Design and simulation of double-heterojunction solar cells based on Si and GaAs wafers

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Keywords: Si and GaAs wafers, ZnSe window, simulation, Al_{0.8}Ga_{0.2}Sb and AlAs_{0.9}Sb_{0.1}, back surface field, SCAPS-1D

Abstract

This article demonstrates the novel designs of Si and GaAs wafer-based double-heterojunction (DH) solar cells using SCAPS-1D simulator. Simple five-layer solar cells are proposed here: cells comprised of a cathode metal layer, three layers of semiconductor materials in the III–V, II–VI and group IV families—and a layer of anode metal. The device structures have been optimized for the analysis of the power-conversion efficiency (PCE) of the Si and GaAs solar cells considering high defect densities at and near each heterojunction. The PCEs predicted are 38% and 38.9% for \( n-ZnSe/p-Si/p^+-Al_{0.8}Ga_{0.2}Sb \) and \( n-ZnSe/p-GaAs/p^+-AlAs_{0.9}Sb_{0.1} \) cells, respectively which stay entirely within the PCE limits set by the Shockley–Queisser theory of multi-junction cell. These results reveal that high efficiency and hence cost-effective Si and GaAs wafer-based DH solar cells can be fabricated in the near future.

1. Introduction

Solar cells as renewable energy sources are widely used technologies for producing electricity from sunlight. Among the several types of solar cells, silicon solar cells cover over the 90% of the global market [1]. In 2017, the highest efficiency of a silicon solar cell module with 180.4 cm\(^2\) area has been reported to be \( \approx 26\% \) [2]. On the other hand, single junction GaAs solar cell has reached an efficiency of 29.1% [3]. However, the manufacturing costs of Si and GaAs modules of the order of 0.185–0.380 and 3.5–4.5 USD/W\(_p\), respectively have limited their widespread use for the production of electricity [4, 5]. The rapid development of PV industry and widespread utilization is possible once the price of the PV systems is low enough to compete with the price of the electricity produced by combined-cycle natural gas and coal.

However, the reduction of cost of the solar cell is possible when the efficiency of the cell is significantly enhanced. The Shockley–Queisser (SQ) detailed-balance theory indicates that the efficiency of the double-heterojunction (DH) solar cells can be increased to 42%–46% [6, 7]. However, there is no reports of the fabrication of such a high efficiency DH solar cells. An examination of solar-cell literature shows that tandem and multiple-junction cells have received a lot of attention for the enhancement of the efficiency; whereas the category of 2-terminal non-tandem double-heterojunction cells is relatively unexplored and is ripe for further advancement [8–11]. Recently, there are few theoretical reports on Si wafer and Ge, CdTe, and CIGS thin film based solar cells which reveal that the of the efficiency of the double-heterojunction solar cell can be greatly increased to 38%–47% with the employment of suitable BSF layers [12–16].

Herein, the design and simulation of Si and GaAs wafer-based high efficiency double-heterojunction solar cells have been demonstrated, and in that context, we propose for the absorber a commercial monocrystalline Si or GaAs wafer because that could provide a pathway to low-cost solar cell construction by the reduction of USD/W\(_p\) of the modules due to the highest efficiencies of the solar cells. The n-type ZnSe and p-type Al\(_{1-x}\)Ga\(_x\)Sb and AlAs\(_{1-y}\)Sb\(_y\) thin films have been used as a window and back surface field (BSF) layers, respectively for the design of Si and GaAs wafer-based double-heterojunction solar cells. Fabrication of these solar cells requires the growth of single-crystalline thin films of n-type ZnSe, p-type Al\(_{1-x}\)Ga\(_x\)Sb and p-type AlAs\(_{1-y}\)Sb\(_y\), respectively. Zinc selenide (ZnSe) is a wide band gap (2.7 eV) n-type chalcogenide semiconductor with electron and hole mobilities of 50 and 20 cm\(^2\) V\(^{-1}\) s\(^{-1}\), respectively which is suitable to be used as a window layer in solar cells [17].
Although molecular-beam epitaxy is traditionally used, ZnSe can be grown by electro-chemical deposition [17], thermal evaporation [18], and metal-organic chemical vapor deposition [19]. On the other hand, Al₁₋ₓGaₓSb is a III–V ternary alloy compound composed of two binary compounds AISb and GaSb, respectively which can be used as a BSF layer in Si solar cells. The Al₁₋ₓGaₓSb growth is linked essentially to that of AlSb where chemical vapor deposition [20, 21] thermal evaporation [22] pulsed-laser deposition [23] and screen printing [24] have been employed for the deposition. In addition, AlₐSb is also a ternary compound composed of two binary compounds and AlAs and AlSb, respectively which can be used as a BSF layer in GaAs solar cells. The growth of AlₐSb is linked essentially to that of AlAs where metal-organic chemical vapor deposition [25], and pulsed laser deposition [26] have been employed for the deposition.

This paper demonstrates the novel design of Si and GaAs wafer-based n-ZnSe/p-Si/p⁺-Al₀.₈Ga₀.₂Sb and n-ZnSe/p-GaAs/p⁺-Al₀.₉Sb₀.₁ double-heterojunction solar cells, respectively. The effect of different physical parameters on the photovoltaic performance of the designed solar cells has been investigated in details. This study indicates that use of ZnSe as window and Al₀.₈Ga₀.₂Sb and Al₀.₉Sb₀.₁ as BSF layers in Si and GaAs wafer-based double-heterojunction solar cells are highly promising for the fabrication of highly efficient wafer-based solar cells in future.

### 2. Theoretical concepts and device structure

In 1961, Shockley–Queisser (SQ) proposed the detailed balance theory of a single junction solar cell that predicted the PCE of ~30% for an energy gap of about 1 eV [6]. The theory was further modified to predict the PCE of the multi-junction solar cells [6, 7]. The SQ limit for tandem solar cell structure with two cells is 42%, with three cells is 49%, etc [6]. However, the SQ limit for the series connected two-terminal multi-junction unconstrained cells with AM 1.5 Global radiation is 32.9% for one cell, 45.7% for two cells etc [7]. In 2015, Marti et al have theoretically shown that a three-terminal double-heterojunction solar cell with bipolar transistor structure can achieve a PCE of ~54.7% [27]. Therefore, there is a possibility to fabricate a high efficiency double-heterojunction solar cell with a PCE of 42%–46%. Here, we propose Si and GaAs wafer-based n-ZnSe/p-Si/p⁺-Al₀.₈Ga₀.₂Sb and n-ZnSe/p-GaAs/p⁺-Al₀.₉Sb₀.₁ double-heterojunction solar cells that serve the purpose of two-terminal two-junction cells with efficiency towards the SQ limit [28, 29].

In this paper, we employed the software package known as Solar Cell Capacitance Simulator (SCAPS-1D) [30] for the simulation of Si and GaAs double-heterojunction solar cells. This simulator works based upon the drift-diffusion method where solar-induced voltage and current are calculated by solving the Poisson equations, taking into account of different parameters. The SCAPS-1D can be employed to compute the J-V, C-V, C-f characteristics and quantum efficiency of the solar cells. The simulator computes these parameters of the designed solar cell using the following three equations:

\[
\text{Poisson’s equation}\ \frac{\partial^2 \Psi}{\partial x^2} + \frac{q}{\varepsilon} \left[ p(x) - n(x) + N_D - N_A + \rho_p - \rho_n \right] = 0
\] (1)

\[
\text{Hole continuity equation} \ \frac{1}{q} \frac{\partial p}{\partial x} = G_{op} - R(x)
\] (2)

\[
\text{Electron continuity equation} \ \frac{1}{q} \frac{\partial n}{\partial x} = -G_{op} + R(x)
\] (3)

where, $\varepsilon$ denotes the dielectric constant, $q$ represents the electron charge, $N_A$ and $N_D$ are the ionized acceptors and donors density, $\Psi$ denotes the electrostatic potential, $J_p$ is the hole current density, $J_n$ is the electron current density, $G_{op}$ denotes the carrier generation rate, $R$ represents the total recombination rate, $p$ denotes free hole density, $\rho_p$ and $\rho_n$ denote distribution of hole and electron, respectively.

The transport properties of holes and electrons of the semiconducting material can be represented by the following drift-diffusion equations:

\[
J_p = -\frac{\mu_p n}{q} \frac{\partial E_{fp}}{\partial x}
\] (4)

\[
J_n = -\frac{\mu_n n}{q} \frac{\partial E_{fn}}{\partial x}
\] (5)

where, $\mu_p$ and $\mu_n$ denote mobilities of hole and electron, $E_{fp}$ and $E_{fn}$ are the Fermi level of p-type and n-type carrier, respectively.

Figure 1(a) presents the cross-sectional view of the proposed npp⁺ Si double-heterojunction solar cell (DHJSC) with its three active layers, ZnSe, Si, and Al₁₋ₓGaₓSb, including the optimized layer thicknesses. To optimize this five-layer device, the aspect of ‘band alignment engineering’ has been added when selecting the
metals and the semiconductors. The valence band (VB) and conduction band (CB) band offsets have been deliberately chosen at each hetero-interface to give ‘selective collection’ of photo-generated electrons and holes. That was done by considering the electron affinities and the band gaps of the candidate materials. For the candidate metals, the work function of each candidate was examined to give favorable positioning of the two Fermi levels in the heterostructure. The wide band gap that is chosen for the window material minimizes its parasitic absorption. The Si wafer absorber is much thicker than the thin-window and BSF layers. The Ti metallic grid electrode was used at the ZnSe front surface, together with a uniform Ni metal contact on the Al$_{1-x}$Ga$_x$Sb BSF back surface.

Figure 1(b) presents the equilibrium energy band diagram of the cell during one-sun solar illumination. The quasi Fermi energy levels $E_{Fp}$, and $E_{Fn}$ for electrons and holes, respectively, are indicated in figure by dashed lines. Both the window and BSF were selected to give approximately type-II band offsets at the hetero-interface with Si. The five materials in figure 1(b) were selected to create a favorable ‘energy map’ for photo-generated electron-hole pairs; that is, the electron affinities of the three semiconductors, together with the band offsets, together with the metals’ work functions, give a valence-and-conduction-diagram yielding selective and efficient collection of photo-created electron-hole pairs. The Fermi level $E_{Fp}$ in figure 1(b) enters ZnSe below its CB edge, while the Fermi level $E_{Fn}$ enters the Al$_{1-x}$Ga$_x$Sb above its VB edge. In the figure 1(b) approach, the Ti front electrode readily collects electrons from the Si absorber, whereas electrons traveling to the Al$_{1-x}$Ga$_x$Sb encounter the CB blocking barrier. Similarly, the Ni back electrode will extract holes from the Si absorber (over a small barrier), while holes traveling to the ZnSe window interface will be blocked by the large VB-offset barrier. The 2.70 eV band gap, $E_g$ of ZnSe produces type-II band alignment with Si due to ZnSe’s electron affinity (EA) of 4.09 eV compared with 4.05 eV EA of Si. Regarding the choice of BSF material, we require $E_g$ for this material to exceed the 1.12 eV $E_g$ of Si by 0.2 or 0.3 eV, and a type II offset is also needed. The ternary alloy Al$_{1-x}$Ga$_x$Sb looks quite suitable here because its individual semiconductor components AlSb and GaSb offer $E_g$ of 3.60 eV (0.70 eV, 4.06 eV), respectively. When determining the ($E_{p}$, EA) of Al$_{1-x}$Ga$_x$Sb, a linear interpolation has been used between the AlSb and GaSb values. After examining several trial values of alloy composition, it is concluded that the 80% AlSb alloy Al$_{0.8}$Ga$_{0.2}$Sb was the best choice because it offered ($E_{p}$, EA) of (1.42 eV, 3.69 eV) which gave the desired band alignments.

To form a suitable Ohmic contact to ZnSe in figure 1(b), the work function (WF) of the cathode metal should be less than 4.0 eV, and here Ti is a good choice; while for the anode metal, its WF should be greater than 5.1 eV for suitable Ohmic contact to the Al$_{0.8}$Ga$_{0.2}$Sb. That suggests that (111) Ni at 5.24 eV [31] is an economical choice; more cost-effective than Au (WF = 5.3 eV).

Solar radiation is primarily absorbed in the Si. There is very little parasitic absorption in ZnSe because of its wide 2.70 eV band gap (The ZnSe absorption overlaps only a tiny portion of the solar spectrum). In principle, the parasitic absorption is zero in the Al$_{0.8}$Ga$_{0.2}$Sb BSF because the Si transmits to the BSF only photons ‘below the Si gap’ and these are also ‘below the BSF gap’ because $E_g$(Al$_{0.8}$Ga$_{0.2}$Sb) > $E_g$(Si). Regarding the absorber-BSF band offsets in the Si cell, for intrinsic Si and intrinsic Al$_{0.8}$Ga$_{0.2}$Sb, the CB hole barrier at the interface was (4.05–3.69 = +0.36) eV and the $E_g$ = 1.42 eV for Al$_{0.8}$Ga$_{0.2}$Sb induced a VB anti-barrier of (4.05 + 1.12) - (3.69 + 1.42) = 0.06 eV. However, the actual doping of $10^{16}$ and $10^{17}$ cm$^{-3}$ for absorber and BSF, respectively, increased the built-in potential at the Si/Al$_{0.8}$Ga$_{0.2}$Sb interface, which then modified the hetero-offsets to
and blende lattice of ZnSe helpful in understanding the band structure of this Si-wafer based DH solar cell. Si-based micro-photonic devices used in biosensing and monitoring system and electro-optic sensors might be simulation. The three semiconductors in the GaAs cell have closely matched lattices, but that is not the case for shunt resistances were set to ideal values and no radiative recombination coef...cells were illuminated by the AM 1.5 G spectrum at an operating temperature of 300 K. The values of series and intrinsic AlAs$_{0.9}$Sb$_{0.1}$, the CB hole barrier at the interface was...for AlAs$_{0.9}$Sb$_{0.1}$ induced a VB anti-barrier of 1.42 eV, 4.07 eV of GaAs will be absorbed in the BSF; hence no parasitic absorption there. To form a suitable Ohmic contact to AlAs$_{0.9}$Sb$_{0.1}$ in...type-II offset of 0.4 to 0.5 eV in the CB, with an Eg of around 1.9 eV. Here we identified the material AlAs$_{1-x}$Sbx as the best BSF because its constituents AlAs and AlSb offer (Eg, EA) of (2.16 eV, 3.50 eV) and (1.60 eV, 3.60 eV), respectively. Using linear interpolation to determine AlAs$_{1-x}$Sbx properties, we then found that the composition choice x = 0.1 gives the desired band offsets because that ternary alloy provided (Eg, EA) of (1.656 eV, 3.59 eV) as shown in figure 2(b). Because the AlAs$_{0.9}$Sb$_{0.1}$ BSF layer has Eg = 1.656 eV, very few photons with energy below the Eg (1.42 eV) of GaAs will be absorbed in the BSF; hence no parasitic absorption there. To form a suitable Ohmic contact to AlAs$_{0.9}$Sb$_{0.1}$ in figure 2(b), the WF of the anode metal should be greater than 5.2 eV, and here again Ni is a good choice. Regarding the absorber-BSF band offsets in the GaAs cell, for intrinsic GaAs and intrinsic AlAs$_{0.9}$Sb$_{0.1}$, the CB hole barrier at the interface was (4.07–3.59 = +0.48) eV and the Eg = 1.66 eV for AlAs$_{0.9}$Sb$_{0.1}$ induced a VB anti-barrier of (4.07 + 1.42)–(3.59 + 1.66) = 0.24 eV. However, the actual doping of 10$^{16}$ and 10$^{19}$ cm$^{-3}$ for absorber and BSF, respectively, increased the built-in potential at the GaAs/AlAs$_{0.9}$Sb$_{0.1}$ interface, which then modified the hetero-offsets to become +0.147 eV at CB and +0.098 eV at VB.

Regarding the lattice mismatches that are present in figure 2(b), the ZnSe (a = 5.671 Å) has a 0.4% larger lattice than GaAs (a = 5.650 Å) while the GaAs is mismatched by 1.0% with respect to the AlAs$_{0.9}$Sb$_{0.1}$ alloy that has a = 5.708 Å. These mismatches are very small.

3. Simulation of solar cells and assumptions

The SCAPS-1D version 3.3.07 was used to simulate the Si and GaAs double-heterojunction solar cells. The solar cells were illuminated by the AM 1.5 G spectrum at an operating temperature of 300 K. The values of series and shunt resistances were set to ideal values and no radiative recombination coefficients were considered in the simulation. The three semiconductors in the GaAs cell have closely matched lattices, but that is not the case for...
Table 1. The physical parameters used in the simulation for the Si and GaAs wafer-based DH solar cells.

| Parameters                        | n-ZnSe [17, 41] | p-Si [42] | p⁺ - Al₀.₉Ga₀.₁Sb [43, 44] | p - GaAs [45, 46] | p⁺ - AlAs₀.₉Sb₀.₁ [47, 48] |
|-----------------------------------|-----------------|-----------|---------------------------|------------------|-----------------------------|
| Thickness (μm)                    | 2               | 350       | 2                         | 200              | 2                           |
| Band gap (eV)                     | 2.70            | 1.12      | 1.42                      | 1.42             | 1.656                       |
| Electron affinity (eV)            | 4.09            | 4.05      | 3.69                      | 4.07             | 3.59                        |
| Dielectric permittivity (relative)| 10              | 11.90     | 12.04                     | 13.18            | 10.1                        |
| CB effective density of states (1/cm³) | 1.5 × 10¹⁸     | 2.82 × 10¹⁹ | 7.8 × 10¹⁷              | 4.7 × 10¹⁷       | 1.5 × 10¹⁹                  |
| VB effective density of states (1/cm³) | 1.8 × 10¹⁹     | 1.83 × 10¹⁹ | 1.8 × 10¹⁷              | 7.0 × 10¹⁸       | 1.7 × 10¹⁹                  |
| Electron thermal velocity (cm s⁻¹) | 1.00 × 10⁷      | 2.30 × 10⁷ | 1.7 × 10⁷               | 1.0 × 10⁷        | 1.7 × 10⁷                   |
| Hole thermal velocity (cm s⁻¹)     | 1.00 × 10⁷      | 1.65 × 10⁷ | 1.4 × 10⁷               | 1.0 × 10⁷        | 1.4 × 10⁷                   |
| Electron mobility (cm² V⁻¹ s⁻¹)   | 50              | 1400      | 200                       | 4600             | 200                         |
| Hole mobility (cm² V⁻¹ s⁻¹)       | 20              | 450       | 420                       | 239              | 100                         |
| Shallow uniform donor density, Nᵥ (1/cm³) | 10¹⁸        | 0         | 0                         | 0                | 0                           |
| Shallow uniform acceptor density, Nₐ (1/cm³) | 0          | 10¹⁶      | 10¹⁷                      | 10¹⁷             | 10¹⁹                        |
| Defect density (cm⁻³) (above Eᵥ w.r.t. E₀f (eV)) | 10⁻¹³       | 10⁰       | 10¹³                      | 10¹⁰             | 10¹³                        |

| Defect Type                        | Single Acceptor | Single Donor | Single Donor/Acceptor | Single Donor | Single Donor/Acceptor |
|-----------------------------------|-----------------|-------------|-----------------------|-------------|-----------------------|
| Capture Cross section Electrons (cm²) | 10⁻¹⁵           | 10⁻¹⁵       | 10⁻¹⁵                 | 10⁻¹⁵       | 10⁻¹⁵                 |
| Capture Cross section Holes (cm²)  | 10⁻¹⁵           | 10⁻¹⁷       | 10⁻¹⁵                 | 10⁻¹⁷       | 10⁻¹⁵                 |
| Reference for defect energy level Eᵥ | Above Eᵥ (SCAPS, <2.7) | Above Eᵥ (SCAPS, <2.7) | Above Eᵥ (SCAPS, <2.7) | Above Eᵥ (SCAPS, <2.7) | Above Eᵥ (SCAPS, <2.7) |
| Energy level with respect to Reference (eV) | 1.35           | 0.65        | 0.80                  | 0.71         | 0.80                  |

Note: The number in the [ ] indicates the reference numbers.

the Si cell. A large concentration of defects within window and BSF films with Gaussian distribution having characteristic energy of 0.1 eV were considered for Si and GaAs DH solar cells.

The relevant physical parameters of the three semiconductors in each cell were collected from the literatures for both the Si and GaAs cells. The film thickness in the 'micron range' for both window and BSF films, and a wafer thickness in the range of 200 to 400 μm were used in the simulation. A high volume concentration of defects of the order of 10¹³ cm⁻³ in both window and BSF layers and a much lower density of defects of the order of 10⁹ and 10¹⁰ cm⁻³ in the commercial Si and GaAs absorber wafers, respectively were considered in the simulation. The interface defect density of the order of 10⁸ cm⁻² was considered at each interface for Si and GaAs solar cells. The complete list of physical parameters that were used in solar-cell simulations is presented in table 1, for Si and GaAs, respectively. The optical absorption coefficient data of each semiconductor used in the simulations were taken from the following literature references for ZnSe [34], Si [35], GaAs [36], AlSb [37, 38] GaSb [39] and AlAs [40].

The physical parameters such as the electron and hole mobilities and densities-of-states of the Al₀.₈Ga₀.₂Sb and AlAs₀.₉Sb₀.₁ BSF materials were used with the similar values as those of AlSb, and AlAs, respectively. The nᵖ⁺ dopings used in the simulations were rather modest at 10¹⁸, 10¹⁶ and 10¹⁷ cm⁻³ for Si solar cell whereas nᵖ⁺ dopings for GaAs solar cell were 10¹⁸, 10¹⁶ and 10¹⁹ cm⁻³, respectively.

An approximation was made to determine the optical absorption spectrum of the ternary BSF alloys for simulations. The absorption edges of AlSb and GaSb are found at 775 and 1771 nm wavelengths, respectively. For Al₀.₈Ga₀.₂Sb, using linear interpolation, the spectrum of AlSb was shifted by 199 nm along the wavelength axis that yielded the absorption edge of the ternary spectrum at 974 nm. Similarly, the spectrum of AlAs₀.₉Sb₀.₁ was set by shifting the spectrum of AlAs rigidly along the wavelength scale by 20 nm to 594 nm (linear interpolation), as the AlAs and AlSb absorption edges are at 574 and 775 nm, respectively. No reflectance at the front surface of the solar cell was considered during the simulation [49].

4. Results and discussion

We embark upon a study of how the physical parameters of the Si wafer effects the photovoltaic performance of the n-ZnSe/p-Si/p⁺ -Al₀.₉Ga₀.₂Sb DH solar cell. We examined the dependence of PV parameters upon the bulk defect density, doping density, and thickness of Si wafer and the results are presented in figure 3.
As shown in figure 3(a), the $J_{SC}$ of the Si solar cell increases with thickness of the Si wafer. The value of $J_{SC}$ is $\sim 38.83 \text{ mA cm}^{-2}$ at a thickness of 150 $\mu$m which increases to $\sim 40.82 \text{ mA cm}^{-2}$ at a thickness of 450 $\mu$m of Si wafer. This is resulted as the enhanced photon absorption in the thicker Si wafer causing the increased electron-hole pairs (EHPs) and hence the higher $J_{SC}$\cite{13, 50}. On the other hand, the $V_{OC}$ and FF of the solar cell slightly decrease with thickness of the Si wafer. It is also noted that the value of $V_{OC}$ is $\sim 1.13 \text{ V}$ which is resulted due to the higher built-in potentials developed at the n-ZnSe/p-Si and p-Si/p$^+$-Al$_{0.8}$Ga$_{0.2}$Sb heterointerfaces\cite{14}. However, as seen in the figure, the PCE ($\eta$) of the Si DH solar cell is almost independent of absorber thickness over the 150 to 450 $\mu$m range. The doping density of the Si wafer was varied from $10^{14}$ to $10^{17}$ cm$^{-3}$ and it is observed that $\eta$ is almost independent of p-doping concentration over the range as depicted in figure 3(b). This indicates that intrinsic recombination rate (radiative and Auger recombination) in the p-Si layer is not dominant and hence PCE does not change in this range of doping\cite{51}. Figure 3(c) shows that $\eta$ has moderate dependence on defect density over the $10^8$ to $10^{11}$ cm$^{-2}$ range. It is observed in the figure that $J_{SC}$ is almost constant with the
change in defect density. Whereas, the $V_{OC}$ and FF decrease markedly due to the increase in Si defects which may happened due to the increase in dark current density with defects by recombination of charge carriers \[50\]. The linear decrease in $V_{OC}$ with defect density indicates that total number of defects in the absorber layer rather than defect density determines the $V_{OC}$ and hence PCE in the Si DH solar cell \[52\].

The optimized result obtained for the Si DH solar cell is a PCE of 38.3% with $V_{OC} = 1.13$ V, $J_{SC} = 40.57$ mA cm$^{-2}$ and FF = 83.69%, respectively when a bulk defect density of $10^9$ cm$^{-3}$ is assumed for the 350 μm wafer, assuming also $10^{13}$ cm$^{-3}$ defects in window and in BSF.

Figure 4 delineates the effect of different physical parameters in GaAs wafer on the photovoltaic performance of the \textit{n-ZnSe/p-GaAs/p-AlAs$_{0.9}$Sb$_{0.1}$} double-heterojunction solar cells. Figure 4(a) shows the effect of

![Figure 4](image-url)

\textbf{Figure 4.} Impact of the wafer/absorber properties upon the power conversion efficiency of the \textit{n-ZnSe/p-GaAs/p-AlAs$_{0.9}$Sb$_{0.1}$} double-heterojunction solar cells solar cell.
thickness of GaAs wafer on the PV performance of $n$-ZnSe/$p$-GaAs/$p^+\text{-AlAs}_0.9\text{Sb}_{0.1}$ double-heterojunction solar cells. As observed in the figure, both JSC and VOC are almost independent of the thickness of the GaAs wafer. It is noted that the VOC of the GaAs DH solar cell is ~1.31 V. This higher value of open circuit voltage is produced due to the higher built-in potentials developed at the $n$-ZnSe/$p$-GaAs and $p$-GaAs/$p^+\text{-AlAs}_0.9\text{Sb}_{0.1}$ heterointerfaces [14]. The FF of the solar cell slightly decreases with the thickness of the GaAs absorber layer. Therefore, the PCE of the slightly decreases with the GaAs absorber thickness over 150 to 300 $\mu$m. Figure 4(b) indicates that both JSC and VOC are almost independent of the doping concentration of the GaAs absorber layer. However, it is also seen in the figure that only FF negligibly decreases at a doping after $10^{16}$ cm$^{-3}$. Therefore, it is almost independent of $p$-doping concentration over $10^{14}$ to $10^{17}$ cm$^{-3}$. Figure 4(c) shows that JSC of the GaAs DH solar cell is almost independent with the defect density over $10^9$ to $10^{12}$ cm$^{-3}$. It is also observed that both VOC and FF are almost constant up to a defect density of $10^{10}$ cm$^{-3}$, after that they start to decrease with the increase in defects as a result of the increase in dark current due to recombination [50].

The result obtained for the GaAs wafer DH solar cell is a PCE of 38.9% with VOC = 1.31 V, JSC = 33.00 mA cm$^{-2}$ and FF = 90%, respectively when a bulk defect density of $10^{10}$ cm$^{-3}$ is assumed for the 200 $\mu$m GaAs wafer, assuming also $10^{13}$ cm$^{-3}$ defects in window and in BSF.

5. Conclusion

Silicon and Gallium Arsenide wafer-based $n$-ZnSe/$p$-Si/$p^+\text{-AlAs}_0.9\text{Sb}_{0.1}$ and $n$-ZnSe/$p$-GaAs/$p^+\text{-AlAs}_0.9\text{Sb}_{0.1}$ double-heterojunction solar cells, respectively have designed and simulated using SCAPS-1D simulator with experimental data taken from literatures. The solar cell structures have been optimized considering thicknesses, adequate bulk and interface defects and proper metallizations. The optimized Si DH solar cell provides a PCE of 38.3% with VOC = 1.13 V, JSC = 40.57 mA cm$^{-2}$ and FF = 83.69%, respectively for a wafer thickness of 350 $\mu$m. On the other hand, The GaAs wafer DH solar cell yields a PCE of 38.9% with VOC = 1.31 V, JSC = 33.00 mA cm$^{-2}$ and FF = 90%, respectively for a wafer thickness of 200 $\mu$m. The higher efficiency in both the solar cells is mainly produced due to the higher VOC developed in the devices. The PCEs of both the Si and GaAs wafer-based DH solar cell remain efficiency limit set by the Shockley–Queisser detailed-balance theory. These results indicate the potential of the fabrication of wafer-based cost-effective double-heterojunction solar cells in the future.

Acknowledgments

The author appreciates many helpful discussions with Professor Richard Soref of the University of Massachusetts at Boston. The author also wishes to thank Professor Marc Burgelman of the Department of Electronics and Information Systems, University of Gent, Belgium for providing the SCAPS software package, version 3.3.07. The author also acknowledges Mr Bipanko Kumar Mondal, Department of Electrical Engineering, University of Rajshahi, Bangladesh for his help in simulations.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Disclosures

The authors declare no conflicts of interest.

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