Optimization of pin GaAs/AlGaAs Heterojunction Nanocone Array Solar Cell based on its Photovoltaic Properties

Sambuddha Majumder, Sooraj Ravindran

Abstract—In this paper, we have designed and investigated the performance of radial GaAs/AlGaAs pin junction nanocone array solar cells by performing coupled optoelectronic simulations to obtain the most optimal design configuration based on its photovoltaic properties. Each model has been compared with its GaAs shell counterparts for different levels of surface passivations. It has been observed that the nanocones with the AlGaAs shell has a much better performance compared to those having GaAs shell. AlGaAs shell acts as a strong barrier restricting most of the photogeneration to the inner GaAs regions and it also acts as a strong passivation layer, reducing the recombination losses due to surface effects. Further, it is observed that the nanocones achieve their highest photoconversion efficiency when they are sparsely packed, with a constant i-shell thickness of 7-9 nm and have an angle of tilt of 5°. This enhanced performance is attributed to a more effective and extended photogeneration throughout the nanowire length, a strong overlapping built-in electric field, and lower recombination losses.

Index Terms—Nanowires (NWs), Nancones (NCs), Nanocone solar cell (NCSC), Radial solar cells, Photovoltaics, GaAs/AlGaAs nanowire, Device simulation.

I. INTRODUCTION

SEMICONDUCTOR nanowires (NWs) have become a vast frontier of extensive research in the nanowire industry with their use in LED [1][2], Lasers [3][5], Photodetectors [6][7], Solar cells [8][13] etc. This is attributed to their small structure and excellent light confining abilities. Particularly, nanowire solar cells have been a key area of research in the field of photovoltaics over the past few years. A large number of nanowires have been investigated using materials like Si, GaAs, GaN, AlGaAs, etc., for both axial and radial junction nanowires. Radial junction nanowires, having a junction formed in the radial direction, produce very high-efficiency solar cells with very low material consumption. In contrast to its axial and planar counterparts, radial pin junction serves as an efficient mechanism to decouple light absorption from carrier extraction in the radial direction, leading to lower recombination losses [9][14][16]. Further, NWSC can give their optimal performance with very small diameters [17] and thus can be grown on a large range of lattice-mismatched materials, allowing them to attain efficient multijunction configurations. Extensive work is still going on every day to further optimize each of these designs. Many different optimization strategies have been studied, such as nanowires’ structural properties, different surface passivations, nanowire height and diameter, diameter to period ratio, and so on [17][20].

Recently, a new design methodology has taken over the nanowire solar cell concept, and that is the nanocone solar cells [7][21][23]. It is seen that despite the various methods to optimize the light absorption in the GaAs nanowires, most of the photoabsorption is confined to the top of the nanowires [18][19]. In contrast, absorption in the depletion region, which spreads throughout the nanowire height, is not sufficient, which leads to only minor improvements to the conversion efficiency. It is observed that providing a taper to the nanowires can increase the absorption properties dramatically. The light absorption in NWs is dominated by resonant modes, which are very closely related to the NW diameter [23][25]. In nanocones, the NW diameter continually changes across the nanowire height, with the top diameter being very smaller than the bottom diameter. Due to this unique geometry, it can support only a few long-wavelength modes in the top, and absorption (particularly for long wavelengths) shifts towards the thicker middle regions of the structure [23]. This even distribution of light throughout the structure increases the effective absorption length, improves the photogeneration, and reduces recombination losses. Also due to the presence of this taper, the NCs acts as a gradual refractive index profile that improves anti-reflection. Therefore, the nanocones must be studied in detail and optimized to improve their performance further. To date, different types of nanocones have been designed and fabricated to investigate the optical properties of the nanocones [7][21][22][24][27]. However, very little focus has been given to the photovoltaic properties of these nanocones in solar cells. Previous work by Zhang et al. [25] investigates the properties of pin GaAs nanocones; however, GaAs are prone to large surface recombination losses. Previous studies have highlighted the importance of proper radial geometry and good surface passivations for NWSC [18][28]. For GaAs NWs, epitaxial passivation by AlGaAs is an effective method to achieve that. In contrast, AlGaAs have lower absorption allowing the photogeneration to be confined to the inner GaAs region and acts as a barrier preventing the carriers generated inside from reaching the surface, thus reducing recombination losses [19][30][32].

In this dissertation, coupled three-dimensional (3D) optical and electrical simulations are done to observe the effect of different nanocone angles on the optical and photovoltaic properties of radial pin junction GaAs and GaAs/AlGaAs nanocones. Four design configurations are chosen for this study, emphasizing the thickness and position of the i-GaAs shell; the best design is then selected and optimized. Finally, a period study is done to observe the effect of dense and...
sparse packing of the nanocones on their performance. In Section II, the various electronic and optical properties of the materials and the different design models and methods are discussed. Section II-A examines the effect of the nanocone angle on different nanocone properties. Section II-B compares the different nanocone design models, and the best model is then decided and optimized. Finally, in Section II-C a study of the nanocone period is done.

II. MODELING AND METHODS

In this dissertation, we have modeled a pin GaAs/AlGaAs heterojunction nanowire solar cell (NCSC) array. For this purpose, a unit cell of the structure is first designed, and then periodic boundary conditions are used to simulate the entire square lattice [33]. Fig. 1 shows the schematic diagram of the modeled nanowire solar cell. p-Al_{0.5}Ga_{0.5}As is used as the outer shell material; the inner regions are made of GaAs. The mean NC diameter is 360 nm with a period of 720 nm [23]. For the optimal performance of cylindrical nanowires, the mean diameter should be 180 nm with D/P = 0.5 [17]. However, we won’t be able to appreciate the effect of nanocone angles for such small diameters. Moreover, due to tapering, the top diameter will be very small and will not be able to accept any wavelength modes. Therefore, a larger mean diameter is chosen. A period study is done on Section II-C to observe the effect of dense and sparse packing on nanowire performance.

The height of the nanocones is taken to be 2 μm [18, 20]. The thickness of the GaAs substrate was made semi-infinite with appropriate PML boundary conditions [18]. Doping is a very important parameter as it decides the behavior of the solar cell, the doping concentration of the p-type shell for ‘good passivation’ (cm\(^{-3}\)) is 1 x 10\(^{17}\) and for ‘poor passivation’ (cm\(^{-3}\)) is 5 x 10\(^{18}\). While, it has been reported previously that high doping is favorable for core–shell NWSCs [18, 19, 28, 34], we have done systematic study [18] to check if this doping satisfies the desired performance characteristics. For bulk GaAs substrate, concentration-dependent mobility is assumed. However, for the radial nanowires, due to the unavailability of such a systematic study that relates mobility to doping, the mobility is chosen from the work of Joyce et al. [18, 21]. For AlGaAs, the mobility is chosen from [35]. The ‘nanocone angle’ or the ‘angle of tilt’ (θ) is defined as the angle between the sidewall and the normal to the bottom surface.

For our work, four different models have been simulated; d1: Intrinsic region width = 10 nm, here the core and the shell
have same radial thickness (t_e = t_s = t_i = 10 nm); d2: Intrinsic region, the shell and the core have the same thickness (t_e = t_s = t_i); d3: The thickness of the intrinsic region is double to that of the and shell (2t_e = 2t_s = t_i); d4: The thickness of the intrinsic region is triple to that of the core and shell (3t_e = 3t_s = t_i). For these designs, as we go from design ‘d1’ to design ‘d4’, the volume of AlGaAs decreases and volume of GaAs increases, also the width of the i-GaAs shell increases, which will result in more absorption; however, if the photogenerated carriers can be efficiently extracted or not, is what we wish to observe. For each, we have changed the angle from 0 to 9° by varying the top and bottom radius (R_MIN and R_MAX), respectively keeping the mean nanowire radius (R_MNW) constant.

For optical simulations, ‘Lumerical FDTD’ software package is used. The absorption per unit volume is calculated using the Poynting vector \( \vec{P} \) as:

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

Which can be written in a more numerically stable form:

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

Where, \( \varepsilon' \) is the imaginary part of permittivity, \( \omega \) is the angular frequency of the incident light, and \( \vec{E} \) is the electric field intensity. Assuming that each photon absorbed generates an equal number of electron-hole pairs, we can write the photogeneration rate as:

\[
G_{ph} = \frac{\nabla \cdot \vec{S}}{2\hbar \omega} = \frac{\varepsilon' |\vec{E}|^2}{2\hbar}
\]

Where \( \hbar \) is the reduced Plank’s constant, \( G_{ph} \) is weighed by the AM 1.5G solar spectrum and integrated over the entire simulation spectrum. The complex refractive index of GaAs and AlGaAs has been taken from the Sopra database. The reflectance and transmittance spectra normalized to the source power are measured using the ‘Frequency-Domain Field and Power’ monitors at the top and bottom of the simulation region respectively.

For electrical simulations, the software package ‘Lumerical CHARGE’ is used. The simulated photogeneration profile is incorporated into a finite-element mesh of the nanocones, which self-consistently solves the carrier continuity equations coupled with the nonlinear Poisson’s equations in 3D. The details and working of the FDTD and CHARGE solver can be found here [36][37]. For our study, we have assumed the interface between GaAs and AlGaAs is perfect without any additional recombination centers, which can be achieved by lattice-matched epitaxy [38]. The surface effects have only been considered for the interfaces between air and the NW. For AlGaAs as the outer surface, a good SRV of 1300 cm.s\(^{-1}\) is chosen. For GaAs surfaces, two SRV cases are considered; good SRV: 1300 cm.s\(^{-1}\) and poor SRV: 10\(^7\) cm.s\(^{-1}\) with the same SRV for both electrons and holes. Radiative, Auger, and SRH recombination models and bandgap narrowing models are also considered. We have used top and bottom ohmic contacts for our structure [28]. The auger recombination coefficients, SRH recombination lifetime, and radiative recombination rates are taken to be the same for GaAs and AlGaAs.

Fig. 2. The photogeneration profiles of radial pin nanocone design ‘d1’ for (a) \( \theta = 0^\circ \), (b) \( \theta = 1^\circ \), (c) \( \theta = 2^\circ \), (d) \( \theta = 3^\circ \), (e) \( \theta = 4^\circ \), (f) \( \theta = 5^\circ \), (g) \( \theta = 6^\circ \), (h) \( \theta = 7^\circ \), (i) \( \theta = 8^\circ \), (j) \( \theta = 9^\circ \).

Fig. 3. (a) Reflectance, (b) Absorptance, (c) The integral of absorptance, reflectance and transmittance of the radial pin junction nanocone ‘d1’ for different nanocone angles.

The various key simulation parameters are listed in Table I.

III. ANALYSIS AND RESULTS

A. Nanocone Angle Study

For this study, the design model ‘d1’ is chosen. In this design, the intrinsic region has a constant thickness of 10 nm, the thickness of core and shell is the same throughout the nanocone’s height. The nanocone angle is varied from 0 to 9 degrees by varying the top and bottom radius, keeping the mean radius constant at 180 nm with a D/P (duty cycle) = 0.5 [23].

1) Optical Properties: Fig 2 shows the photogeneration profiles of the nanocone solar cell for different nancone angles. It is observed that when the angle of the nanocone is less, the photogeneration hotspot is mostly confined to the top of the nanowires. By introducing a tapered structure, we observe that as the nanocone angle increases, the photon absorption shifts downward and spreads across the nanocone’s length, leading to enhanced effective absorption. However, this process increases the absorption till a certain angle, and after a certain angle, the absorption tends to decline. From the
B. Nanocone Design Study

Since the overlap of the optical absorption with the i-GaAs region is the key to the nanocone’s performance, four designs have been tested to find the optimal thickness profile of the i-GaAs shell. In design 1, we have a constant intrinsic photovoltaic performance.

2) Electrical Properties: In Fig 5(a), we observe the efficiency of the NCSC varies vs the nanocone angle for structures with AlGaAs shell with good passivation, GaAs shell with good passivation, and GaAs shell with poor passivation. It can be seen that the designs with AlGaAs shells have superior performance than the GaAs counterparts for the entire range of angles. For small angles, the optical generation hotspot is situated in the top of the solar cell [19] but due to lack of electric field to drive those photogenerated carriers, the carrier extraction will be poor [24,40,41]. This results in significant recombination of photocarriers and loss of absorbed power. This loss is less when AlGaAs are used as the outer shell material. Due to its large bandgap and less absorptivity, minimal absorption will occur in AlGaAs, and most of the absorption will stay confined to the inner GaAs regions [19]. Thus, reducing the surface recombination losses present in GaAs and improving the solar cell performance [30,32,33,42]. AlGaAs also acts as a barrier preventing the photogeneration carriers that are generated in the inner GaAs regions from reaching the surface, and it also acts as an effective passivation layer reducing surface recombination [31,32].

As the nanocone angle increases, the photogeneration is more evenly spread out throughout the length of the structure and therefore it overlaps with the radial intrinsic region, thereby allowing efficient carrier extraction. As a result, the $J_{sc}$ increases with the increase in angle from 0 - 5 degrees (Fig 5(b)) with a corresponding improvement in conversion efficiency. However, after a certain angle, the efficiency reaches its maximum value, and then it starts to decrease, which is probably because the useful photogeneration reduces. At large angles, the top of the structure becomes very thin to support long wavelength modes, and even though the longer modes get absorbed towards the middle, it is offset by the decrease in absorption in the top, thus resulting in a reduction of efficiency.

Fig. 5. (a) Conversion efficiency of the radial pin junction nanocone 'd1' with AlGaAs shell, GaAs shell (Good and Bad passivation) for different nanocone angles. (b) Short circuit current density ($J_{sc}$) of the radial pin junction nanocones with AlGaAs shell.
Fig. 6. The integral of (a) reflectance, (b) transmittance, (c) absorptance of the nanocone with different nanocone angles for different design configurations.

region. From designs 2 - 4, the intrinsic GaAs region thickness increases across the nanocone’s height. This is done to obtain the profile of the intrinsic region that provides a more efficient overlap of the photogeneration with the intrinsic region and better optical and electrical properties.

1) Optical Properties: On Fig 6, the effect of different designs on the optical properties (the net absorptance, reflectance, and transmittance) of the NCSCs are observed. It can be seen that the design ‘d1’ has the lowest absorption and highest transmittance for all the nanocone angles, followed by ‘d2’ with better absorption and lower transmission, and with ‘d4’ having the best absorption and least transmission. Such a trend is expected as ‘d1’ has the highest volume of AlGaAs and ‘d4’ has the lowest, and GaAs have much larger light-absorbing properties than AlGaAs. The structure’s reflectance for different configurations remains almost the same because the overall geometry is not changed. Therefore, in terms of the optical properties, design ‘d4’ has a better performance than the other designs.

2) Electrical Properties: Fig 7a,b,c shows the conversion efficiencies of different NCSC arrays for designs ‘d2’, ‘d3’, and ‘d4’. We can see that the different designs follow a similar profile; initially, the efficiency increases, then it gradually starts to decrease (similar to the design ‘d1’). Further, it’s observed that NCs with AlGaAs shell has better efficiency than the one with a GaAs shell for all the cases. Hereby emphasizing the improved performance of GaAs/AlGaAs nanocones. We can apply the same reasoning as in the case of ‘d1’. In Fig 7d, the conversion efficiencies for all the designs with AlGaAs shell have been compared. In contrast to the trend in the optical properties, we see that the overall efficiency of design ‘d1’ is the greatest for all the angles, and efficiency decreases as we go from design ‘d1’ to ‘d4’. The efficiency increases monotonically from 0° to 5° then it saturates followed by a decrease for larger angles.

One reason for such a contrasting behavior is the presence of the built-in electric field. We can see it from Fig 8a, b, c that the electric field mostly exists around the interface between the (n-core) - (i-shell) interface but as the thickness of the i-GaAs region increases from design ‘d1’ – ‘d4’ (for nanocone angles: 3°, 5°, 7°), the magnitude of the electric field continually decreases and has a maximum value for the case of ‘d1’ (constant intrinsic region). As a result, when we go from ‘d1’ to ‘d4’, the extraction of the photogenerated carriers decreases, and the recombination rate rises. Further, the built-in electric field generated in the 1st case (‘d1’) may overlap with the maximal photogeneration region. Compared to the other designs, a large shell allows the photogeneration
The overlap of the built-in electric field with photogeneration hotspots, which may also change depending on the position and thickness of the radial junction. Therefore, considering all these constraints, we get an optimized thickness satisfying all the factors.

C. Period Study

In this section, we observe the effect of dense and sparse packing of the nanocone array on its optical and electrical properties. Fig 11-a shows the net absorbance, reflectance, and transmittance of the nanocone array for different unit cell periods, keeping the cell diameter constant at 180 nm. It is observed that as the period decreases (D/P increases), there is an increase in absorption with an overall absorbance of \( \sim 80 \% \) at \( D/P = 0.4 \) to a \( \sim 90 \% \) at \( D/P = 0.6 \) with a corresponding decrease in total reflection and transmission. The difference in the anti-reflective properties between the dense and sparse models is attributed to the different effective refractive index mismatches at the air/SC interface [43] and enhanced multiple scattering effects in the dense NCs [22,44].

From this observation alone, one can easily expect the nanowires having smaller periods to perform better. In order to verify that, we need to analyze the structure’s photovoltaic properties as well. Fig 11-b shows the IV curves and the conversion efficiencies of the GaAs/AlGaAs nanocone solar cell arrays as D/P is varied from 0.6 to 0.4 with a constant diameter of 180 nm. In contrast to the optical properties, we see a huge increase in the efficiency from around 13 \% to 27 \% as the period is increased, i.e. for sparse NCSCs, the higher efficiency is obtained despite the better anti-reflective properties of the dense NCs. This change in efficiency comes from the improvement in \( J_{sc} \) as seen from Fig 11-c. This behavior is similar to the behavior of SiNW/ PEDOT: PSS cells [22]. With the same reasoning, we can say that the increased \( J_{sc} \) can be attributed to the more effective filling of AlGaAs into the sparse NCs versus the dense NCSCs.

3) Design Optimization: Now that we have decided on the optimal design configuration, we now look forward to optimizing it. Since the key to this design is the constant thickness of the intrinsic shell, we need to find the most optimal thickness which can give us the best performance. For that, we have done a parametric sweep of the thickness of the i-shell (\( t_i \)) from 5 nm to 20 nm and observed its effect on the solar cell efficiency. From Fig 9, we can see that, with the increase in \( t_i \), the efficiency first increases and attains the maximum at a thickness of 8 - 9 nm and then decreases. The possible reason for this type of efficiency profile could be due of a trade-off between photogeneration and carrier extraction. As the thickness of i-GaAs increases, the thickness of the AlGaAs shell decreases, and thus the overall absorption (which primarily happens in GaAs) increases leading to improved performance. On the other hand, with a large increase in thickness, the electric field magnitude across the pin junction decreases as seen from Fig 10 leading to poor carrier extraction and degrading efficiency. Also, one crucial factor is the surface away thus reducing recombination. Both these factors primarily happen in GaAs increases leading to improved performance. For that, we have done a parametric sweep of the thickness of the i-shell (\( t_i \)) from 5 nm to 20 nm and observed its effect on the solar cell efficiency. From Fig 9, we can see that, with the increase in \( t_i \), the efficiency first increases and attains the maximum at a thickness of 8 - 9 nm and then decreases. The possible reason for this type of efficiency profile could be due of a trade-off between photogeneration and carrier extraction. As the thickness of i-GaAs increases, the thickness of the AlGaAs shell decreases, and thus the overall absorption (which primarily happens in GaAs) increases leading to improved performance. On the other hand, with a large increase in thickness, the electric field magnitude across the pin junction decreases as seen from Fig 10 leading to poor carrier extraction and degrading efficiency. Also, one crucial factor is
This improvement in efficiency results from an improved optical generation rate and the corresponding decrease in the net recombination rate of the photogenerated carriers in the sparse structures. For sparse structures, even though the overall absorption is less, the photogeneration profile, which comes from the useful absorption spectra, spreads across the entire structure and results in improved effective absorption and photogeneration as seen from Fig. 12. Here, we can see that when the D/P ratio is low (the period is large), the photogeneration spreads out across the entire length of the solar cell. This helps us attain a longer absorption length. Which in this case, is better than the photogeneration at large solar cell. This helps us find the configuration for best solar cell performance, and it is seen that a thickness of 8 - 9 nm provides the best efficiency. A period study is done to see the effect of dense and sparse packing of NCs in the array, and it has been observed that sparse NCs with larger periods had much larger efficiency than the densely packed ones because of more effective filling of AlGaAs, large effective photogeneration throughout the structure (it behaves similar to the cells having large nanocone angles w/o the loss incurred due to the thin top region) and the decreased net recombination of the photogenerated carriers.

Fig. 12. Photogeneration profiles of the radial pin junction nanocone ‘d1’ with D/P : (a) 0.6, (b) 0.5, (c) 0.4.

Fig. 13. Net photo-carrier recombination profiles of the radial pin junction nanocone ‘d1’ with D/P : (a) 0.6, (b) 0.5, (d) 0.4.

**IV. Conclusions**

An extensive study of the optical and photovoltaic properties of pin junction GaAs/AlGaAs nanoarray solar cells has been done. It is observed that with the increase in the nanocone angle, the photogeneration, which is generally confined to the top for cylindrical NWs, spreads out along the length of the structure. This happens because the top of the cell becomes too thin to support many long-wavelength modes, which get absorbed towards the bottom, increasing the absorption length. However, having a very large angle is also detrimental to the cause; as for angles $\geq 5$ - 7 degrees, the loss of light absorption at the top becomes greater than the light absorbed at the bottom. Four different designs have been studied to observe the effect of the variation of the intrinsic shell position and thickness on the nanowire performance. The efficiency curves for all the structures follow a similar trend, i.e. they increase for small angles, then saturate and decrease for larger angles. It is observed that the design with a constant i-region delivers the best electrical results because of its strong built-in electric field throughout the structure and its overlap with the photogeneration. For all the cases, the NCs with AlGaAs shells have better overall performance than NCs with GaAs shells, highlighting the importance of AlGaAs passivation and confinement. The thickness of the i-region is further optimized to find the configuration for best solar cell performance, and it is seen that a thickness of 8 - 9 nm provides the best efficiency.

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