

Impact of Doping Concentration and Temperature on Carrier Mobilities in 4H-SiC Based Semiconductor Devices: A Sentaurus TCAD Simulation Study

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ABSTRACT

This study examines the influence of doping concentration and temperature on carrier mobilities in semiconductor device development. The introduction of small quantities of dopants during crystal growth or device fabrication significantly affects the device's electrical properties. Using the Sentaurus Technology Computer Aided Design(TCAD) modeling tool, the work simulates and evaluates device characteristics, focusing on parameters like electron and hole mobilities. Doping concentration and temperature emerge as crucial factors shaping device behavior in both the epitaxial and bulk regions. Findings show that higher doping concentrations lead to reduced mobility, with electron mobility consistently exceeding hole mobility, underscoring electrons' role as the majority carriers in n-type devices. Schottky and ohmic contacts in different regions further illustrate the impact of doping on electrical properties. Additionally, the study reveals a linear relationship between temperature increases and reduced electron and hole mobilities, attributed to mechanisms such as impurity-induced defects and lattice vibrations. The stability of the detector's performance is emphasized at constant temperatures. Ultimately, this research offers valuable insights for optimizing semiconductor devices and advancing electronic technology.

1.0 INTRODUCTION

Doping in semiconductors device involves introducing a small quantity of foreign atoms, called dopants, into a semiconductor material. This process typically occurs during crystal growth or device fabrication to modify the material's electrical properties(Tan et al., 2022)

Consequently, the influence of doping on the electrical properties of the material is dependent on some important factors such as the type of dopant, its concentration and the method by which dopants are integrated into the crystal structure(Bekaddour et al., 2023).The optimal scenario for doping in a crystal occurs when the lattice structure remains basically intact, with only a fraction of lattice atoms being replaced by the dopant(Puglisi, 2019). Ideally, this occurs when two or more semiconductor materials, either belonging to the same group or different groups in the periodic table are combined to create a compound semiconductor(Owens, 2012). Similar processes take place when fabricating a semiconductor device, introducing active concentrations (N or P type) to the substrate in epitaxial or bulk regions(Idris et al., 2021). When, a doping is carefully performed in a well-defined manner to ensure that the electrical, chemical and structural properties of the material remain unchanged (Popovych et al., 2021). These processes may be

referred to as crystal growth or film deposition (Capan, 2022).

In developing a semiconductor device, Sentaurus TCAD device modeling tool is utilized for the evaluation of its interfacial characteristics. The sentaurus proved to be one of the robust simulation software (Nabil et al., 2020). Simulations are performed to analyze and explore crucial parameters, including electron and hole mobilities in relation doping concentration and Temperature. These parameters play a vital role in understanding the charge transport in the 4HSiC semiconductor Radiation detector(Berger et al., 2022).

2.0 METHOD

Modeling and Simulation of Semiconductor Devices in Sentaurus TCAD is carried out in this study, silicon carbide (4H-SiC) with two distinct surface orientations the silicon-rich face and the carbon-rich face (C-face) was utilized. A uniformly doped epitaxial layer was employed to establish an n-type region, facilitating the formation of a Schottky contact. The substrate featured nitrogen doping with active concentrations of $3 \times 10^{17} \text{ cm}^{-3}$ and $5 \times 10^{20} \text{ cm}^{-3}$. Nickel (Ni) and titanium (Ti) were chosen as contact metals, each applied in a rectangular geometry as also addoted by Garba et al., (2024).

The simulations were conducted using Sentaurus TCAD, a physics-based simulation tool incorporating models for key electronic device parameters (Nabil et al., 2020; Synopsys, 2015). These 2D simulations provided insights into the surface, electrical, and thermal characteristics of the semiconductor device (Parent, 2014; Folkestad et al., 2017).

A rectangular 2D model of a 4H-SiC detector with dimensions $0.25 \mu\text{m} \times 0.21 \mu\text{m}$ was developed within the Sentaurus TCAD environment. The device was designed as an n-type semiconductor, incorporating a nitrogen-doped epitaxial region with an active concentration of $3.0 \times 10^{17} \text{ cm}^{-3}$. This epitaxial layer, measuring $0.25 \mu\text{m} \times 0.075 \mu\text{m}$, was formed on the Si-face of the substrate without an intermediate buffer layer.

Additionally, the substrate region was doped with nitrogen at a higher concentration of $5 \times 10^{20} \text{ cm}^{-3}$, spanning dimensions of $0.25 \mu\text{m} \times 0.2 \mu\text{m}$. Nickel ($0.25 \mu\text{m} \times 0.005 \mu\text{m}$) was deposited on top of the epitaxial layer, while titanium ($0.25 \mu\text{m} \times 0.005 \mu\text{m}$) was applied at the bottom, ensuring proper electrical contact (Garba et al., 2024).

3.0 RESULT

Doping concentration is a key factor in the development of semiconductor devices, significantly affecting

junction characteristics by precisely defining the separation between the epitaxial and bulk regions. In Figure 1, the doping concentration is shown to vary, with values of $3 \times 10^{17} \text{ cm}^{-3}$ in the epitaxial region and $5 \times 10^{20} \text{ cm}^{-3}$ in the bulk region of the semiconductor.

The epitaxial region of the device, illustrated in the blue segment of Figure 1, is doped with a Nitrogen concentration of $3 \times 10^{17} \text{ cm}^{-3}$ and has a thickness of 20 nm. Equally, the red region represents the bulk region of the detector, doped with a Nitrogen concentration of $5 \times 10^{20} \text{ cm}^{-3}$ and a thickness of 180 nm. The distribution of doping concentration at the junction reveals the depletion region, showcasing a drop in doping concentration towards the epitaxial region due to lower doping levels in contrast to the bulk region.

The reduction in doping concentration results in the formation of a Schottky contact between the metal at the top and the epitaxial region, while creating an ohmic contact between the metal and the bottom of the bulk region of the detector. Notably, doping concentration significantly affects device performance by enhancing key electronic properties, such as electron and hole mobility, carrier velocity, and temperature-dependent behavior, as revealed by Stefanakis and Zekentes (2014).

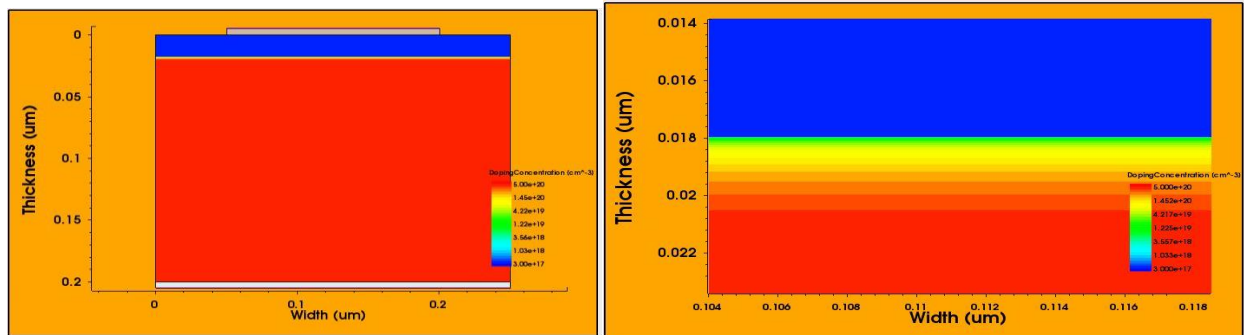


Figure 1: Doping concentration characteristics

3.

1 Carrier (Electron and Hole) Mobilities

This section of the results examines the behavior of electrons and holes at the junction between the metal (Ni) and the semiconductor material (4H-SiC), focusing on relevant physical parameters. The roles of electrons and holes as charge carriers at this interface are vital for the conduction process of the device, influenced by the impurities introduced and the temperature.

Figure 2 illustrates the relationship between electron mobility and doping concentration. The doping

concentration varies at the interface between the epitaxial layer and the bulk region of the simulated device, particularly in areas where the doping concentration differs. The reddish region indicates high electron mobility, while the blue region represents lower mobility. A transitional zone, approximately $0.015 \mu\text{m}$ to $0.025 \mu\text{m}$ thick, is observed between the epitaxial and bulk regions, characterized by a yellow area (a blend of red and blue). This suggests a gradual transition at the interface, with a decline in electron mobility toward the bulk region due to varying doping concentrations. These

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variations at the interface consequently impact the electrical properties of the developed device as also corroborated by Capan & Brodar, (2022).

While exhibiting similar trends, electrons, as the majority carriers, demonstrate a higher mobility of $4.25 \times 10^2 \text{ cm}^2/\text{Vs}$, surpassing the hole mobility of $9.167 \times 10^1 \text{ cm}^2/\text{Vs}$. Figure 2 shows that electron mobility

is highest in the epitaxial region and decreases gradually toward the bulk region, ranging from $4.25 \times 10^2 \text{ cm}^2/\text{Vs}$ to $4.25 \times 10^1 \text{ cm}^2/\text{Vs}$. This decline in mobility at higher doping densities is attributed to increased collisions among electrons, leading to Coulombic interactions. This observation aligns with expectations regarding carrier behavior in semiconductor materials which is in line with findings by Shen (2012) and Spieler (2005).

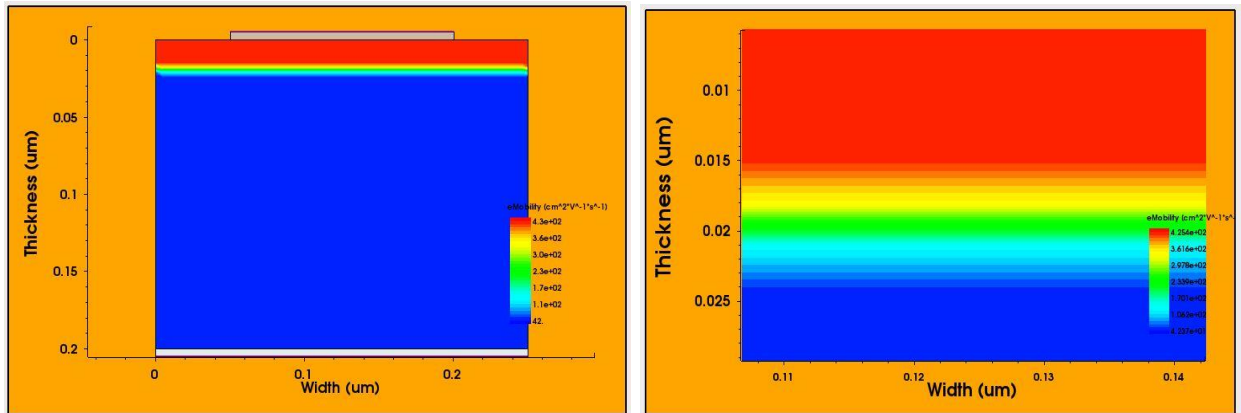


Figure 2: Electron Mobility

As a result, Figure 3 shows characteristics of hole mobility that are similar to those observed for electron mobility in Figure 2. However, the magnitude of hole mobility is lower than that of electron mobility due to the higher effective mass of holes compared to electrons, as well as the predominance of electrons as majority carriers in the n-type device. This indicates that hole mobility is greater in the epitaxial region than in the bulk region, with values decreasing from $9.167 \times 10^1 \text{ cm}^2/\text{Vs}$ in the epitaxial region to $2.781 \times 10^0 \text{ cm}^2/\text{Vs}$ in the bulk region.

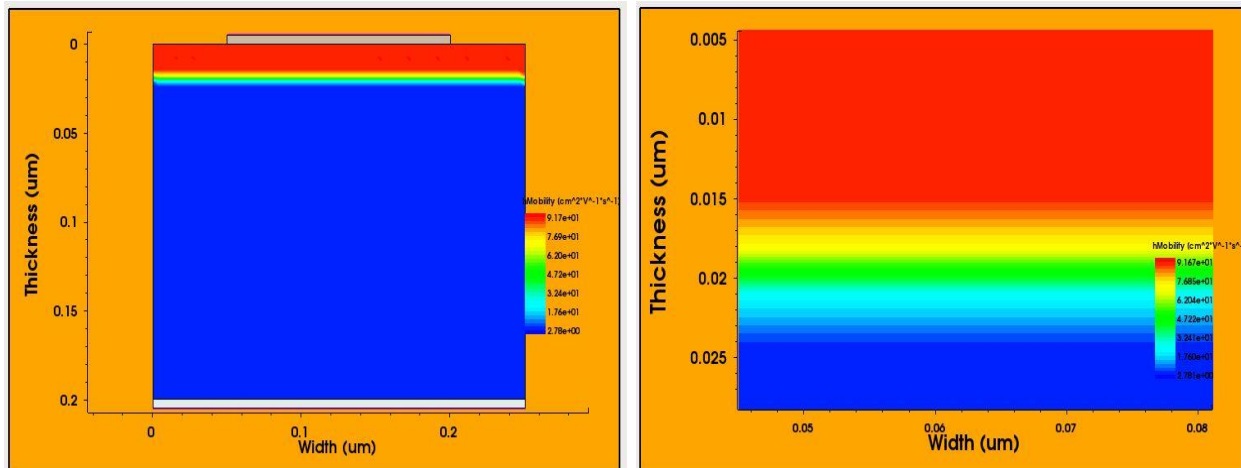


Figure 3: Holes Mobility

Observations from both Figure 2 and 3 indicate that electron mobility is consistently higher than hole mobility. This observation supports the notion that when the device is doped with n-type material, then the electrons serve as the majority carriers. Additionally, it is noteworthy that the effective mass of holes is higher than the effective mass of electrons, a fact supported by Shao, (2021).

In light of these findings, the movement of electrons in one direction and holes in the opposite direction induces the flow of charge within the detector. Furthermore, the relationship between carrier mobilities (i.e., electron mobility and hole mobility) depicted in Figure 4 demonstrates a directly proportional behavior. This alignment suggests that the device is optimal, displaying no defective characteristics. This is attributed to the coordinated movement of holes in the negative direction and electrons in the positive direction, whereas any contrary behavior may result in defective device characteristics.

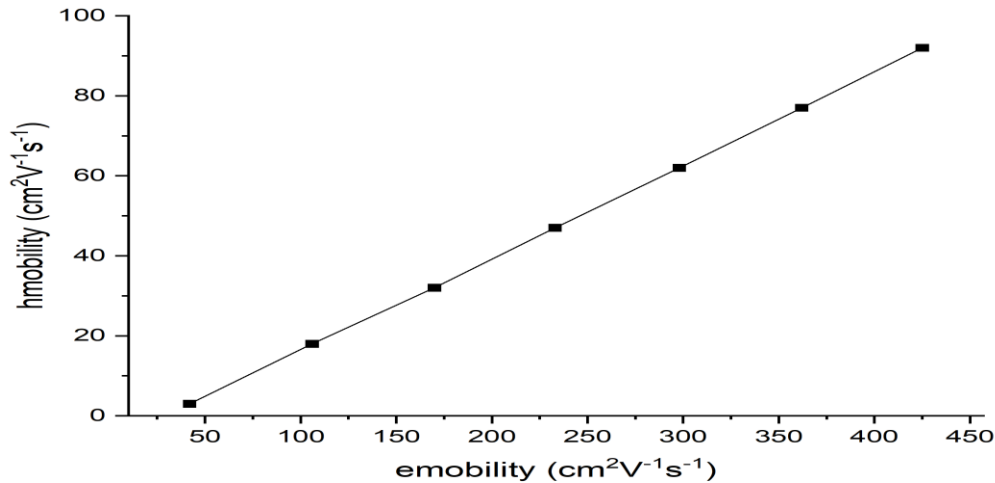


Figure 4: Relationship between Electrons and Holes Mobilities

3.2 Doping Concentration and Carrier Mobilities

The developed detector exhibits homogenous doping, with uniform dopant of the same concentration material (Nitrogen Active concentration) throughout, differing only in magnitude between the Epitaxial and Bulk regions. Another important observation in the device is that an increase in doping concentration leads to a decrease in carrier (both hole and electron) mobility. This decline is attributed to the frequent collisions of charge carriers with impurities, as illustrated in Figure 5. This aligns with the conclusions drawn by Ha et al. (2020).

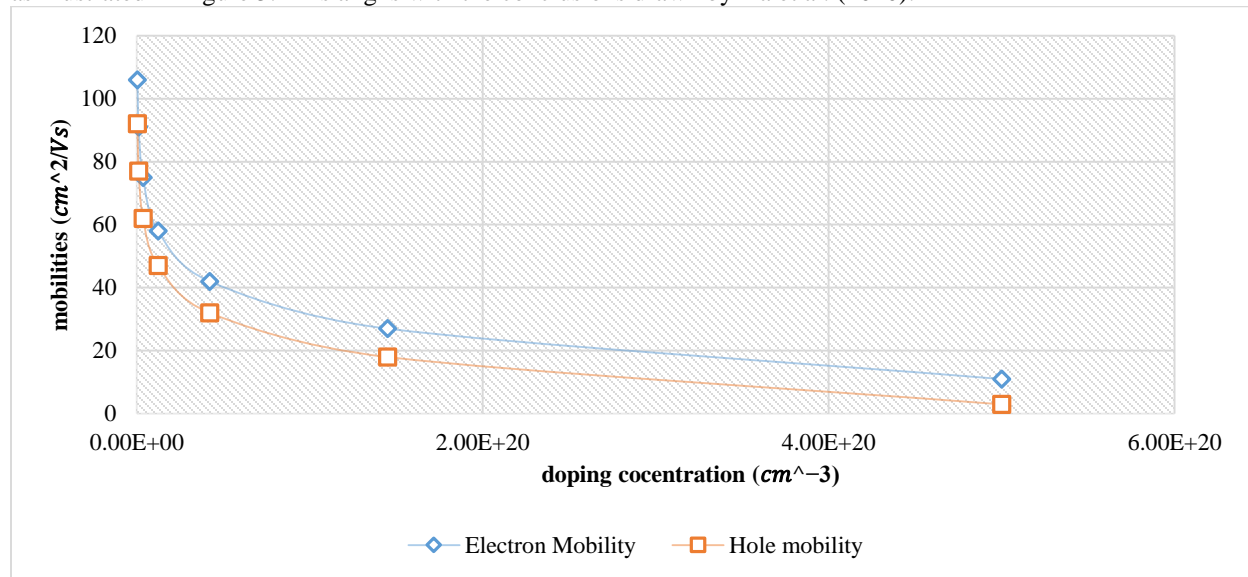


Figure 5: Characteristics of Doping Concentration and Carrier Mobility

Figure 5 illustrates that an increase in doping concentration results in a decrease in carrier mobility, confirming the findings of Tobehn-Steinhäuser et al. (2021). Consequently, it becomes evident that with an increase in doping concentration, the Schottky contact has the potential to change into an ohmic contact. This is due to the reduction in resistance at each doping state.

3.3 Carrier Mobilities and Temperature

Figure 6 presents the mobilities of electrons and holes which are crucial carriers for signal transmission. This study examines the mobilities regarding an increase in temperature ranging from 300 K to 700 K. The results indicate that temperature has a notable impact on both electron and hole mobilities in the simulated device, as depicted in Figure 6. The observed trend reveals a consistent decrease in both electron and hole mobilities with rising temperature, establishing a linear

relationship. This finding aligns with the work of Hamaguchi (2021), which also reports declines in mobility with increasing in temperature.

Several mechanisms, including defects due to impurity and lattice vibrations (phonons), may contribute to this behavior. As temperatures rise, lattice vibrations increase, leading to a decline in carrier mobility, as illustrated in Figure 6. This highlights that the conduction characteristics of the detector remain stable only at a constant temperature, as indicated by Abubakar *et al.*, (2015). The conductivity in the detector decreases as temperature increases, emphasizing that the stability of the detector's performance is reliant on a consistent temperature rather than a fluctuating one, as demonstrated in this study (from 300 K to 700 K). This observation is consistent with the findings of Noor Mohammad et al. (1993).

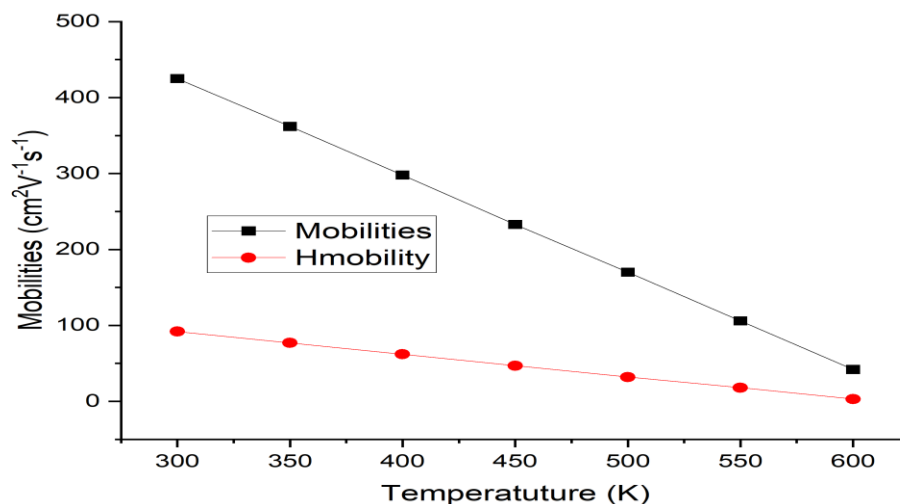


Figure 6: Electrons and holes characteristics in terms of temperature

4.0 CONCLUSION

In conclusion, this study delves into the impact of doping concentration and temperature on carrier mobilities in semiconductor device development. Doping, as the introduction of minute quantities of different atoms (dopants) into a substrate or material during crystal growth or device fabrication, significantly influences the electrical properties of the material. The careful execution of the doping process ensures the stability of electrical, chemical, and structural properties, whether in crystal growth or film deposition.

Sentaurus TCAD modeling tool for the device development is used in which simulations are conducted to assess device characteristics. The concentration of

doping emerges as a critical factor in semiconductor device development, influencing the separation between epitaxial and bulk regions. The intricate relationship between doping concentration and carrier mobility is evident, with high concentrations leading to decreased in both electrons and holes mobilities.

The establishment of Schottky and ohmic contacts in different regions of the device further demonstrates the nuanced impact of doping concentration on electrical properties.

The relationship between carrier mobilities, specifically electrons and holes in a directly proportional manner, affirming the optimal performance of the device. An increase in doping concentration is found to decrease

carrier mobility, offering insights into the potential transition from Schottky to ohmic contact.

Temperature, explored within a range from 300 K to 700 K, emerges as a crucial factor influencing carrier mobilities. The study reveals a linear relationship between temperature and a consistent decrease in both electron and hole mobilities.

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