Abstract—In this study, we designed and optimized the performance of pin junction GaAs/AlGaAs heterojunction nanowire solar cell arrays. It is done by performing coupled optoelectronic simulations to find the optimal doping for the GaAs core and AlGaAs shell, and to see the influence of GaAs and AlGaAs shell thickness and junction positions on the solar cell performance. Further, the impact of different surface effects that exist at the semiconductor interface such as surface traps, surface recombination velocities, and associated lifetime degradation are also investigated. It has been observed that a high core and shell doping is essential to achieve the appropriate band configuration and carrier extraction. Further, it is observed that having a larger doping density is more important than having a larger lifetime. The importance of the thickness and the passivation properties of the radial and axial AlGaAs layer is also examined and it has been observed that having a thick AlGaAs shell at the cost of the i-GaAs region can be detrimental to the performance due to increased local carrier generation and recombination. Finally, the effect of having different Aluminium compositions (on the shell) on the photogeneration inside the nanowire is examined and it has been observed that having a large Aluminium composition can confine most of the photogeneration to the inner GaAs regions, thus potentially allowing for thicker Aluminium shells which can more efficiently prevent surface recombination.

Index Terms—Nanowires (NWs), Radial Solar cells, Photovoltaics, GaAs/AlGaAs Nanowire, Device simulation.

I. INTRODUCTION

SEMICONDUCTOR nanowires (NWs) is a topic of intense research and development these days as they find their application in a wide range of devices, including lasers [1–3], photodetectors [4,5], LEDs [6,7] and solar cells [8–13]. In particular, semiconductor nanowire based solar cells have gained significant attention due to their ability to realize much higher efficiency than conventional thin-film planar solar cells at a lesser cost [14]. The superior performance of the NW photovoltaic devices is attributed to their efficient photon absorption, carrier generation, and carrier transport mechanisms [15,16]. Among various nanowire designs, structures having a radial junction serves as an efficient means to decouple light absorption from carrier extraction [9,17]. In such a junction, the absorption of light primarily occurs in the vertical direction, while the electric field that is present in the radial direction separates the photo-generated carriers in the radial direction. This decoupling of light absorption and carrier separation allows us to have taller structures (which enables more light absorption) and smaller diameter (which reduces carrier recombination and allows better charge separation [18]). Further, due to their smaller diameter, the radial junction nanowires can be easily grown on a large range of lattice-mismatched materials which allows them to attain efficient multi-junction configurations.

For many years, Silicon (Si) due to its low cost has been considered as a prime material choice for realizing thin-film and NW based solar cells, however, Si based solar cells are less efficient as Si is an indirect bandgap material. High efficiency solar cells are made out of direct bandgap III-V materials like Gallium Arsenide (GaAs) [8,19–22] due to their ideal bandgap [23], high coefficient of absorption, and its ability to be implemented in multi-junctions. However, due to their relatively higher cost, III-V based solar cells have been mostly considered only for space-grade applications. Since NWSC can offer efficient performance with lower material usage (GaAs NWSCs have been shown to attain ≥ 92% efficiency just by a height of 3 µm, while indirect bandgap materials need to have much larger heights to attain the same [24]), the cost of the device considerably reduces. Thus, by using NWSCs made of III-V semiconductor materials, high-efficiency cost effective solar cells can be realized that can be used for both terrestrial and space applications.

Though III-V based NWSCs have several advantages to offer, unfortunately, they have not been not commercially successful. It has been shown that surface recombination (caused by traps formed due to dangling bonds from the sudden discontinuation of the semiconductor crystal) present in NWs captures the photogenerated carriers and prevent them from being collected by the metal contacts and thus poses a serious threat in reducing the device efficiency. A study done by Joyce et. al. [25] compared the electronic properties of different III-V based nanowires and they measured picosecond-long carrier lifetimes in GaAs based nanowires, finding that the lifetime of photogenerated carriers is extremely short due to high surface recombination velocity. This indicates the importance of surface passivation in GaAs NWSCs. Different studies have highlighted the importance of adopting proper radial geometry and good surface passivation for NWSC [26,27] to overcome these drawbacks. In particular, for GaAs NWs, epitaxial passivation by AlGaAs is shown to be an effective method to overcome these surface effects [28,29]. It has been demonstrated that AlGaAs (due to their higher bandgap and low absorption coefficient) have less photogeneration and acts as a barrier preventing the carriers generated inside from reaching the surface, thus confining the photogeneration to the inner GaAs regions [29,31].

In this paper, we have performed coupled optoelec-
tronic simulations on radial GaAs/AlGaAs pin heterojunction nanowire solar cell to find the optimal doping and other surface parameters which allows us to achieve the best solar cell performance [26, 29]. Section II looks into the modelling of this solar cell, the different structural and optical parameters, and the material properties used in this study. In Section III-A, a thorough study on doping has been done to find the optimal doping density for GaAs core and AlGaAs shell of this solar cell with the objective to attain proper band energy configuration, carrier separation, and extraction. Section III-B looks into the change in the solar cell’s performance due to the change in lifetime caused by different doping levels. In Section III-C, studies have been done to see the influence of AlGaAs axial and radial shell thickness and junction position along with the influence of different surface passivations (i.e., different surface recombination velocity and their corresponding lifetime), and based on this study, an optimal radial and axial shell thicknesses have been obtained. Further, a study of axial intrinsic GaAs shell thickness has also been done, and its effect on the NW design has been highlighted. In Section III-D, to account for the nanowire height with the existing literature [24], the impact of nanowire height on our solar cell performance is observed. Finally, section III-E observes the effect of different shell Aluminium compositions on the photogeneration inside the NWSC.

II. Modeling and Methods

For our study, we have modeled the nanowire array (NWA) using a single cell GaAs/AlGaAs pin junction heterojunction nanowire solar cell with periodic boundary conditions. A square lattice has been used [32] with the individual cells having a circular cross-section, this is because it is shown that a cylindrical geometry is a good approximation of a more realistic hexagonal geometry [20] and a circular cross section also simplifies the computation because the problem can be reduced to a 2D simulation. The schematic diagrams of our NW is shown in Fig. 1 and Fig. 2. The NW diameter is taken as 180 nm with a duty cycle (D/P) = 0.5, which has been shown to be ideal for optimal absorption and performance of nanowires [18]. The height is taken as 2 µm, as it has been observed that beyond the height of 2 µm, there is no significant improvement in light absorption for direct bandgap materials [24, 26]. In Section III-D we have confirmed that this result holds true for our solar cell as well. The thickness of the GaAs substrate is taken to be semi-infinite according to PML boundary conditions in the FDTD simulations. A cross-sectional figure of photogeneration profile across the nanowire is shown in Fig. 3.

A crucial material parameter that has to be chosen carefully to achieve proper solar cell behavior is the doping density (the doping density controls the carrier inversion and sets the effective band alignment, it also controls the electric field across the junction). In this paper, we have done a systematic study to find the optimal doping density for our NWSC. As the starting point, a similar doping density for both p and n regions were set as 5 x 10^{18} cm^{-3} [26, 27, 33] and also used for AlGaAs passivation layers [29]. Further, higher doping density can be assumed for the n-type substrate to achieve good Ohmic contacts. As the carrier mobility varies with doping density, a concentration-dependent mobility model can be considered for bulk GaAs substrates, however, for nanowires, there has been no systematic study that relates mobility with doping density. Therefore, in our study, we have chosen the value based on previous work by Joyce et al. [25], where the
carrier mobility was measured for GaAs NWs (with doping concentration at around \(10^{16}\) cm\(^{-3}\)). Finally for AlGaAs, we have used mobility given by ref: [34].

The axial and radial AlGaAs shell thickness has been initially set to 20 nm, however, in Section III-C1 and Section III-C2 we have carried out systematic studies to find their most optimal thicknesses. We have used top and bottom contacts for our nanowire [27]. The Auger recombination coefficients, SRH recombination lifetime, and radiative recombination rates are taken to be the same for GaAs and AlGaAs [25][27][29], however, the lifetimes have been varied in some cases during the study (Section III-B, Section III-C2), which has been mentioned accordingly. The various geometrical, optical, and electrical parameters that are used in the simulation are summarized in Table I

For optical modeling, the ‘Lumerial FDTD’ software package with ‘Solar Generation Rate’ analysis group has been used to calculate the light absorption and photogeneration profiles in the NWSC. We have used periodic boundary conditions on all four sides of the single NW unit cell to generate the entire square array. The absorption is calculated from the divergence of Poynting vector \(\mathbf{S}\) as:

\[
P_{\text{abs}} = -0.5 \text{real}(\nabla \cdot \mathbf{S})
\]

This can also be written in a numerically more stable form :

\[
P_{\text{abs}} = 0.5 \text{real} \left( \omega \mathbf{E} \cdot \mathbf{D} \right) = 0.5 \omega \varepsilon^{*} |\mathbf{E}|^2
\]

Where, \(\varepsilon^{*}\) is the imaginary part of permittivity, \(\omega\) is the angular frequency of the incident light, \(E\) is the electric field intensity. Assuming each absorbed photon generates one electron-hole pair, the Generation Rate is given by:

\[
G_{ph} = \frac{\nabla \cdot \mathbf{S}}{2h\omega} = \varepsilon^{*} |\mathbf{E}|^2 / 2h
\]

The complex index of refraction of GaAs and Al\(_{0.3}\)Ga\(_{0.7}\)As have been taken from the Sopra database \(G_{ph}\) is initially calculated using a CW normalization which is then weighted using the AM 1.5 and integrated over the entire spectrum.

For electrical modeling, we have used the device simulation software ‘Atlas’ of ‘Silvaco TCAD’. The different simulation programs that have been used are ‘Blaze’ and ‘Device 3D’ for modeling the semiconductor materials and their properties. ‘Luminous 2D’ and ‘Luminous 3D’ for doing the optoelectronic simulations. Atlas solves Poisson’s equations and carrier continuity equations self-consistently. Further equations are still required to specify the physical models for various recombination mechanisms and carrier transport. Earlier studies based on the Boltzmann transport theory have shown that the current densities in the continuity equations may be approximated by a drift-diffusion transport model [35][36]. Since we are working with heterojunctions, the Drift-diffusion model used here is modified to account for the non-uniform band structure. The procedure for the same can be found on [35][37].

We have also taken into account thermionic emission-dominated current [36][38][39].

| Parameter | Values (GaAs) | Values (AlGaAs) |
|-----------|--------------|-----------------|
| Band Gap (eV) | 1.42 | 1.80 |
| Affinity (\(\chi\)) (eV) | 4.07 | 3.74 |
| Radiative recombination coefficient \((C_{\text{rad}})\) (cm\(^3\)s\(^{-1}\)) | \(7.2 \times 10^{-10}\) | \(7.2 \times 10^{-10}\) |
| SRH lifetimes \((\tau_{n}, \tau_{p})\) (ns) | 1 * | 1 * |
| Auger recombination coefficient \((A_{n}, A_{p})\) (cm\(^6\)s\(^{-1}\)) | \(1 \times 10^{-30}\) | \(1 \times 10^{-30}\) |
| Electron mobility \((\mu_{n})\) (cm\(^2\)V\(^{-1}\)s\(^{-1}\)) | 1200 | 2300 |
| Hole mobility \((\mu_{p})\) (cm\(^2\)V\(^{-1}\)s\(^{-1}\)) | 100 | 146 |
| Electron relative effective mass | 0.067m\(_{0}\) | 0.0919m\(_{0}\) |
| Hole relative effective mass | 0.485m\(_{0}\) | 0.690m\(_{0}\) |
| Doping concentration \((n)\) | \(1 \times 10^{18}\) * | \(5 \times 10^{18}\) * |
| Axial shell thickness \((t_{A}\) respectively)(nm) | 20* | 20* |

* Parameters are varied as per the study. The change in the value is mentioned during each study.
** For core-GaAs material.

The recombination paths in this study include Radiative recombination, Auger recombination, and Shockley–Read–Hall (SRH) recombination [4]. The values of the respective recombination coefficients can be found in Table 1.

In the SRH model, we have assumed the interface between GaAs and AlGaAs to be perfect without any additional recom-
bination centers, which can be achieved by lattice-matched epitaxy [40]. The surface effects have only been considered for the interfaces between air and the NW. Therefore, for the NW surface, the surface band bending due to surface traps has been included.

For simplicity, we have chosen the trap density as the same for electrons and holes \((N_{TD} = N_{TA})\), and all were assumed to be at the intrinsic Fermi level. The e-h capture cross-section is not explicitly available, so a typical average value is taken from ref: [41]. The presence of surface traps now acts as surface recombination centers. The surface recombination rate has also been modelled \([\] and \(S_n\) and \(S_p\) are the surface recombination velocity (SRV) for electrons and holes, respectively. For our study, we have kept the same SRV of electrons and holes, and three different values of SRV have been used for different levels of passivation, which have been mentioned accordingly in the upcoming sections.

Finally, we have assumed Ohmic contacts for metal electrodes which are implemented as simple Dirichlet boundary conditions. This completes the modeling of our NWSC. In section III, we will look into the analysis and the results of our study.

III. ANALYSIS AND RESULTS

A. Effect of doping

It can be seen from the literature that for conventional p-n junction solar cells, the doping densities for the p and n region should be medium-to-high for efficient carrier extraction. Following this trend, previous work done with GaAs/AlGaAs NWSCs has used doping densities of the order \(10^{17} - 10^{18}\) cm\(^{-3}\) however, no systematic studies were carried out to determine how the doping densities influence the performance of these solar cells. Therefore, in this section, we intend to check the influence of the various core-shell doping densities and obtain the optimal doping densities for the efficient performance of GaAs/AlGaAs NWSCs. The procedure followed here is inspired by the work done by Li et. al. [26] for GaAs nanowire solar cells.

To save computation time, we made a 2D model for our NW solar cell (the final results were once again verified for the 3D solar cell model and used in the later sections).

The axial and radial shell thickness were fixed at 20 nm. The surface is given a good passivation (SRV = 1300 cm.s\(^{-1}\) and \(N_{TD} = N_{TA} = 2 \times 10^{11}\) cm\(^{-2}\)). The carrier lifetime is taken as 1 ns and is assumed to be the same for both electrons and holes. The solar cell efficiency is then calculated by varying the doping concentration from \(1 \times 10^{16}\) cm\(^{-3}\) to \(5 \times 10^{18}\) cm\(^{-3}\) for two cases: in one case, the doping of the GaAs core region is fixed (at \(5 \times 10^{18}\) cm\(^{-3}\)) and the doping for the AlGaAs shell region is varied, and in the other case, doping of the AlGaAs shell region is fixed (at \(5 \times 10^{18}\) cm\(^{-3}\)) and doping for the GaAs core region is varied. It can be observed from Fig 4a that for a given core doping density, the NW performance is not degraded significantly even when the shell doping density is low. Thus, we can say that the NWSC has better tolerance to the variation in shell doping rather than core doping. Therefore, for the remaining discussions, the effect of variation in core doping densities on the performance of the solar cell will be investigated for a fixed shell doping density of \(5 \times 10^{18}\) cm\(^{-3}\).

As seen from Fig 4a, the performance of the solar cell is poor when the core doping is less, and the efficiency increases sharply when the core doping increases from \(1 \times 10^{17}\) cm\(^{-3}\) to \(1 \times 10^{18}\) cm\(^{-3}\), followed by a slower increase in efficiency with further increase in doping density to \(1 \times 10^{19}\) cm\(^{-3}\). Fig 4b depicts the variation in short current density \((J_{sc})\) as a function of core doping density, and we see that \(J_{sc}\) follows the same trend as the efficiency. It can be seen that \(J_{sc}\) increases rapidly when the doping density is increased from \(1 \times 10^{17}\) cm\(^{-3}\) to \(1 \times 10^{18}\) cm\(^{-3}\), followed by a slower increase. This shows that the performance of GaAs/AlGaAs NWSC follows the same trend as that of \(J_{sc}\). This result is similar to the result obtained by Li et al. [26] for GaAs NWSC. Therefore radial GaAs p-n junction nanowires and radial GaAs/AlGaAs p-n junction nanowires follow a similar trend in efficiency and \(J_{sc}\) to variation in doping density.
all the regions is close to the valence band edge as seen in Fig. 5a. Therefore, for core doping densities of $1 \times 10^{16}$ cm$^{-3}$ and $1 \times 10^{17}$ cm$^{-3}$, the core, i-region and shell effectively behave as if they have the same doping type (p-type), and the resulting band alignment does not allow for a good flow of the photogenerated minority carriers. Thus the photovoltaic contribution from the junction is poor [26].

When core doping is increased to $1 \times 10^{18}$ cm$^{-3}$, the structure finally attains a p-AlGaAs / i-GaAs / n-GaAs configuration, and the photovoltaic contribution becomes significant. As the core becomes more n-doped, the Fermi level splitting becomes more significant, resulting in improved $J_{sc}$. This unusual behavior of carrier inversion/compensation is an attribute of the small radial dimension of nanowires.

From Fig 5 (d) we can also see that when the core doping is as large as $5 \times 10^{18}$ cm$^{-3}$, the Fermi-level within the core lies above the conduction band edge, making the core degenerate. Even though a large core doping is good, having degenerate doping can be detrimental. At degenerate doping the Fermi level is expected to lie in the conduction or valence band rather than in the forbidden region. Semiconductors can act like a metal if the Fermi level lies in the conduction band even at absolute zero K (usually observed in metals).

In other words, the electrical conductivity decreases with the increase in temperature. Further, Unlike non-degenerate semiconductors, these kind of semiconductor do not obey law of mass action, which relates intrinsic carrier concentration with temperature and bandgap.

To further support our analysis, we have calculated the electric field and equilibrium electron-hole concentrations at the dark conditions and at the same NW height (1600 nm from the bottom of the NW). From Fig 6 plot (a), we can see that for a core doping of $1 \times 10^{16}$ cm$^{-3}$, the electric field lies across the i-GaAs/p-AlGaAs interface, thus giving a very narrow space-charge region. With the increase in n-doping of the core, it can be seen from Fig 6 plot (b), (c), that the electric field extends across the entire intrinsic GaAs region, in other words, the depletion region now extends along the entire intrinsic region. This results in efficient separation of the electron-hole pairs that are generated in that intrinsic region.

When core doping is increased to $1 \times 10^{18}$ cm$^{-3}$, the Fermi level splitting becomes more significant, resulting in improved $J_{sc}$. Excellent carrier confinement is observed.

We also observed that the doping concentration of AlGaAs shell does not significantly influence the performance of the solar cell unlike the doping concentration of GaAs core. Nevertheless, we still need to maintain a large doping concentration for the shell ($\geq 1 \times 10^{18}$ cm$^{-3}$). As seen from Fig 7 plot (a), with low shell doping, the structure loses its p-AlGaAs / i-GaAs / n-GaAs configuration and behaves as a n-AlGaAs / n-GaAs configuration due to large electron injection from the largely n-doped core into the lightly p-doped shell. The structure works effectively only when the shell doping is made as large as $5 \times 10^{18}$ cm$^{-3}$. 

The reason for such variation in $J_{sc}$ can be explained by observing Fig 5 where the energy band diagrams at equilibrium are plotted at the height of 1600 nm (from the bottom of the NW), along the diameter of the nanowire, for different core doping levels. It can be seen that when the n-doping density of the core is $1 \times 10^{16}$ cm$^{-3}$, instead of having a p-AlGaAs / i-GaAs / n-GaAs structure, we effectively have a p-AlGaAs / p-GaAs / p-GaAs configuration, which is formed due to large hole injection from the largely p-doped shell into the lightly n-doped core. As a result, the Fermi level inside the core lies above the conduction band edge, making the core degenerate. Even though a large core doping is good, having degenerate doping can be detrimental. At degenerate doping the Fermi level is expected to lie in the conduction or valence band rather than in the forbidden region. Semiconductors can act like a metal if the Fermi level lies in the conduction band even at absolute zero K (usually observed in metals).

In other words, the electrical conductivity decreases with the increase in temperature. Further, Unlike non-degenerate semiconductors, these kind of semiconductor do not obey law of mass action, which relates intrinsic carrier concentration with temperature and bandgap.

To further support our analysis, we have calculated the electric field and equilibrium electron-hole concentrations at the dark conditions and at the same NW height (1600 nm from the bottom of the NW). From Fig 6 plot (a), we can see that for a core doping of $1 \times 10^{16}$ cm$^{-3}$, the electric field lies across the i-GaAs/p-AlGaAs interface, thus giving a very narrow space-charge region. With the increase in n-doping of the core, it can be seen from Fig 6 plot (b), (c), that the electric field extends across the entire intrinsic GaAs region, in other words, the depletion region now extends along the entire intrinsic region. This results in efficient separation of the electron-hole pairs that are generated in that intrinsic region. 

When core doping is increased to $1 \times 10^{18}$ cm$^{-3}$, the Fermi level splitting becomes more significant, resulting in improved $J_{sc}$. Excellent carrier confinement is observed.
incorporate that change in our study. However, we have done a comparative study to observe how different carrier lifetimes influence the NWSC efficiency when the core doping density is varied. In Fig 8(a), we have plotted the change in efficiency of the NW vs different core doping densities for five different lifetimes: 1 ns, 0.8 ns, 0.4 ns, 0.2 ns, 0.05 ns. We observe that as the lifetime decreases, the efficiency also decreases. This decrease is more when the doping concentration is less (1×10\(^{16}\) cm\(^{-3}\)), whereas, when the doping concentration is high (1×10\(^{18}\) cm\(^{-3}\)), the drop in efficiency due to a decrease in lifetime is lesser as compared to the reduction observed at low doping levels, thus highlighting the importance of having a larger doping density for the core.

The reason for such a trend in the efficiency can be understood from the JV curves plotted in Fig 8(b) for different lifetimes for a fixed core doping of 1×10\(^{18}\) cm\(^{-3}\). A significant reduction in the open circuit voltage (\(V_{oc}\)) is observed when the lifetime is decreased. This decrease is expected, because for a smaller carrier lifetime, there will be more recombination in the depletion region, leading to a higher saturation current density and low \(V_{oc}\), similar to the results obtained by Li et al. \cite{26} for GaAs nanowires.

If we consider the decrease in efficiency due to lifetime degradation coupled with the increase in efficiency due to increase in core doping, we are expected to find a more optimal value for the core doping. Since there are no studies correlating the carrier life time and doping density for GaAs/AlGaAs heterojunction nanowires, choosing an optimal core doping density is not possible at this stage. However, from our analysis, we can safely conclude that the effect of low carrier lifetime on the efficiency of the NWSC is not as adverse as compared with the case where the core doping densities are low. Therefore, for the rest of our study, the core doping is fixed as 1×10\(^{18}\) cm\(^{-3}\).

C. Shell Study

Now that we have decided the doping densities of core and shell, we will now look at the influence of the axial AlGaAs shell thickness (\(t_A\)) and radial AlGaAs shell thickness (\(t_{rad}\)) and their junction positions on the performance of NWSC. Several studies have shown the effect of shell thickness of NWSC \cite{26,27,29}. We performed a similar study for our radial pin junction GaAs/AlGaAs NWSC. In addition, a study was also done to observe the influences of the thickness of intrinsic axial GaAs shell (\(t_i\), refer Fig. 1) on the NWSC behavior.

1) Axial AlGaAs Shell: We investigated the effect of the thickness of axial p-AlGaAs layer (\(t_A\), refer Fig. 1) present on the top of NW, as this thickness influences the amount of light absorption and carrier extraction. The core and shell doping is set as 1×10\(^{18}\) cm\(^{-3}\) and 5×10\(^{18}\) cm\(^{-3}\), respectively. The carrier lifetime is kept at 1 ns and a good surface passivation (SRV = 1300 cm.s\(^{-1}\)) and \(N_{TD} = N_{TA} = 2 \times 10^{11} \text{ cm}^{-2}\) \cite{28}) is considered.

In Fig 9(a), we observe the change in the efficiency of the NW when the thickness of the axial p-AlGaAs shell layer

![Fig. 8](image)

Fig. 8. (a) Efficiency dependence on the nanowire core doping for different carrier lifetimes.

(b) \(J-V\) characteristics for different carrier lifetimes at a fixed core and shell doping of 1×10\(^{18}\) cm\(^{-3}\) and 5×10\(^{18}\) cm\(^{-3}\) respectively.

(Fig 7 plot (b), (c)). The same reasoning can be applied as before.

We can thus infer that GaAs/AlGaAs heterojunction nanowire solar cells having a low doping concentration for core and shell region leads to insufficient photovoltaic contribution from the junction. We need to maintain a large core and shell doping to maintain the p-i-n configuration and have efficient carrier extraction. We have determined the optimal core and shell doping as 1×10\(^{18}\) cm\(^{-3}\) and 5×10\(^{18}\) cm\(^{-3}\) respectively. It is worth noting that, for our study of core doping dependence, we have kept the shell doping at 5×10\(^{18}\) cm\(^{-3}\). Varying the doping concentration of the shell might lead to different optimal doping concentration for the core. However, the inference obtained in this section would still be valid.

B. Effect of Carrier Lifetime

It is known that with increase in doping, the carrier lifetime is expected to decrease \cite{42}. Due to the unavailability of a systematic study on how the lifetime varies as a function of doping density for nanowires in literature, we could not
Fig. 9. (a) Efficiency dependence of the nanowire on axial shell thickness at three different radial shell thicknesses. (b) $J - V$ characteristics of the nanowire for different axial shell thicknesses at a fixed radial shell thickness of 20 nm.

is varied from 10 nm to 400 nm for three different radial p-AlGaAs shell thicknesses (10 nm, 20 nm and 30 nm). It is seen that for a given radial shell thickness, the efficiency of the NWSC decreases with increase in the axial shell thickness and the NW shows the best performance when the axial shell thickness is the least. It is also observed from Fig 9(a) that for a given axial shell thickness, the efficiency decreases when the thickness of the radial shell increases. The reason for a decrease in the efficiency with the increase in axial shell thickness can be associated to the decrease in the $J_{sc}$ as seen from Fig 9(b). To further understand why $J_{sc}$ decreases with increasing thickness of the axial shell layer, we have plotted the photogeneration profile across the NW cross-section in Fig 10.

We can see from Fig 10 (a)-(c) that for smaller values of AlGaAs thickness, the optical generation hotspot lies inside the GaAs region. This means that majority of the photogenerated carriers are swept by the electric field present. However, with a large increase in the thickness of the AlGaAs shell, the entire hotspot occurs only in the AlGaAs shell, which means that these generated carriers are not under the influence of the electric field, and hence the probability that they will be collected at the contacts is extremely small, which is undesired.

To further support our claim, in Fig 11 the recombination rate along the central axis (BC, ref. fig 1) of the axial shell is plotted for different axial shell thicknesses. It can be seen that as the axial shell thickness increases from 10 nm to 120 nm, the bulk recombination rate in the AlGaAs shell increases by two orders, and that results in a decrease in the solar cell performance.

Thus, we can conclude that having a thin AlGaAs shell sets the upper limit to the performance of the NWSC as there is less carrier generation-recombination in the shell and more carrier generation in the intrinsic region and the core.

We have also studied the effect of the thickness of the axial i-GaAs shell on the performance of the NWSC and it was observed that the there is no significant change in the solar cell parameters with the change in the Axial GaAs shell thickness, therefore its kept fixed at 20 nm for the rest of our study.

2) Radial AlGaAs Shell: This section explores the influence of the radial shell thickness on our GaAs/AlGaAs NWSC with different surface passivations and the effects associated with...
variation in lifetime. Surface effects are predominantly present in the radial shell, and therefore we investigate the influence of various structural and electrical parameters of the radial shell on the performance of NWSC, keeping the axial thickness fixed at 20 nm.

Existing literature highlights the importance of proper radial geometry (position of the radial shell and its thickness) along with the need for proper surface passivation [26, 27]. In practice, epitaxially growing a passivation layer helps in attaining this goal. In addition, it also acts as a barrier confining the optical generation on inner GaAs regions.

Fig 12 shows the change in the efficiency of the NWSC with the radial shell thickness varied from 10 nm to 40 nm, keeping the overall nanowire radius fixed at 180 nm. The simulations were done for ‘best surface passivation’ with SRV = 0 cm.s\(^{-1}\) and \(N_{TD}, N_{TA} = 0\) cm\(^{-2}\), ‘good surface passivation’ with SRV = 1300 cm.s\(^{-1}\) and \(N_{TD}, N_{TA} = 2 \times 10^{13}\) cm\(^{-2}\) (which has been experimentally demonstrated for AlGaAs passivation [28]) and ‘poor surface passivation’ with SRV = \(10^7\) cm.s\(^{-1}\) and \(N_{TD}, N_{TA} = 1 \times 10^{12}\) cm\(^{-2}\) (typical for surfaces with no passivation). For three cases (Fig 12 (a), (c), (d)), we are interested in observing the efficiency of the NWSC purely due to different SRV and trap densities, therefore, all these simulations were done for a carrier lifetime of 1 ns. Later, we considered two realistic cases (Fig 12 (b) and (e)), where simulations were carried out for the good and poor surface passivation cases, with a reduced life time of 400 ps [43] and 50 ps [28], respectively.

All the plots in Fig 12 follows a general trend in which the efficiency decreases as the radial shell thickness increases. With the increase in the radial shell thickness, while keeping the NW radius constant, the depletion region width in the core-shell junction decreases as the width of the i-GaAs region decreases. Thus, the total number of photocarriers generated overall is less since more carriers are being generated in the AlGaAs shell, and the wide quasi-neutral region in the shell allows the photogenerated carriers to undergo bulk recombination, leading to a reduction in efficiency.

Figure 12 - (a), (c), (d) shows the change in efficiency of the NWSC with varying Radial shell thickness (\(t_{Rad}\)) for three cases of surface passivations. For these cases, the lifetime of the carriers is assumed to be 1 ns. It can be seen that for a given radial shell thickness, there is hardly any difference in the efficiency among the two surface passivation cases (best (no surface effects) and good), however, for the case of poor passivation, the efficiency is smaller. It is also observed that with increasing radial shell thickness, the efficiency decreases for all the considered cases; and this rate of decrease in efficiency is much larger when the passivation is poor, whereas, for the case of good passivation, the rate of decrease is similar to best passivation (the ideal case where there are no surface effects).

These two trends i.e, the decrease in the efficiency of the NWSC with the increase in \(t_{Rad}\) and the increasing rate of efficiency degradation with the increase in surface effects (SRV and trap densities) can be associated to the increase in the photogeneration within the shell (we desire the photogeneration to happen inside the core and intrinsic region rather than in the shell) with the increase in \(t_{Rad}\), and the corresponding increase in the bulk and surface recombination. To support our claim, in Fig 13 we have plotted the photogeneration
rate profiles across the NW cross-section for four radial shell thicknesses (10 nm, 20 nm, 30 nm, 40 nm). It can be observed that with the increase in the thickness of the radial AlGaAs shell, a large amount of photogeneration what was initially in the GaAs region (i.e. intrinsic region) now happens in the AlGaAs shell. These photocarriers in the AlGaAs shell, as they are not under the influence of the built-in electric field at the junction are not swept away, and therefore are more prone to recombination. In Fig 14, we have plotted the recombination rates of carriers along the width of the radial AlGaAs shell for different shell thickness (10 nm, 20 nm, 30 nm and 40 nm). It is observed that, as the width of the radial shell increases from 10 nm to 40 nm, the recombination rate not only increases in the bulk of the shell but there is also an increase in the recombination rate near the surface, which explains a larger efficiency degradation for the poor passivation case.

It is worth noting that, for NWSC with AlGaAs shells, the decrease in efficiency due to poor passivation of the AlGaAs shell is still much smaller than the decrease seen on NWSC with poorly passivated GaAs shell for the same shell thickness [26-29], where the reported efficiency is 7 - 8 % smaller than our results with AlGaAs shells. This improved behavior shown in our NWSC is attributed to the fact that the outer shell is made of AlGaAs material which has a larger bandgap compared to GaAs, and thus resulting in a smaller carrier generation in the shell layer. Thus, most of the photogenerated carriers are confined in the inner GaAs regions, and the AlGaAs shell acts as a barrier [29] and prevents these carriers from reaching the surface and undergo recombination.

However, as observed in our structure, the decrease in the efficiency of a NWSC due to a poorly passivated surface, should not be neglected if we want to obtain an optimal design for the NWSC.

Figure 12 thus highlights the importance of having a good passivation layer along carrying out a optimized design for the radial structure. It can be inferred that a thicker shell that are well passivated provides more efficiency than a thinner shell that are poorly passivated.

There is a decrease in the lifetime with the decrease in surface passivation. So the effect of lifetime degradation can be seen from Fig 12 - (b) and (e), and we can see that the decrease in efficiency due to lifetime degradation is not as significant as the reduction due to the geometric and surface effects.

From our analysis, we can therefore conclude that we need to have a thin radial shell so that the photogeneration mainly lies within the core-shell interface, as a result, the photogenerated carriers can be properly collected at the electrodes. The shell layer of the NW also needs to be well passivated and should also be made out of a material having a large band gap (compared to the inner layers) so that the photogeneration is more confined to the inner core and intrinsic regions. This will prevent the carriers from reaching the surface and recombine, thus improving the solar cell efficiency, signifying the importance of choosing a proper NW radial geometry along with a proper surface passivation to achieve optimal performance for the NWSC.

D. Height Study

Several studies have been done to observe the influence of the NWSC height on its performance. A study done by Li et al. [26] has observed that only minor efficiency improvement can be achieved for GaAs NWSC having a height above 2 µm. An extensive study regarding the influence of the NW height on their efficiency have been done by Huang et al. [24]. The study had shown that for NWs made of direct bandgap materials (GaAs, InP, In0.48Ga0.52P and CdTe), the efficiency remains almost the same for heights above 5 µm and an efficiency ≥ 92 % can be obtained by a nanowire array of height 3 µm. Thus, for the sake of completeness, we checked if our GaAs/AlGaAs NWSC design is consistent with this result. Keeping all the other parameters fixed, we varied the nanowire height (H_NW) from 0.5 µm to 7 µm. From Fig 15 we see that there is not much variation in the efficiency of the NWSC for heights above 2 µm, and the efficiency remains relatively the same, indicating that our results are consistent with what observed in [24,26].

Thus, choosing the NW height to be 2 µm is optimal for our NWSC structure as it provides efficient light trapping effects; yielding high broadband absorption while using much less semiconductor material than planar solar cells.

E. Aluminum Composition Study

This section looks into the photogeneration inside the NWSC as a function of the Aluminium Composition in Al_xGa_{1-x}As (shell layer). From Fig 16 we see that as the composition of Al is varied from 0.3 to 0.8, the amount of photogeneration in the shell layer decreases, and most of the photogeneration is limited to the inner GaAs regions. This happens mainly because with the increase in Aluminium composition, the bandgap of AlGaAs increases from 1.8 eV (at Al composition = 0.3) to a bandgap of 2.07 eV (at Al composition = 0.8). As a result, the spectrum of light that can be absorbed decreases which results in less photogeneration in AlGaAs.
From Fig [17] we see that, as the axial shell thickness is increased, the photogeneration hotspot moves down and lies inside the GaAs material even for large shell thickness. At the same time, the photogeneration inside the AlGaAs shell is still less, thus allowing a thicker AlGaAs axial shell and a long top region which could facilitate the fabrication and contacting of the NWSC array. However, a thicker axial shell also means that the carriers generated inside the GaAs will have to travel a much larger distance to be collected, which can increase the probability of recombination. Thus, an optimal estimate of shell thickness is still necessary, which can be determined by evaluating the electrical performance of the solar cell.

Figure [18] shows the photogeneration profiles across the the NWSC cross-section (for an Al composition of 0.8 in the shell) for different radial shell thicknesses. Here, in contrast to our previous study (section C-2), we observe that even if a thick radial shell is used, the photogeneration is still confined to the inner GaAs regions, allowing for a thicker AlGaAs shell to be fabricated. This will prevent the radially transported photocarriers from reaching the NW surface where they are prone to surface recombination and thus improve carrier extraction. However, the influence of the variation of Al composition on the electrical properties of the NWSC is yet to be explored.

IV. Conclusions

In this paper, coupled optical and electrical simulations have been done to understand the influence of core-shell doping, different shell thicknesses and junction positions, and Aluminium composition on the performance of GaAs/AlGaAs pin junction heterojunction nanowire solar cells. It has been observed that the NWSC is more sensitive to core doping than shell doping. When the core doping is less, due to large carrier injection from the heavily doped shell, the structure behaves as a p-p-p structure instead of a p-i-n structure, which is corrected only when the core and the shell both have a sufficiently large doping of the order $10^{18}$ cm$^{-3}$. Based on this, an optimal doping level has been decided for both the core ($1 \times 10^{18}$ cm$^{-3}$) and the shell ($5 \times 10^{18}$ cm$^{-3}$). It is seen that there is a decrease in the NWSC efficiency due to lifetime degradation at high doping levels, however, from our analysis, we can safely conclude that the effect of low carrier lifetime on the efficiency of the NWSC is not as adverse when compared to the case where the core doping densities are low. Further highlighting the importance of having high doping in the NW core. However, both of these effects need to be considered to obtain an optimal doping. It is seen that when the axial thickness of the AlGaAs shell increases, there is a decrease in the NWSC efficiency due to a reduction in $V_{oc}$ and that’s because, when the axial shell thickness increases, the photogeneration rate in the AlGaAs shell also increases. Hence, the carriers that were supposed to be generated in the core or the intrinsic region, to be collected radially are now being generated in the axial AlGaAs shell, which now has to travel a larger axial distance to be collected, further the carriers generated in the AlGaAs shell is not under the influence of the built-in electric field and thus face a high probability of recombination, as a result a minimal thickness of the axial AlGaAs shell is preferred. Similarly, keeping the overall nanowire radius constant and increasing the thickness of the AlGaAs radial shell, the GaAs/AlGaAs interface moves further inside the NW, as a result, the volume of the intrinsic GaAs region decreases and there is more carrier generation...
inside the AlGaAs, which undergoes more bulk and surface recombination, reducing the NWSC efficiency. Thus, even though AlGaAs have great carrier confining ability due to their low absorption coefficient and high bandgap, having a thick AlGaAs shell at the cost of the i-GaAs region reduces the solar cell performance. This reduction in SC performance is more pronounced when the surface has poor passivation. Therefore having a thin AlGaAs shell with proper passivation is necessary for better performance of the device. This, once again highlights the importance of a proper NW geometry is necessary for better performance of the device. This reduction in SC performance though AlGaAs have great carrier confining ability due to their low absorption coefficient and high bandgap, having a thick AlGaAs shell, which can potentially allow the fabrication of thicker axial or radial AlGaAs shells, which will allow the dominant photogeneration inside the shell, which can potentially allow the fabrication of thicker axial or radial AlGaAs shells, which will allow the dominant photogeneration to lie in the inner GaAs layers and at the same time push the radial surface further away from the junction, reducing the probability of surface recombination.

REFERENCES

[1] X. Duan, Y. Huang, R.argarwal, and C. M. Lieber, “Single-nanowire electrically driven lasers,” Nature, vol. 421, no. 6920, pp. 241–245, 2003.
[2] D. Saxena, S. Molkapati, P. Parkinson, N. Jiang, Q. Gao, H. H. Tan, and C. Jagadish, “Optically pumped room-temperature gaas nanowire lasers,” Nature photonics, vol. 7, no. 12, pp. 963–968, 2013.
[3] C. E. Wilhelm, M. I. B. Utama, G. Lehoucq, Q. Xiong, C. Soci, D. Dolfi, A. De Rossi, and S. Combréi, “Broadband tunable hybrid photonic crystal-nanowire light emitter; ,” IEEE Journal of Selected Topics in Quantum Electronics, vol. 23, no. 5, pp. 1–8, 2017.
[4] X. Dai, S. Zhang, Z. Wang, G. Adamo, H. Liu, Y. Huang, C. Couteau, and C. Soci, “Gaas/algaas nanowire photodetector; ,” Nano letters, vol. 14, no. 5, pp. 2688–2693, 2014.
[5] H. Wang, “High gain single gaas nanowire photodetector; ,” Applied Physics Letters, vol. 103, no. 9, p. 093101, 2013.
[6] W. Guo, M. Zhang, A. Banerjee, and P. Bhattacharya, “Catalyst-free ingan/gan nanowire light emitting diodes grown on (001) silicon by molecular beam epitaxy,” Nano letters, vol. 10, no. 9, pp. 3355–3359, 2010.
[7] F. Qian, S. Gradecek, Y. Li, C.-Y. Wen, and C. M. Lieber, “Core/multishell nanowire heterostructures as multicolor, high-efficiency light-emitting diodes,” Nano letters, vol. 5, no. 11, pp. 2287–2291, 2005.
[8] E. C. Garnett, M. L. Brongersma, Y. Cui, and M. D. McGehee, “Nanowire solar cells; ,” Annual Review of Materials Research, vol. 41, pp. 269–295, 2011.
[9] B. M. Kayes, M. Filler, M. Henry, J. Maiolo Iii, M. Kelzenberg, M. Putnam, J. Spurgeon, K. Plass, A. Scherer, N. Lewis et al., “Radial pn junction, wire array solar cells,” in 2008 33rd IEEE Photovoltaic Specialists Conference. IEEE, 2008, pp. 1–5.
[10] A. I. Hochbaum and P. Yang, “Semiconductor nanowires for energy conversion,” Chemical reviews, vol. 110, no. 1, pp. 527–546, 2010.
[11] S. Sandhu, Z. Yu, and S. Fan, “Detailed balance analysis and enhancement of open-circuit voltage in single-nanowire solar cells,” Nano letters, vol. 14, no. 2, pp. 1011–1015, 2014.
[12] K. Sun, A. Kargar, N. Park, K. N. Madsen, P. W. Naughton, T. Bright, Y. Jing, and D. Wang, “Compound semiconductor nanowire solar cells,” IEEE Journal of Selected Topics in Quantum Electronics, vol. 17, no. 4, pp. 1033–1049, 2011.
[13] R. LaPierre, A. Chia, S. Gibson, C. Haapamaki, J. Boulanger, R. Yee, P. KYyanov, J. Zhang, N. Tajik, N. Jewell et al., “Ii–vi nanowire photovoltaics: review of design for high efficiency,” physica status solidi (rRL)–Rapid Research Letters, vol. 7, no. 10, pp. 815–830, 2013.
[14] Y. Zhang and H. Liu, “Nanowires for high-efficiency, low-cost solar photovoltaics,” Crystals, vol. 9, no. 2, p. 87, 2019.
[15] J. Kupec and B. Witzigmann, “Dispersion, wave propagation and efficiency analysis of nanowire solar cells,” Optics express, vol. 17, no. 12, pp. 10390–10410, 2009.
[16] J. Kupec, R. L. Stoop, and B. Witzigmann, “Light absorption and emission nanowire array solar cells,” Optics express, vol. 18, no. 26, pp. 27589–27605, 2010.
[42] S. M. Sze, Y. Li, and K. K. Ng, *Physics of semiconductor devices*. John wiley & sons, 2021.

[43] P. Parkinson, Y.-H. Lee, L. Fu, S. Breuer, H. H. Tan, and C. Jagadish, “Three-dimensional in situ photocurrent mapping for nanowire photovoltaics,” *Nano letters*, vol. 13, no. 4, pp. 1405–1409, 2013.