Optimization of a CNT-based SiGe Thin Film Solar Cell Structure

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Optimization of a CNT-based SiGe thin film solar cell structure

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Abstract
In this paper, a SiGe thin film solar cell structure based on the carbon nanotube (CNT) and with a back surface field (BSF) layer is proposed. The efficiency of this structure is 40.36%, which is higher than conventional structures without CNT layer. We optimize this structure by changing the base layer thickness and determining the ratio of the width of the upper contact to the width of the entire cell. The cell efficiency after this optimization reaches 41.08%. Furthermore, the performance of this cell is evaluated using two types of CNT layers with sheet resistances of 128 Ω/□ and 76 Ω/□. The results of numerical simulation show that the SiGe thin film solar cell using CNT layer with 128 Ω/□ sheet resistance has better performance parameters. Finally, the number of metal electrodes above the cell is optimized due to the shading effect and we show that the contact distance in the presence of CNT layer can be increased up to 2000 μm.

Keywords: Solar cell, SiGe thin film, Carbon nanotube (CNT), Optimization.

1-Introduction
Solar cell technology is one of the most interesting types of renewable energy and seems to be the solution for environmental problems such as global warming. It is believed that the share of photoelectric system (PES) in electricity consumption will increase to 25-30% by 2030 [1]. The Si solar cells lead the real photovoltaic (PV) market due to their abundance of raw materials, stability, fabrication technology development and high efficiency. Si solar cells currently control approximately 90% of the total PV market [2, 3]. It has been shown that the SiGe material has better properties than the Si material, such as higher absorption coefficient at higher wavelengths, higher conductivity, production at lower cost, higher mechanical strength, suppresses the high-intensity degradation of the solar cell under illumination and the ability to change the band gap by changing the fraction of germanium [4]. Also, there is expected to be a significant increase in photocurrent in the SiGe solar cell because the photon absorption is increased. On the other hand, the decrease in open circuit voltage (V_{OC}) is seen due to the reduction of the SiGe band gap, which should be considered and prevented in optimizing cell behavior [5].

SiGe and GaAs-SiGe dual-junction solar cells are widely used as bottom layers of multi-junction or tandem solar cells due to their high mobility, production process compatibility, adjustable lattice constant and the ability to absorb light with wavelengths up to 1800 nm [6-8].

On the other hand, carbon nanotubes (CNTs) are promising candidates for a variety of electronic and photonic applications in nanoscale. The presence of nanotubes leads to increase the carrier’s mobility and conductivity [9]. Many researchers have focused on CNT applications in solar cells to reduce the total resistance and shading effect. Due to the special properties of CNTs such as semi-transparent conductor, anti-reflect coating, self-cleaning, they used as emitter or p-layer in Si-based solar cells [10-12]. Also, the use of CNT layer has been reported in many other types of solar cells [13-19]. Some of the reported CNT-based solar cell structures are listed in Table 1.
We recently reported a CNT- based SiGe thin film solar cell structure and showed that this cell in the presence of the CNT layer as a charge collector can have an efficiency about 40.05%, which is about 5.3% higher than the structure without CNT [20]. In this paper, the aim is to improve the characteristics of the solar cell by optimizing this structure. Optimizing the structure contains some step, first of all adding a layer of GaAs as a back surface field (BSF) to prevent the carrier recombination then choosing the appropriate CNT according to the sheet resistance and transparency, finally we optimize the thickness of the base layer and the distance between the top metal contacts.

The rest of this paper is organized as follows. Section 2 describes the proposed CNT-based SiGe thin film solar cell structure. In section 3, we present the employed theoretical model for simulation of the device. Section 4 covers the results and discussions for the simulation and optimization of the cell structure. Finally, we conclude this paper in section 5.

2- The proposed structure of CNT-based SiGe thin film solar cell

Figure 1(a) shows a schematic of the base structure of CNT-based SiGe thin film solar cell. The solar cell heterostructure consist of a SiGe layer with a thickness of 12 μm as the substrate, 8 μm -thick SiGe as the base layer, 400 nm-thick SiGe as the emitter layer, 500 nm-thick GaAs as the window layer, and a CNT layer with thickness of 100 nm as the charge collector. Also, gold layer with a thickness of 100 nm is used as the electrodes.

Single-walled carbon nanotubes (SWNTs) are one-dimensional conductors and narrow-band semiconductors with a diameter of about 1 nm and a length of several micrometers. SWNT networks have been successfully used in various devices as an alternative to transparent conductive oxides (TCOs). Due to the difficulty of manufacturing and the cost of producing high quality TCOs, the CNTs are good alternative to these transparent conductors [21]. Using a more conductive and transparent material as a top layer in the solar cell can improve the overall efficiency. Because CNTs can reduce the surface area of solar cells covered by the top metal girds, on the other hand, we can increase the distance between the metal mesh lines that collect current. Using the CNT layer as the charge collector and the transparent layer helps us to create a low-resistance path for the carriers, which can reduce the series resistance of the cell. This ultimately leads us to reduce the number of front electrodes and the shading effect. All of these can improve the solar cell performance [22, 23].
Figure 1(b) shows a schematic of the proposed CNT-based SiGe thin film solar cell structure with a back surface field (BSF) layer. The GaAs layer with thickness of 2 μm, as the BSF, prevents the carrier recombination and is expected to play a significant role in increasing the cell efficiency. The layer thickness and doping profile of these structures are summarized in Table 2.

![Figure 1(b) schematic of the proposed CNT-based SiGe thin film solar cell structure with a back surface field (BSF) layer.](image)

Table 2. Layer thickness and doping profile

| Structure Cell | Layer        | Material | Thickness (µm) | Doping (cm$^{-2}$) |
|---------------|--------------|----------|----------------|--------------------|
| a)            | Electrode    | Au       | 0.1            | -                  |
|               | Semi-transparent | CNT | 0.1            | -                  |
|               | Window       | GaAs     | 0.5            | P type-1e18        |
|               | Emitter      | SiGe     | 0.4            | P type-1e18        |
|               | Base         | SiGe     | 8              | N type-1e17        |
|               | Substrate    | SiGe     | 12             | N type-3e18        |
|               | Electrode    | Au       | 0.1            | -                  |
|               | Semi-transparent | CNT | 0.1            | -                  |
|               | Window       | GaAs     | 0.5            | P type-1e18        |
|               | Emitter      | SiGe     | 0.4            | P type-1e18        |
|               | Base         | SiGe     | 8              | N type-1e17        |
|               | Substrate    | SiGe     | 10             | N type-5e17        |
|               | Substrate(BSF) | GaAs | 2              | N type-1e18        |

Fig1:(a) The CNT- based thin film SiGe solar cell structure, (b) The CNT- based thin film SiGe solar cell structure with the BSF layer.
3- Theoretical modeling

For simulation of the solar cell structure, the dynamics of the carrier can be described by the one-dimensional equations of drift-diffusion, the current continuity equations and the Poisson equation. The Poisson equation is shown below:

\[ \nabla^2 V = \frac{q}{\varepsilon_r \varepsilon_0} (n - p - N) \]  

(1)

where \( V \) is the potential, \( q \) is the initial charge, \( \varepsilon_r \) and \( \varepsilon_0 \) are the relative dielectric constant and the vacuum dielectric constant, respectively. \( n \) and \( p \) are the electron and hole concentration, respectively. The drift-diffusion equation and the current continuity equation are expressed as follows:

\[ J_n = -qn \mu_n \nabla V + qD_n \nabla n \]

\[ J_p = -qp \mu_p \nabla V - qD_p \nabla p \]  

(2)

where \( J_n \) and \( J_p \) are the electron and hole current density, respectively. \( \mu_n \) and \( \mu_p \) are the electron and hole mobility and \( D_n \) and \( D_p \) are the electron and hole diffusion constant, respectively.

\[ \frac{1}{q} \nabla.J_n - R_n + G_n = 0 \]

\[ \frac{1}{q} \nabla.J_p - R_p + G_p = 0 \]  

(3)

where \( G_n \) and \( G_p \) are the electrons and hole generation rate because of light illumination. \( R_n \) and \( R_p \) are the recombination rate of electrons and holes, respectively [24-26].

Also, the charge carrier statistics in the CNT layer can be described as follows [22]:

\[ p - n = \text{sign}(E_D - E_F) \frac{1}{\pi \eta F} \frac{1}{\nu_F^2} (E_F - E_D)^2 \]  

(4)

Where \( p \) and \( n \) are the holes and electrons density in the CNT layer, \( E_D \) and \( E_F \) are the Dirac point and the Fermi level of the CNT layer, respectively. Also, \( \hbar \) is the reduced Planck's constant and \( \nu_F \) is the Fermi velocity in the CNT layer. The height of the junction barrier in the CNT/SiGe can be inferred by matching the JV curves (in the dark mode) in the Schottcky CNT/SiGe diode:
\[ J = J_0 \left( \exp \left( \frac{qV}{N_{IF}KT} \right) - 1 \right) \]  

(5)

where \( K \) is Boltzmann's constant, \( N_{IF} \) is the ideal factor of the junction, and \( T \) is temperature. Based on the thermionic-emission theory, the saturation current density, \( J_0 \), is described as follows:

\[ J_0 = A^*T^2 \exp(-\frac{q\Phi_{\text{barrier}}}{KT}) \]  

(6)

where \( A^* \) is the effective Richardson constant and is \( 127 \text{ A/cm}^2\text{K}^2 \) for the n-type SiGe layer [22, 27].

By solving the above equations, the different performance parameters of the solar cell are determined. The I-V curve of the solar cell is the superposition of the I-V curve of the solar cell diode (in the dark mode) with the current generated by light [22].

\[ I = I_0 \left[ \exp\left( \frac{qV}{nKT} \right) - 1 \right] - I_L \]  

(7)

The I-V characteristic and the open circuit voltage (\( V_{oc} \)) of the solar cell are as follows:

\[ I = I_0 \left[ \exp\left( \frac{qV}{nKT} \right) - 1 \right] \]  

(8)

\[ V_{OC} = \frac{nKT}{q} \ln\left( \frac{I_L}{I_0} + 1 \right) \]  

(9)

where \( I_L \) is the light output, \( n \) is ideality factor of junction, \( K \) is Boltzmann's constant and \( T \) is the temperature.

In general the power delivered from a power source can be \( P = IV \). If the current density of \( J \) is used in this relation, we obtain the power density (\( P_d = JV \)). The maximum power density occurs somewhere between \( V = 0 \) (short circuit) and \( V = V_{oc} \) (open circuit) at \( V_m \) voltage. The corresponding current density is called \( J_m \), so the maximum power density is \( P_m = J_mV_m \). The efficiency of a solar cell is as follows [22, 28]:

\[ P_{max} = V_{OC}I_{SC}FF \]  

(10)

\( FF \) is fill factor that used to describe a solar cell performance. The fill factor can be defined as follows:

\[ FF = \frac{V_{OC} - \ln(V_{OC} + 0.72)}{V_{OC} + 1} = \frac{I_mV_m}{I_{SC}V_{OC}} \]  

(11)

Using \( FF \) we can write the efficiency as follow:
\[ \eta = \frac{V_{oc}I_{sc}FF}{P_{in}} = \frac{P_{\max}[W] \times 100}{1000[W/m^2] \times CellArea[m^2]} \]  \hspace{1cm} (12)\\

where \(V_{oc}\) and \(I_{sc}\) are open circuit voltage and short circuit current respectively and \(P_{in}\) the input light power density, which is assumed to be 1000 Wm\(^{-2}\) in our simulation.

4- Results and discussions

In this section, the proposed structure of CNT-based SiGe thin film solar cell with BSF layer and also the structure of CNT-based SiGe thin film solar cell without BSF layer are simulated and the performance characteristics of cells such as short circuit current, open circuit voltage and efficiency of two structures are calculated. The material parameters used in our simulation are given in Table 3.

| layer identifier | CNT     | Window | Absorber         |
|------------------|---------|--------|------------------|
|                  | 128Ω/□ | GaAs   | SiGe(x=0.1)      |
| \(E_g\) (eV)     | 0.026   | 1.42   | 1.08             |
| Affinity (eV)    | 5.8     | 4.07   | 4.045            |
| Permittivity \(\varepsilon\) (Fcm-1) | 5.4     | 13.1  | 12.15            |
| \(\mu_n\) (cm\(^2\)/vs) | 8138.2  | 8000  | 1000             |
| \(\mu_p\) (cm\(^2\)/vs) | 8138.2  | 400   | 500              |
| Conduction band effective density of state NC (cm\(^3\)) | 3×10\(^{17}\)  | 4.7×10\(^{17}\)  | 2.62×10\(^{19}\) |
| Valence band effective density of state NV (cm\(^3\)) | 3×10\(^{17}\)  | 7×10\(^{18}\)  | 0.996×10\(^{19}\) |

The numerical simulation results are presented in Table 4. For further comparison, the characteristics of the conventional SiGe solar cell structure without the CNT layer are shown. As can be seen, the proposed structure has a higher efficiency than the other two structures.

| Solar structure               | \(I_{sc}\) | \(V_{oc}\) | \(V_m\) | \(I_m\) | \(P_{\max}\) | FF   | eff  |
|-------------------------------|------------|------------|--------|--------|-------------|------|------|
| Conventional SiGe solar cell  | 0.061      | 0.6732     | 0.59   | 0.061  | 0.0385      | 85.65| 34.67|
| 'a' structure                 | 0.069      | 0.7099     | 0.61   | 0.066  | 0.0413      | 83.94| 40.05|
| 'b' structure                 | 0.069      | 0.7121     | 0.62   | 0.067  | 0.0416      | 83.95| 40.36|
In the proposed CNT-based SiGe thin film solar cell structure, using the high doped GaAs material as the back surface field (BSF) layer creates the energy offset between the SiGe and GaAs layers on the conduction and valence bands. Hence, this BSF layer greatly reduces the recombination rate due to a barrier against carriers and increases cell efficiency. The $E_V$ and $E_C$ band offset depends on the concentration of Ge in the SiGe layer. In addition to the lower surface recombination rate, and the smaller band gap, at higher concentrations of Ge in SiGe, the light absorption coefficient is higher, which can lead to the production of more electron-hole pairs and could increase $J_{SC}$ and both of these factors can increase the efficiency of SiGe-based solar cells [30].

The energy band diagram of the proposed solar cell structure is shown in Figure 2.

![Energy Band Diagram](image)

**Fig 2.** The energy band diagram of the proposed solar cell structure.

As mentioned earlier, in these structures the CNT layer plays an important role in the cell performance. The rapid transfer of electron-hole pairs which was created in the absorber layer to the contact well done by the CNT layer. In the next step, we intend to use two different types of CNT to simulate the proposed structure of the solar cell and calculate and compare the performance characteristics of the cell.

The two types of CNT used to simulate the proposed cell structure were developed by the Canadian Institute of Microstructural Sciences with sheet resistances of 76 and 128 Ω/□. In the heterogeneous CNT network, 1/3 of the nanotubes are metal and 2/3 of them are semiconductors. This layer is used as a charge collector in the cell structure and creates a low resistance path for the carrier to reach the high contact surface. The simulation parameters of the two types of CNTs used are presented in Table 5.

| Table 5. Simulation parameters of CNTs with different sheet resistances |
|--------------------------------------------------|------------------|
| Layer identifier | CNT 128 Ω/□ | CNT 76 Ω/□ |
| $E_g$ (eV) | 0.026 | 0.026 |
| Affinity (eV) | 5.8 | 5.8 |
| Permittivity $\varepsilon_r$ (Fcm$^{-1}$) | 5.4 | 5.4 |
| $\mu_n$ (cm$^2$/vs) | 8138.2 | 13889 |
|                           | \(\mu_p\) (cm\(^2\)/Vs) | 8138.2 | 13889 |
|---------------------------|---------------------------|-------|------|
| Conduction band effective density of state NC (cm\(^3\)) | \(3 \times 10^{17}\)     | \(3 \times 10^{17}\) |
| Valence band effective density of state NV (cm\(^3\))    | \(3 \times 10^{17}\)     | \(3 \times 10^{17}\) |

Figure 3 shows the current density of electrons and holes in the proposed cell structure. As shown in the figure, the current density near the CNT layer is the maximum value. Indeed, the charge carriers were created in the absorber layer are separated and sent to the contacts through the CNT layer. This is the important role of the CNT layer in the solar cell performance.

For simulating different structures of solar cells and the ability to compare their performance, incoming light with standard AM0 or AM1.5 spectra is considered. In this simulation, we considered the CNT layer to be completely transparent and modeled the input power spectrum of the cell using the information of the CNT layer transmission spectrum for 128 and 76 Ω/□ sheet resistances [22]. Figure 4 shows the transmission spectra of two different CNT layers with resistances 128 and 76 Ω/□. Also, the modified AM1.5 spectrum is shown in Figure 5 by considering the transmission coefficient of two different CNT layers with different sheet resistances 128 and 76 Ω/□, which we use as the input power spectrum in the simulation.

Figure 4. Transmission spectra of two different CNT layers [23]
In order to select the appropriate CNT layer, the proposed cell structure is simulated with two types of CNT layers with different sheet resistances, 76 and 128 $\Omega/\square$, and the voltage-current characteristic and efficiency in both cases are compared. Higher sheet resistance means lower density of metal nanotubes and consequently more transparency of the layer. On the other hand, the small sheets resistance means higher nanotubes concentrations which decrease light absorption and can reduce the performance of the whole cell. Figure 6 shows the I-V characteristics using two types of CNT layers with different Sheet resistances, also the efficiencies of these two cell types are also shown in Table 6. According to these results, the CNT layer with sheet resistance of 128 $\Omega/\square$ leads to a better result and higher efficiency.

Next, for the proposed CNT-based SiGe solar cell structure in the presence of a CNT layer with a sheet resistance of 128$\Omega/\square$ as the charge collector layer, we optimize the thickness of the base layer and try to find the best thickness of this layer. Figure 7 shows the cell efficiency for changes in the base layer thickness from 12 microns to 0.3 microns. As can be seen, the efficiency of the solar cell is maximized for a thickness of 0.5 microns.
In addition, cell performance parameters including efficiency, short-circuit current, and cell open circuit voltage for different base layer thicknesses are listed in Table 7.

![Graph showing efficiency of the solar cell for different base layer thicknesses](image)

**Fig 7. Efficiency of the solar cell for different base layer thicknesses**

| Base Thickness (µm) | $J_{sc}$ (A) | $V_{oc}$ (V) | Efficiency% |
|---------------------|--------------|--------------|-------------|
| 0.4                 | 0.068        | 0.73         | 41.07       |
| 0.5                 | 0.068        | 0.73         | **41.08**   |
| 1                   | 0.068        | 0.721        | 41.06       |
| 4                   | 0.069        | 0.721        | 40.79       |
| 8                   | 0.069        | 0.72         | 40.36       |
| 12                  | 0.069        | 0.7          | 39.95       |

In the final part, we optimize the distance of the metal contacts above the cell. In the initial structure, the width of the upper contact of the cell was considered to be 50 µm and the total width of the cell was considered to be 200 µm, it means 25% of the cell was covered by the upper contact. Here, to optimize the distance between the top electrodes of the cell to reduce the shadowing effect, we change the total width of the cell from 200 to 6000 µm, while the width of the upper contact of the cell in all stages of the simulation is considered a constant value of 50 µm. Figure 8(a) shows the short-circuit current density for a change in the total width of the cell. As can be seen, the short-circuit current density increases with increasing cell width. This result is acceptable because by increasing the cell width and keeping the contact width constant, the percentage of cells covered by the contact decreases and therefore the absorption due to the contact decreases. Figure 8(b) shows the open circuit voltage for the changes in total cell width. As the figure shows, as the cell width increases, the cell open circuit voltage will increase slightly. This small increase in open circuit voltage is due to the generation of more charge carriers in the cell structure.
Figure 9 shows the maximum cell voltage curve for changes in cell width. As can be seen, the $V_{\text{max}}$ of the cell will decrease significantly as the cell width increases. As the width of the cell increases, the distance traveled by the charge carriers to reach the top contact of the cell increases and therefore the voltage drop due to series and shunt resistance increases and this reduces the maximum voltage of the cell. Decreasing $V_{\text{max}}$ reduces the maximum power ($P_{\text{max}}$) in larger the cell width. Therefore, to increase cell efficiency, the cell width cannot be increased too much. Because for large amounts of cell width, the $V_{\text{max}}$ value decreases and hence the $P_{\text{max}}$ decreases.

Figure 10 shows the cell fill factor (FF) for changes in the cell width. As the figure shows, increasing the cell width increases the internal resistance of the cell and thus decreases the FF. Reducing FF can also reduce the maximum available cell power. Therefore, according to the obtained results, the optimum cell width is about 2000 $\mu$m with a top contact width of 50 $\mu$m.
5- Conclusion

In this paper, a CNT-based SiGe thin film solar cell structure with a back surface field (BSF) layer is proposed. We first simulated a CNT-based SiGe solar cell structure without BSF layer and showed that it has an efficiency of about 40.05%. Then, by adding a high doped GaAs as the BSF layer, we increased the efficiency of this structure by 40.36%. We also showed that the CNT layer with higher sheet resistance and greater transparency is more suitable for this structure. Then, by optimizing the thickness of the base layer, we increased the efficiency of the proposed structure to 41.08%. Finally, the distance between the upper contacts was optimized. According to the simulation results, by using the CNT layer on the cell surface, we can increase the distance between the metal contacts without changing their thickness to reduce the shadowing effect. In this proposed cell structure, we obtain an efficiency of 41.08% for a total cell width of 2000 μm and a width of 50 μm for the upper contact.

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**Declarations (Not Applicable)**

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