the limit approaching 0. Based on the constant surface area normal to the x-axis of 1μm², the tabulated data in Table 3 shows the results clearly.

| Table 3. DR of GaN and GaAs result from doping concentrations change |
|---------------------------------------------------------------|
| **Doping Concentration (cm⁻³)** | **GaAs (μm x 1μm²)** | **GaN (μm x 1μm²)** |
|---------------------------------|----------------------|---------------------|
| 1e13                            | 1.9990               | 1.9990              |
| 5e13                            | 1.5890               | 1.9990              |
| 1e14                            | 1.2710               | 1.9990              |
| 5e14                            | 1.0230               | 1.0730              |
| 1e15                            | 0.6060               | 0.5880              |
| 5e15                            | 0.3320               | 0.3090              |
| 1e16                            | 0.1740               | 0.1580              |
| 5e16                            | 0.0890               | 0.0790              |

Referring to Table 4, GaN can maintain higher values of DR when the doping concentrations are low, but it starts to decrease rapidly at doping concentration $\geq 5 \times 10^{14}$ cm⁻³. Then as the doping concentration is increased further, $DR_{GaN}$ becomes smaller than $DR_{GaAs}$. Nevertheless, it can be accepted here that, GaN can withstand a higher current density environment compared to GaAs. This occurs when GaN has lower intrinsic carrier concentration compared to GaAs, so it can receive more dopants while
maintaining its active region, initially. An extensive thorough investigation regarding the fundamental of material science should be done to clearly explain this behavior.

The effects of doping concentration on the BE and resulting DR of semiconductors have been investigated. The BE increases rapidly while the DR decreases drastically when the doping concentrations increase until both resulting variables reached their saturation values. Any increment of doping concentration would not affect both of them anymore. This is true for both of the materials.

Furthermore, by applying these effects to the light-emitting diode (LED) and solar cells semiconductor, one will realize the importance of investigating them. Firstly, the efficiency of LED mainly depends on the recombination process. The changes in DR will affect the recombination process greatly because the region where the recombination process has taken place, is changing rapidly with the changing of doping concentration [8],[14],[15]. Secondly, the BE determines the photoluminescence of LED as well. The color of light emitted depends on its wavelength produced by the LED. Based on the energy spectrum of light wavelength, the color of visible-light changes with different wavelengths of light-wave. This can be compared with the blue-LED finding [16], where the ultraviolet-LED (UV-LED) of GaN emits the blue-colored light by having the Indium as its dopant (making its bandgap energy lower than the original UV-LED level).

The visual overview of these behaviors can be seen in the EBS that is based on DDM. This is because it shows a whole picture of the changes in the DR and BE. Undoubtedly, EBS with DDM-based is comprehensive as it considers various dynamic principles related to the epitaxial layer’s materials, such as the effective mass of carriers, the effective density of states of the bands, Fermi energies, electrons piezo-polarization, etc.

4. Conclusion
A numerical simulation that study the correlations between BE and DR with the doping concentration based on GaAs and GaN materials properties, has been done. They were deductively derived from the process to construct EBS which are based on different doping concentration values as well. Both of GaN and GaAs behave differently when the doping concentrations are increase, BE increases significantly until it reaches a saturation value. On the contrary, DR decreases drastically when doping concentration are increase, where it can reach to 0 value of active region where recombination process would unlikely occur. The changes of BE and DR as the doping concentrations change for GaN are much larger compared to GaAs. Thus, this clearly shows that the donor and acceptor carriers in semiconductor affect the BE and DR.

One must realize that using DDM, one can construct, calculate, or provide numerous information aside from EBS. In other words, DDM is not restricted or limited to EBS discussion only. Yet for now, our research can achieve fruitful findings by merely discussing the EBS. Nevertheless, these preliminary findings requires a more extensive discussion that are based on the carriers mechanism or the fundamental of solid state physics to achive much more clarity than the ongoing study.

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Appendices

Energy Band Structure

Figure 5(a). The energy band diagram of GaAs against the doping concentration

Figure 5(b). The energy band diagram of GaN against the doping concentration

Bandgap Energy

Figure 6(a). The band energy of GaAs against the doping concentration.

Figure 6(b). The band energy of GaN against the doping concentration.

Depletion

Figure 7(a). The depletion region of GaAs against the doping concentration

Figure 7(b). The depletion region of GaN against the doping concentration
Validation

The simulation was done in Octave environment and referred to the manuscript [10]. There are various equations involved to construct the EBS and calculate the valence and conduction bands, such as the discrete form of the Poisson’s equation, Bernoulli’s equation, conduction and valence bands equations, carriers concentration equation etc. Since the calculation of valence band is directly calculated with bandgap energy difference to the conduction band or vice-versa, Figure. 5 shows the ratio between the simulated and referred data of the conduction band.

![Figure 8](image.png)

Figure 8. The ratio of the simulated conduction band to the referred conduction band values.

Based on the Figure 5, the highest value of ratio is about 1.22 and the lowest is around 0.91. Where the rest of ratio values are close to the value 1, which indicate the similarities between the referred and simulated data for validation. The parameters used in the validation are the same in Table 1 and both of the dopant concentration $N_a$ and $N_d$ of $1\times10^{16}$cm$^{-3}$ are set. The referred manuscript used the MATLAB software to simulate the data.

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