Mathematical Analysis of the C-V of Nanowires Based on Si and GaAs

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Abstract. In this study the electrical properties of the GaAs/Si radial heterojunction by measuring them at various temperatures of 50 K to 500 K separated by 50 K at a time and considering the values of band gap narrowing (BGN), built-in potential, band gap difference between GaAs and Si, capacitance-voltage (C-voltage) curves. Precisely, we study shell radii 500 nm and 1000 nm in the structure. We find that the thickness of the depletion region of the GaAs/Si radial heterojunction increases with temperature. The BGN decreases by 2 meV as the doping concentration changes by $2 \cdot 10^{-1}$ to $2 \cdot 10^{-2}$. Furthermore, the capacity power charge of the GaAs/Si radial heterojunction rises by 3 nF with hike in temperature between 50 K and 500 K. The inherent potential of the GaAs/Si radial heterojunction reduces by 1.5 volts with rise in temperature.

1 Introduction

The unabated growth in research concerning semiconductor electronic devices has over the years prompted incredible developments in designing, choice of materials, optimization, and functionality of the gadgets. Several advancements have been made in different fields with the most notable being the development of two-dimensional transistors [1-2], nanowires [3] and the most important development being radial p-n and p-i-n junction structures [4-7]. Radial junctions, specifically radial nanowire junctions, have a number of particular benefits over conventional planar junctions, particularly when incorporated into any submicron nanowire applications [4-6]. Such benefits are an increase in internal and external quantum efficiency [7], lowering the rate of recombination by decreasing the diffusion length, and improving the surface to volume ratio. Radial junctions as a category of junctions have received significant attention during the last twenty years because of their outstanding optical and electronic characteristics as the species that can be easily used in a broad variety of applications, such as photodiodes, optical sensors, thermal and photovoltaic detectors [8], and solar cells [9].

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The main advantages of radial p-n junctions include minimization of optical losses through efficient absorption of light and charge carrier collection that, consequently, increases the conversion efficiency. Besides, the normal orientation of light absorption and carrier transport in these junctions is better in working with high frequency and therefore, these junctions are very effective in working with high speed electronics and wireless communication system.

Besides these benefits, radial junctions are now part of the high-speed photodetectors [10], avalanche photodiods, photovoltaic detectors, gamma-ray detectors, and infrared detectors. Their exceptional efficiency, speed and sensitivity are possible because of their unique structural design that is essential in multiple applications of modern semiconductor. Since their potential is extensive, there is a need to explore the electrophysical characteristics of such junctions, especially ionization processes and the behavior of such junctions in a wide temperature range [11]. The theoretical models and experimental validation play a crucial role in the reliability, performance and the accuracy of these devices.

Although the research on radial p-n and p-i-n junctions has been conducted in large scale, research on heterojunction structure is quite under-researched. This work is focused on the GaAs/Si heterojunction structure, where we give a critical theoretical and analytical analysis of the electrophysical characteristics of heterojunction structure. Using mathematical modelling, we study the behaviour of the n-GaAs/p-Si heterojunction structure, which provides an insight on the behaviour of the structure under different temperatures, and voltages applied. Semiconductor electronic devices have undergone major enhancement in design, materials and use over the years due to continuous research on the same. Some of the most important innovations are two-dimensional transistors, nanowires, and most importantly radial p-n and p-i-n junction structures. Radial p-n junctions have several benefits in comparison to conventional planar junctions, especially in nanowire applications, especially with submicron nanowires, including high internal and external quantum efficiency, low recombination rates (because diffusion lengths are short), and a large surface-to-volume ratio. All these have caused radial junctions to be increasingly popular in a wide range of applications such as photodiodes, optical sensors, thermal and photovoltaic detectors, and solar cells. Such junctions are designed to reduce optical losses and maximize light absorption and charge carrier collection as well as operate at high frequencies, so are well adapted to high-speed electronics and wireless communications systems. Even though radial junctions are well researched, little work has been done on heterojunctions, one of them being the GaAs/Si structure. We are engaged in the present work to analyse the electrophysical properties of the GaAs/Si heterojunction by applying mathematical modelling to examine its behaviour with varying temperatures and applied voltages, which will offer a lot of insights into the performance of the heterojunction as far as various applications of semiconductors are concerned.

2 Materials

2.1 Material and Geometric Parameters

In spite of the emergence of new semiconductor compounds, GaAs is still the main material to be used in optoelectronic devices, and Si is still the most common material with its high development technology and the fact that it is found around the earth in large quantities. According to this view, Si and GaAs were chosen to be used in this study. The cross-sectional image of a chosen a radial p-n junction sample, cut along the Z-axis, is presented in Figure 1. We obtained solutions to radial p-n junction structures in which the p-type core radius and the n-type shell radius were 500 nm and 1000 nm respectively. In which, r is the radial dimension and, respectively, is the densities of ionized donor and acceptor atoms, in the interface of the radial p-n heterojunction in the depletion region.

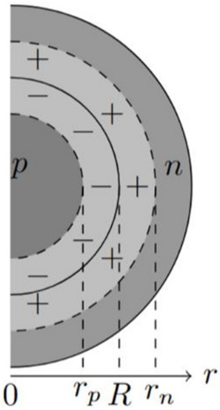


Fig. 1. This figure depicts a 2D cross-sectional view of submicron radial p-n junction structures. The n-type GaAs region is indicated by the light gray area, the p-type Si region by the dark gray area, and the depletion region is represented in very light gray.

In fig. 1, the interval represents the p-type quasi-neutral region (QNR), the interval represents the depletion region in the radial p-n heterojunction junction, the interval represents the n-type quasi-neutral region (QNR).

$$d_{p-h} = \sqrt{\frac{2(\varepsilon_{GaAs}N_A+\varepsilon_{Si}N_D)(\varphi_{bi}(T)-U)}{q\varepsilon_{Si}\varepsilon_{GaAs}\varepsilon_0 N_A \cdot N_D}} \tag{1}$$

The interval represents the depletion region and this depends on temperature and external voltage and is represented by the expression (1): Where, is the built-in potential of the radial p-n junction which is defined by the expression (3), are dielectric constant of the Si and GaAs respectively, electrical constant. Heterojunction p-n structures are fundamental to the development of advanced semiconductor devices, as they significantly improve device performance by optimizing band alignment and minimizing recombination processes. The width of the depletion region is one of the most important things that affects how well these structures work. It directly affects the distribution of charge carriers, the breakdown voltage, and the overall performance of the device. This is especially important for high-frequency and high-power uses, where charge carrier dynamics need to be efficient and the system needs to be strong enough to avoid breaking down. Carefully controlling the depletion region can improve the performance of devices, which is why heterojunction p-n structures are so important in the design of high-performance semiconductor devices. To make devices based on heterojunctions work better and be more reliable, you need to have a good understanding of the depletion region width and be able to control it precisely. The width of the depletion region has a direct effect on how well these devices work, how efficiently they use energy, and how stable they are. This is why it is important to accurately modulate the depletion region to improve device characteristics. Fig. 2 shows how the depletion region changes when the voltage from the outside changes at different temperatures. The data comes from the results of Equation (1). This picture shows how voltage, temperature, and depletion region behavior are all connected. It gives us useful information about how heterojunction-based devices work in different situations. The band gap is one of the most important things to know about semiconductor materials, especially heterojunctions like p-GaAs/n-Si. The difference in the band gaps of GaAs (about 1.43 eV) and Si (about 1.12 eV) at 300K is very important for how these heterojunctions work and what they can do. This difference has a big effect on how charge carriers move, how they recombine, and the junction's overall properties.

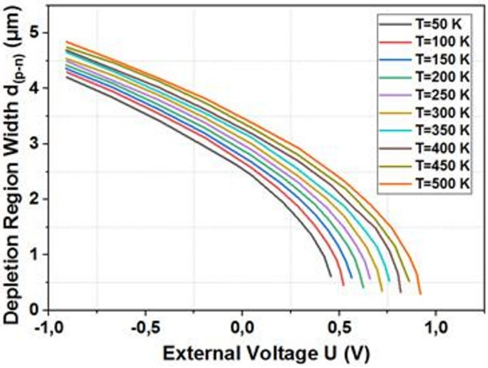


Fig. 2. The differences in the thickness of the depletion region in the p-GaAs/n-Si heterojunction depend on the temperature.

The combination of these properties in GaAs/Si heterojunctions makes them very useful for many different kinds of high-speed electronics and optoelectronic devices.

The expression (2) captures the change in the width of the band gap as a function of temperature variation, providing insights into how temperature influences the electronic properties of the material and, consequently, the performance of the heterojunction.

$$\Delta E_g(T) = \Delta E_g(0) - T^2 \cdot \left(\frac{\alpha_{GaAs}}{T+\theta_{GaAs}} - \frac{\alpha_{Si}}{T+\theta_{Si}}\right) \qquad (2)$$

Where, $\Delta E_g(0)$ is differences of the band gap Si and GaAs at 0 K. θ_{GaAs} and θ_{Si} are Debye temperature GaAs and Si respectively. The Debye temperature can be calculated using the material's properties, but empirical values are often referenced.

$$\varphi_{bi}(T) = \Delta E_g(T) - \frac{kT}{q} \cdot ln\left(\frac{N_A \cdot N_D}{n_{iGaAs} \cdot n_{iSi}}\right) \qquad (3)$$

The charge capacity of the GaAs/Si radial heterojunction depends on the differences in electrostatic potential. The negative charge of the p-type acceptors is balanced by the positive charge of the n-type donors . which is equal to the differential electric capacity derived from the change in charge with respect to voltage. The results of the analytical and mathematical expressions derived above are analyzed in the following section, along with proposed future expectations. Additionally, the obtained results have been calibrated. The charge capacity of the p-GaAs/n-Si heterojunction is expressed by equation (5)

$$C_{p-n} = S\sqrt{\frac{q\varepsilon_{Si}\varepsilon_{GaAs}\varepsilon_0 N_A \cdot N_D}{2(\varepsilon_{GaAs}N_A + \varepsilon_{Si}N_D)(\varphi_{bi}(T) - U)}} \qquad (5)$$

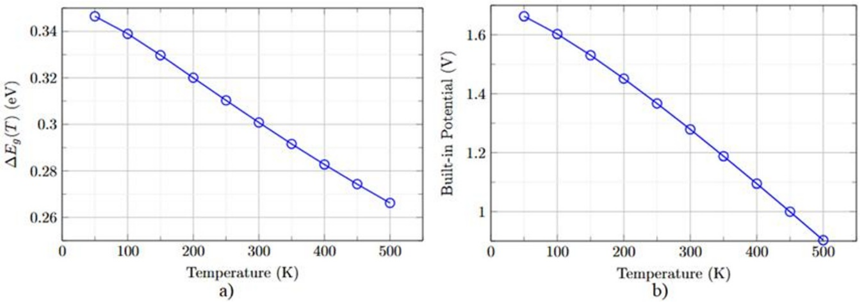
Moreover, the observed decrease in built-in potential by 1.5 volts with increasing temperature provides crucial insights into the stability of the junction. The built-in potential is a key factor in determining the electric field strength within the depletion region, which directly influences carrier recombination and the overall performance of the junction. This behavior shows how important it is to know how temperature affects junction characteristics in order to keep devices running well.

The difference in bandgap energy also changes with temperature, which is important. The bandgap gets smaller as the temperature rises, going from 3.2 eV at 200 K to 3.0 eV at 300 K. This shows that the bandgap is getting smaller. As shown in Fig. 4, this phenomenon, which is common in semiconductors, happens because the lattice vibrations are stronger. As the temperature rises, the bandgap gets smaller, which can change how carriers move. This is very important for how semiconductor devices work.

As the temperature rises, the decrease in built-in potential may lead to a greater thermal generation of electron-hole pairs, which could possibly raise the reverse saturation current. This shows how important it is to manage heat well when designing devices, especially for applications that work in places with changing temperatures. The results show that temperature effects must be taken into account to keep things running smoothly in real-world settings.

This study underscores the complex interplay among temperature, doping concentration, and the electrophysical properties of GaAs/Si radial heterojunctions. The increase in depletion width, the decrease in bandgap narrowing, the increase in charge capacity, and the decrease in built-in potential all give us important information that we can use to improve device performance in different thermal environments.

Future research should concentrate on empirically validating these results and investigating methods to alleviate the detrimental impacts of temperature on the electrical properties of GaAs/Si radial heterojunctions, especially for use in high-performance semiconductor devices.



a) b)

Fig. 3. a) The variations in the band gap change with temperature in the p-GaAs/n-Si heterojunction. b) The built-in potential of the p-GaAs/n-Si heterojunction changes with temperature, going from 50 K to 500 K.

3 Discussion

This part shows and talks about the study's results. A study of GaAs/Si radial heterojunctions over a temperature range of 50 K to 500 K gives us useful information about their electrical properties. Fig. 2 shows that the depletion region gets thicker as the temperature rises and thinner as the external voltage rises. This is an important observation. The behavior can be explained by the natural properties of the semiconductor materials that were used. Thermal energy speeds up the movement of charge carriers as the temperature rises. This lowers the doping concentration in the depletion region. A wider depletion width is needed to keep the charge neutral across the junction. This is necessary for the heterojunction to work properly.

Figure 2 shows how the thickness of the depletion region in p-GaAs/n-Si heterojunctions changes at different voltages, specifically -1 V and 1 V, and at temperatures from 50 K to 500 K in 50 K steps. The findings demonstrate a reduction in the depletion region thickness as voltage and temperature rise. Also, the width of the depletion region has a direct effect on the potential barrier of the p-n junction, which makes the potential barrier change in a noticeable way. This dependence is very important for the performance of devices like thermosensors, photosensors, and solar cells, where precise control over the depletion region is needed for the best performance.

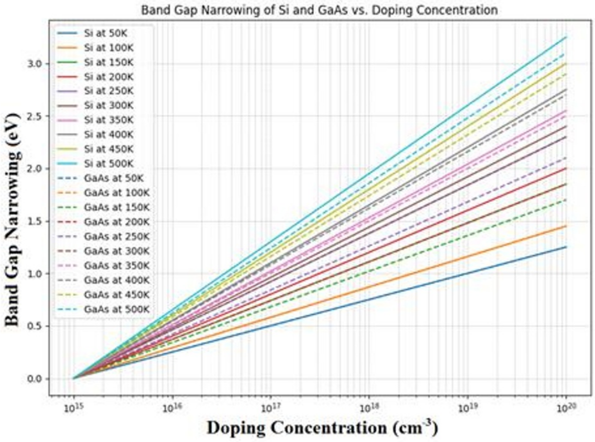


Fig. 4. Band gap narrowing as a function of the logarithmic doping concentration in both n-Si and p-GaAs.

Another important finding is that as the doping concentration goes from 2.10 to 2.18, the band gap narrowing (BGN) goes down by 2 meV. This trend suggests that higher levels of doping make it easier to screen out ionized impurities, which lowers the interactions that cause BGN. BGN has a big effect on how well devices work. For example, a narrower band gap can cause more leakage currents, which can lower the efficiency of devices that use heterojunctions, like solar cells and light-emitting diodes, as shown in Fig. 3. To make high-performance GaAs/Si radial heterojunctions, you need to know how temperature, doping concentration, and band gap narrowing are related. This study's results show how GaAs/Si heterojunctions could help improve semiconductor technology. Manufacturers can make devices that work better, use less energy, and work over a wider range of temperatures and BGN levels by using what they know about these factors. This makes them useful for many different purposes.

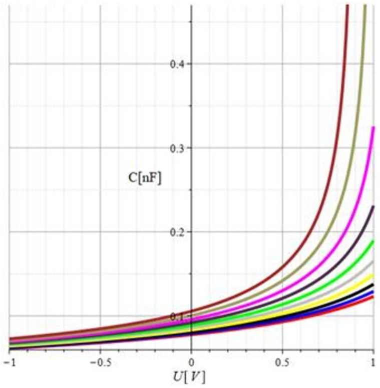
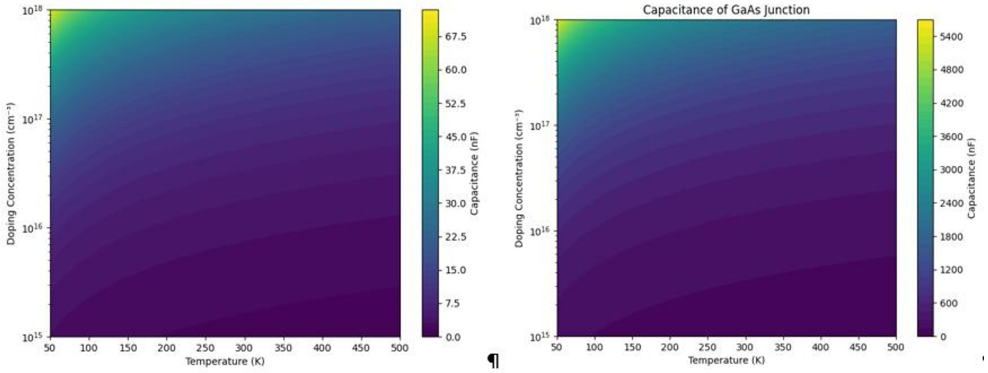


Fig. 5. The charge capacity of the p-GaAs/n-Si heterojunction changes with the outside voltage between 50 K and 500 K. The red line shows the results at 50 K, and the brown line shows the results at 500 K.

The observed increase in charge capacity by 3 nF with rising temperature from 50 K to 500 K reflects the temperature dependence of the capacitance-voltage (C-V) characteristics shown in Fig. 5. When the temperature goes up, carriers gain thermal energy, which makes them more available for conduction. This increases the overall capacitance of the device. This effect is especially important for high-frequency applications, where stable capacitance is necessary for reliable performance. The findings indicate that GaAs/Si radial heterojunctions can be designed to function efficiently over an extensive temperature spectrum. But it's important to think about how the temperature affects other factors, like leakage current and noise, to make sure the device stays stable and works well in different thermal conditions.



(a)¤ ¶ (b)¤

Fig. 6. Capacity depends on Temperature and doping concentration both a) for Si, b) for GaAs.

Fig. 6 shows that the capacitance (C) of both Si and GaAs goes down as the temperature goes up from 50 K to 500 K. The depletion width (W) gets bigger as the built-in potential (Vb) gets smaller. For example, GaAs has a higher capacitance than Si at 300 K because it has a higher permittivity. Effect of Doping Concentration: Capacitance goes up as the doping concentration goes up from 2.10 to 2.10. More doping makes the depletion width smaller, which increases the capacitance. At 1017 cm−3, GaAs has a capacitance that is 10–15% higher than Si's at the same temperature. GaAs has higher capacitance values than Si because it has a higher dielectric constant and a lower intrinsic carrier concentration. GaAs has better capacitance stability over temperature changes than Si. For example, Si's capacitance drops by about 30% from 300 K to 500 K, while GaAs's capacitance drops by only 20–25% in the same range. What this means for applications: Because it has a higher capacitance, GaAs is better for optoelectronic and high-frequency devices. Si is still the best material for semiconductor applications that need to be cheap and easy to scale.

4 Conclusion

In summary, this study offers a comprehensive examination of the electrophysical properties of GaAs/Si radial heterojunctions within a temperature range of 50 K to 500 K, emphasizing the effects of different doping concentrations and shell radii of 500 nm and 1000 nm. Our results show that as the temperature rises, the depletion region thickness also rises. This means that the charge distribution within the junction is better. One interesting thing to note is that the band gap narrowing (BGN) goes down by 2 meV as the doping concentration goes up from $2\cdot10^{15}$ to $2\cdot10^{18}$. This shows how important doping is in changing the electronic properties of the heterojunction. We also discovered that the charge capacity rose by 3 nF with temperature, which suggests that the device works better at higher temperatures. On the other hand, the built-in potential went down by 1.5 volts as the temperature went up, which suggests that the energy barrier for charge carriers went down. These results give us important information about how GaAs/Si radial heterojunctions behave at different temperatures. This is useful for designing and improving semiconductor devices that need to work reliably in a wide range of temperatures.

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