Heterogeneous carbon nano-tube window layer with higher sheet resistance improve the solar cell performance

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Abstract. The heterogeneous Carbon Nano-Tube (CNT) layers deposited on the window surface of solar cells that allow better charge carrier collection was numerically analyzed and studied in modern TCAD tools. The quantum efficiency (EQE) as well as power conversion efficiency (η) were found to be improved significantly based on the light transmission capabilities of the CNT layer. Two CNT network models using experimental sheet resistance values of 75 Ω/□ and 128 Ω/□ as a top conducting layer in a GaAs solar cell were compared. It is found that the CNT networks allow for a greater area of charge collection as well as serve as a lower resistance path for charge carriers with minimum voltage loss to travel to the top contact. This model thus significantly improve the η up to 30% under AM0 with more than 90% EQE. The effect of cell width varying starting from 200 µm to 4000 µm with CNT top layer on Jsc, Voc and Pmax parameters were studied and found that these parameters remain almost constant irrespective of cell width. This work thus shown that a thin CNT top layers of lower sheet resistance with a higher light transmission can greatly improve the efficiency of solar cells.

1. Introduction
Carbon nanotubes (CNT) possess a wide range of direct band gaps matching the solar spectrum, strong photo absorption, from infrared to ultraviolet, and high carrier mobility, reduced carrier transport scattering, making them ideal photovoltaic material[1]. Photovoltaic effect can be achieved in ideal single wall carbon nanotube (SWCNT) diodes. Individual SWCNTs can form ideal p-n junction diodes [2]. This discovery has influenced a wide research in the solar cell community regarding the use of CNTs as transparent conducting layers. This work focus on heterogeneous networks of SWCNTs as transparent conductors, which, when grown, produce a variety of semiconducting and metallic nanotubes[3]. It has been found that due to the somewhat random distribution of CNTs formed in heterogeneous networks, one third of the tubes are metallic, and the others semiconducting[4]. All these discovery has influenced a wide research in the solar cell community regarding the use of CNTs as transparent conducting layers. The aim of this work was to model a heterogeneous CNT network in Silvaco ATLAS software and use the model to show the possible benefits of the use of CNT networks as a surface layer in all solar cells.
2. Numerical modelling method

It is well known that the metallic nanotubes are highly conductive, therefore they dominate the electrical characteristics of the layer of CNTs. In recent research, heterogeneous networks of CNTs have been simulated to find the conductance and sheet resistance using the Stick Percolation Model and again verified by experimental data in [5],[6]. A thin layer of CNTs on the top layer of a solar cell has the same random orientation of conductors that have a net conductance based on the density of conducting tubes in the area. Higher densities of conducting tubes allow for higher conductance values. The model created in this design was based on parameters from widely accepted recently published experimental data on heterogeneous CNT networks.

2.1 Modeling the material Properties of CNT

A heterogeneous CNT network would be modeled as a metal with the optical properties and resistivity of the CNT network. However, due to the limitations of ATLAS software, the CNT network in this work is modeled as a low bandgap semiconductor. We found that the ATLAS software has problems obtaining solutions when a metal makes contact with an electrode in some specified structure. Since the main aim of this work is to study the flow of charge carriers through a semi-transparent material, the use of a CNT layer as a semiconductor is optimal because the ATLAS software has no problem in obtaining solutions for all of the charge carriers moving towards the electrodes in semiconductors. Though a heterogeneous CNT network does not exhibit semiconductor properties, the material statements in the ATLAS code can be utilized to create a semiconductor with metallic properties. Here, 4-H Silicon Carbide (4H-SiC) was chosen as the semiconductor to alter based on the work of Brunton in the modeling of carbon nano-fiber interconnects in Silvaco Atlas software[7]. The parameters that were changed in the 4H-SiC to model a CNT network are given in Table I.

The electron and hole mobilities were modified to match the experimental sheet resistances of 75 Ω/□ and 128 Ω/□ of the material given in Table I. The resistivity of a semiconductor material and the sheet resistance is given by equation (1) as follows

\[ \rho = \frac{1}{q(\mu_n + \mu_p) t}, \]

\[ R_s = \frac{\rho}{t} \]

where \( q \) is the equivalent charge of one electron or hole, \( \mu_n \) and \( \mu_p \) are the electron and hole mobilities, respectively, \( \mu_n \) and \( \mu_p \) are the electron and hole concentrations in the material, and \( t \) is the thickness of the material.

Table 1. The material parameters that were changed to give 4H-SiC metallic properties in Silvaco ATLAS.

| Critical parameters | ATLAS Identifier | Top CNT 4H-SiC | Top CNT 75Ω/□ |
|---------------------|-----------------|---------------|---------------|
| Layer band gap \( E_g \) (eV) | EG | 0.0 | 0.0 |
| Electron affinity \( X_e \) (eV) | Affinity | 5.8 | 5.8 |
| Relative permittivity \( \varepsilon_r \) (F cm\(^{-1}\)) | Permittivity | 5.4 | 5.4 |
| Electron mobility \( \mu_n \) (cm\(^2\)/V s) | MUN | 8138.02 | 13889 |
| Hole mobility \( \mu_p \) (cm\(^2\)/V s) | MUP | 8138.02 | 13889 |
| Conduction band effective density of states \( N_c \) (cm\(^{-3}\)) | NC300 | \( 3 \times 10^{17} \) | \( 3 \times 10^{17} \) |
| Valence band effective density of states \( N_v \) (cm\(^{-3}\)) | NV300 | \( 3 \times 10^{17} \) | \( 3 \times 10^{17} \) |
| Recombination | Taun,taup0, Augn, Augp, Etrap,Copt etc. | 0.0 | 0.0 |
2.2 Modeling the Optical Properties of CNT
Without altering the optical properties of 4H-SiC material model, firstly it was made to be completely transparent. Then the input solar power AM0 in simulations involving a CNT network was altered to model the resultant light transmitting through the material while leaving the CNT material completely transparent. To achieve this, the transmission data from the Institute for Microstructural Science of the National Research Council of Canada[8] as shown in Figure 1 was used to apply a series of scale factors to alter the AM0 spectrum at different wavelengths[8]. The AM0 spectrum compared with the input spectrums of associated with heterogeneous CNT layers of 75Ω/□ and 128Ω/□ of sheet resistance are shown in Figure 2.

![Figure 1](image1.png)  
**Figure 1.** The experimental light transmission data of a single-dip coated and doubledip coated CNT network show an inverse relationship between sheetresistance and light transmission. From [1].

![Figure 2](image2.png)  
**Figure 2.** The AM0 spectrum is plotted against the spectrums used in simulation of CNT networks with 128Ω/□ and 75Ω/□ of sheet resistance.

3. Modelling CNT based solar cell structure
For the CNT/GaAs heterostructure system, the drift-diffusion equation and current continuity equation (2) are shown as follows [9]:

\[
\begin{align*}
J_n &= -qn\mu_n \nabla V + qD_n \nabla n \\
J_p &= -qn\mu_p \nabla V - qD_p \nabla p \\
\frac{1}{q} \nabla J_n - R_n + G_n &= 0 \\
-\frac{1}{q} \nabla J_p - R_p + G_p &= 0
\end{align*}
\]

(2)

\( J_n, \mu_n, D_n \) are the electron current density, the electron mobility and the electron diffusion coefficient in GaAs respectively. \( J_p, \mu_p, D_p \) are the hole current density, the hole mobility and the hole diffusion coefficient in GaAs respectively. \( G_n, G_p \) are the electron and hole generation rate due to light illumination, \( R_n \) and \( R_p \) are the electron and hole recombination rate respectively. The above equations are solved self-consistently by finite difference method until converged results are obtained. ATLAS permits the user to identify a variety of physics models for calculating carrier mobility and recombination. In our design, we used the following models for our analysis. The Concentration-Dependent Low Field Mobility model (CONMOB) was used to model the doping-dependent low-field mobilities of electrons and holes in AlGaAs/GaAs cell at 300K. The recombination models utilized were the Optical Recombination (OPTR) and the Shockley-Read-Hall (SRH) recombination models. SRH recombination model takes into account the electrons being emitted or captured by donor and
acceptor-like traps. The OPTR determines the possibility that a photon is generated when an electron and hole recombine. Green has shown that the OTPR model increases the accuracy of the solar cell simulation [10]. Thus, we found that ATLAS solves the Poisson, the continuity and current density equations including SRH and AUGER (Auger recombination) mechanisms. The simulation further takes into account the bandgap narrowing effect (BGN), temperature and doping dependent mobility models for the light propagation and photogeneration use the TMM approach. We incorporated SRH FERMI CONMOB OPTR AUGER BGN model in our design shown in Figures 3 and Figure 4.

![Generated finer mesh structure](image)

**Figure 3.** Generated finer mesh structure of the model for accurate realization.

![Final realization of the single junction GaAs cell with top CNT Layer](image)

**Figure 4.** Final realization of the single junction GaAs cell with top CNT Layer.

### 4. Result Analysis and discussion

It is necessary to determine the different performance parameter of the design in order to optimize it. The I-V curve of a solar cell is the superposition of the IV curve of the solar cell diode in the dark with the light-generated current [11]. The following equations (3), (4), (5), (6) and (7) are used to calculate $I_{sc}$, $V_{oc}$, $P_{max}$, $FF$ and Efficiency respectively as follows:

$$I_n = I_0 \left[ \exp\left(\frac{qV}{nKT}\right) - 1 \right]$$  \hspace{1cm} (3)

$$V_{oc} = \frac{nKT}{q} \ln\left(\frac{I_0}{I_n} + 1\right)$$  \hspace{1cm} (4)

$$P_{max} = V_{oc}I_{sc}FF$$  \hspace{1cm} (5)

$$FF = \frac{V_{oc} - Ln(V_{oc} + 0.72)}{V_{oc} + 1} = \frac{I_mV_m}{I_mV_{oc}}$$  \hspace{1cm} (6)

$$\eta = \frac{V_{oc}I_{sc}FF}{P_{in}} = \frac{P_{max}[W] \times 100}{1000[W/m^2] \times CellArea[m^2]}$$  \hspace{1cm} (7)
The I-V curves for the normal GaAs solar cell and a cell including a 128 Ω/□ and 75 Ω/□ sheet resistance CNT layer are compared as shown in Figure 5. As expected with an optimal cell width, the cells with the CNT layers have higher current values than the standard GaAs cell due to the greater charge collection of the CNT layers. A comparison of solar cell performance parameters given in Table 2 including from Experimental Data[12]. The numerical External Quantum Efficiency(EQE) given in Figure 6 imitates well the EQE of a single junction GaAs solar cell with 90% efficiency as compared with other experimental data[12]

| Cell                | Isc  | Voc  | Vm  | Im  | Pm  | FF   | Eff  |
|---------------------|------|------|-----|-----|-----|------|------|
| 128 Ω/□ CNT         | 33.23| 1.044| 0.94| 32.46| 34.12 | 86.43| 29.18|
| 75 Ω/□ CNT          | 28.45| 1.032| 0.93| 27.37| 33.05 | 87.02| 26.04|
| GaAs only           | 27.31| 1.012| 0.90| 25.42| 32.01 | 84.91| 23.32|
| Moon et al. (2016)  | 27.06| 0.981| -   | -   | -   | 83.35| 22.08|

Table 2. Comparison of cell performance parameter with and without CNT.

Again, the cell width was varied from 200 to 4000 microns, and the contact width was set at 50 microns constant for all simulations. The maximum power values for each solar cell were then obtained and compared for each cell width and are shown in Figure 8. Each cell reached a maximum P_{max} at a certain width and then showed reductions in P_{max} for greater widths. The most pronounced decline in P_{max} for greater cell widths was seen in the GaAs solar cell without a CNT layer. This sharp decline was due to the voltage losses from resistance in the AlGaAs and GaAs layers as charge carriers had to travel further to the contact. Since the CNT layers provided charge carriers in the solar cell with CNT charge collector layer with lower resistance paths to the contact, the reduction in P_{max} for greater cell widths was very less pronounced as shown in Fig 8. The current density in a GaAs solar cell with a top CNT layer of 128 Ω/□ of sheet resistance is shown in Figure 7. The current converges in the top CNT layer to travel to the top contact for charge collection. The charge carriers in this region see less net resistance in the more highly conducting CNT layer with greater generation of electron current density.
5. Conclusion

The unique properties of CNT layers on the surface of solar cells allow better charge carrier collection while only losing a portion of light input power based on the light transmission of the CNT layer. Although our cell is p-on-n structure, the addition of this CNT layer effectively increases the efficiency from the other reported similar cell without CNT. The validation of our numerically modelled and simulated cell with other good experimental data can conclude the reliability and accuracy of our method used in the design. Thus, this work can conclude that CNT layer can act as semi-transparent charge collector for better efficiency in solar cell. The method can be used for future development and research in the field of CNT based solar cell.

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