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Strained Carbon Nanotube (SCNT) Thin Layer Effect on GaAs Solar Cells Efficiency

Seyed Nooreddin Jafari[1], Abbas Ghadimi[*,2], Saeed Rouhi[3]

[1]Department of Electrical Engineering, Rasht Branch, Islamic Azad University, Rasht, Iran, Email: jafari@iaul.ac.ir
[2]Department of Electrical Engineering, Lahijan Branch, Islamic Azad University, Lahijan, Iran, Email: ghadimi@liau.ac.ir
[3]Department of Mechanical Engineering, Langarud Branch, Islamic Azad University, Langarud, Iran, Email: rouhi@iaul.ac.ir

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Abstract: In this paper, the effect of strain on the efficiency of GaAs solar cell is investigated. It has been shown that the applied strain during the synthesizing of carbon nanotubes (CNTs) leads to changing some of its physical properties. This means that strains can cause numerous changes in the structures. By using a strained layer of the carbon nanotubes on the GaAs solar cell, the effect of this layer on the performance of the GaAs solar cell is evaluated. This CNT layer can be used for several purposes. The first is to create a transparent electrical conductor at the cell surface to increase the output current. This purpose is one of the most important applications of this layer. But the second and more important goal is to capture more photons and reduce the emission or reflection of light emitted onto the cell surface. It is found that the mentioned goals cannot be satisfied simultaneously. Accordingly, to solve this problem, two different layers were used to achieve the ideal conditions. It has been shown that the use of a 10% uniaxial strained CNT layer leads to increase the photon absorption rate onto a non-strained CNT layer for electrical purposes. The efficiency of the single-junction GaAs solar cell with the above conditions reaches about 31% which is about 2% higher than the model without strain.

Keywords: Strained Carbon Nanotubes (SCNT), Gallium-Arsenide (Gaas), Transparent, Single-Junction Solar Cells

* Corresponding author. Email: **ghadimi@liau.ac.ir**

1. Introduction

Carbon nanotubes (CNTs) and graphene are often considered as environment friendly and economical materials to be used in the conventional solar cells [1, 2]. They have found different applications as the back, front, or buffer layers in the solar cells as well as photodetectors and light sensors [3, 4]. This promising application is due to the great optical and electrical properties of the graphene and nanotubes including good electrical conduction, thermal conduction as well as high light transparency in a wide range of the wavelengths. Considering these fantastic physical properties, they have also been used to improve the physical properties of other materials [5-11]. Before realizing these applications, a comprehensive investigation should be done on the physical properties of the nanostrcutures.

The influence of the strain on the physical properties of the CNTs has also been the subject of different researches [12-18]. It has been proven that changes in the cavity impurities can have a significant impact on the electronic properties of graphene. Similarly, the different studies have been performed on the electronic properties of the armchair carbon structure. The parameters of the carbon fiber layer can be modified by using several methods [19]. Moreover, the radiative transfer of light is observed in the symmetric multilayers of the carbon structure [20].

Li et al. [17] represented that the CNT based 3D architectures can change from transparent materials to opaque ones under a very small strain (<0.4%). The dependency of the phonon–phonon scattering rates of SWCNTs on the uniaxial tensile strain was studied by Chu et al. [18]. It was shown that the phonon–phonon scattering rates of SWCNTs can be changed by three orders of magnitude at the presence of the strain. In a computational study on the structural properties of SWCNTs, it was shown that the nanotubes can be adapted to different conditions and highly adaptable for specific applications [21].

The conversion efficiency in solar cells applied in the photovoltaic modules has a significant influence on the cost of electricity generation. Having its high electron mobility as well as direct bandgap, Gallium arsenide (GaAs) has been used for high performance electronics and optoelectronics applications [22-25]. Based on the thermodynamics calculation, the bandgap of GaAs is at the energy which theoretically maximum efficiency of single junction (SJ) solar cells occurs [26]. Therefore, the GaAs solar cells have been investigated extensively [27-34].

Kosten et al. [29] represented that the power conversion efficiencies of the GaAs solar cells with a single junction can be reached upto above 38% by limiting the emission angle. The theoretical limit of the efficiency of the GaAs solar cells was predicted as 33.5% by Shockley–Queisser [31].

Much progress has been made in high-efficiency and low-cost solar cells. It has been shown that the tunnel layer can be used to increase the efficiency of the solar cell based on InGaP/GaAs [35]. This was related to the increasing photon absorption. Wang et al. [32] tried to approach the efficiency of the single-junction GaAs solar cells to this theoretical limit by using the photon recycling and carrier transport simulations. Dimroth et al. [33] reached to the efficiency of 44.7% for the GaInP/GaAs//GaInAsP/GaInAs four-junction solar cell. Steiner et al. [34] proposed a GaAs solar cell with the varying optical properties such as the back reflectance. They obtained the conversion efficiency of 27.860.8% under the global solar spectrum.

Moreover, some researchers have been focused on the influence of the nanomaterials on the performance of the solar cells [36-46]. Also, it has been shown thatby using 2D photonic crystals, the light absorption process was changed. The results showed that flexibility can be used to create nanostructures which are able to control light absorption and passage [47]. A new design for the nanostructured solar cells were proposed by Liang et al. [43]. They obtained the energy conversion efficiency of 17% and open circuit voltage of 0.982 V by the proposed nanostructured window cell. Singh et al. [45] deposited carbon nanotube (CNT) layers on the surface of the solar cells. It was shown that due to the light transmission of the CNT layer, the power conversion efficiency and quantum efficiency of the GaAs solar cells increase. They also showed that depositing a CNT layer on the GaAs solar cells leads to increasing the power conversion efficiency from 26.04% to 29.18% [46].

Furthermore, it has been shown that the performance of GaAs solar cells can be improved by using the CNT [48]. In this work, it was observed that the presence of a thin CNT layer results in increasing the efficiency of the solar cell due to its ability to absorb more surface currents and better electrical conductivity.

In this paper, the performance of the solar cell would be improved based on changes in the CNT structure. For this purpose, different properties such as ohmic resistance, transparency, and light reflectance at the CNT surface would be changed to reach the optimal efficiency for the GaAs solar cell. Besides, a model is searched that is capable of absorbing maximum photons. It has also been attempted to increase the absorption of surface current by creating the lowest ohmic resistance on the surface of the solar cell.

2. Methodology

Here, the single-junction GaAs solar cell is used due to its high performance and compatibility with sunlight spectrum. The efficiency of some of the most important types of the solar cells are compared in Table 1. Considering the larger efficiency of the GaAs solar cell than the other solar cell types given in Table 1, it has been selected for further investigation and it is tried to increase its efficiency.

TABLE 1
Comparison of the efficiency of single-junction cell solar cells irradiated with standard AM1.5G beam at 25 ° C [49]

Classification	Efficiency (%)	Voc (v)	Jsc (mA/cm^2)
Silicon (Crystalline cell)	26.7±0.5	0.73	42.65
GaAs (thin film cell)	28.8±0.9	1.12	29.68
InP (Crystalline cell)	24.2±0.5	0.93	31.15
CIGS (cell)	22.9±0.5	1.04	38.77
Perovskite (cell)	24.9±0.7	1.12	24.92
Dye (cell)	11.9±0.4	0.74	22.47

Different methods have been employed to obtain larger efficiency in single-junction GaAs solar cells. One of the most important methods is to modify the structure of the absorbing surface current. This can be possible by using a current collector layer on the surface of the solar cell. But the important point is that the surface current collector layer that covers the solar cell must be capable of passing through the light beam. Without this ability, the light absorption and the photovoltaic process are prevented. Hence, the transparency of this element is also important. Accordingly, different methods have been used to solve this problem such as the use of a semi-transparent CNT thin layer [46]. This layer can be used both as a surface current collector and as a semi-transparent layer against photon passage. It should be noted that the transparency of the CNT layer affects its surface resistance. It has been shown that the increase in the transparency of the CNT would also increase its ohmic resistance [50].

For this reason, several layers of CNTs can be used instead of one layer, each of which can provide the capabilities needed to improve solar cell performance. It has also been shown that by applying compressive and tensile forces in a photovoltaic process, the amount of current and voltage resulting from the conversion of light are respectively reduced or increased [51] (see Fig. 1).

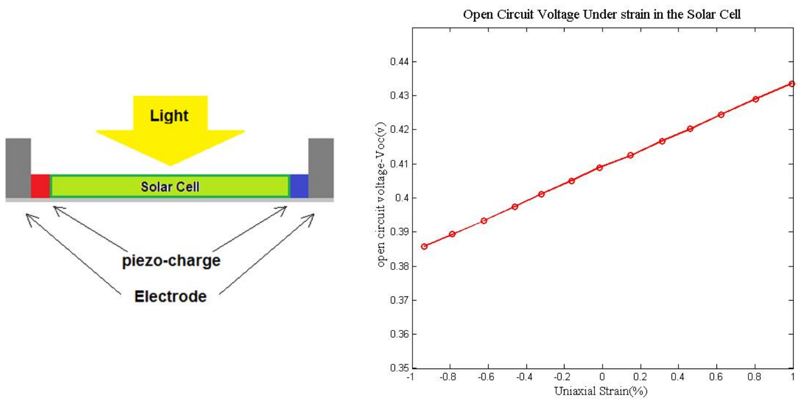

Fig. 1. Influence of the compressive and tensile strains on the open circuit voltage in solar cell [51]

In these conditions, one of the most important parameters affecting solar cell efficiency is the absorption rate of light emitted to the surface of the solar cell. In other words, the number of photons emitted to the solar cell is divided into reflective and non-reflective parts after they hit the surface. Thus, if the reflection on the cell surface layer is reduced, the photon absorption and the photovoltaic process can be increased.

The highest amount of photon scattering occurs when the network potential energy, V possesses its largest value. In the governing relationships of photon scattering it is assumed that the cubic parameters are dominant. In this case, the relationships governing the physics of carbon nanotube for strain analysis can be defined as follows. According to the third statement of Taylor's expansion based on potential V, the force (Ψ) relation can be expressed as [18]:

$$\Psi_{\alpha\beta\gamma} = \frac{\partial^3 V}{\partial u_\alpha\,(lb)\partial u_\beta\,(l'b')\partial u_\gamma\,(l''b'')} \tag{1}$$

where α, β, γ represent the three-dimensional displacement components, and uα, uβ and uγ denote the small displacements of the atoms. Besides, lb is the location order. Using Fourier transform and applying the photon operator, the non-harmonic part of the potential function can be obtained:

$$v_3 = \frac{1}{3!}\frac{i}{(N_0\Omega)^{\frac{3}{2}}}\sum\left(\frac{\hbar^3}{8m_b m_{b'} m_{b''} w(qs) w(q's') w(q''s'')}\right)^{\frac{1}{2}}$$
$$\square\ \delta_{G,q+q'+q''} e_\alpha(b|qs) e_\beta(b'|q's') e_\gamma(b''|q''s'') \tag{2}$$
$$* \ \delta\Psi_{\alpha\beta\gamma}(qb, q'b', q''b'')\ \square\ (a^t_{qs} - a_{-qs})(a^t_{q's'}$$
$$- a_{-q's'})(a^t_{q''s''} - a_{-q''s''})$$

In this function $N_0\Omega$ equals the lattice volume, m_b is the mass of a carbon atom, w_{qs} is the equivalent frequency of the photon with the wave function of q and polarization of s. Besides, G is a cross-lattice function, e(b | qs) is a direct polarization function, and $\Psi_{\alpha\beta\gamma}$ is the third degree of Fourier transform obtained from Eq. (1).

Based on the results of the calculations, it can be concluded that the amount of strain applied to the CNT structure is effective on the scattering rate of the light spectrum. The photon scattering rates for a (10,10) armchair nanotube under different values of strains are given in Table 2. According to the Table 2, it can be seen that in the lowest dispersion occurs at the 10% strain which lead to decreasing in the reflection of the beams and increasing in the non-reflective photons. In other words, the light scattering rate is 2% for a non-strained CNT which decreases to 1.2% by applying the 10% strain. This reduction in the scattering rate can be effective in increasing the efficiency of photovoltaic process.

TABLE 2

Phonon scattering rates for a (10,10) armchair nanotube under different values of strains [18]

Uniaxial Strain	Photon Scattering Rate
0%	**2%**
5%	**1.9%**
10%	**1.2%**
15%	**2%**
20%	**3.1%**

Considering this reduction in the phonon scattering rate by applying the strain on the CNT, a GaAs solar cell is simulated here with a strained CNT (SCNT) layer on its top surface. The chirality of the CNTs is (10,10) and the strain of 10% is applied to it. The proposed model has been shown in Figure 2, in which one SCNT layer is used as the top layer to improve the photons absorption. The next layer is a low-ohmic CNT layer which is used to improve solar cell performance.

This layer actually collects the surface currents produced inside the solar cell. After these two layers, which are referred as the enhancement layers, there are several layers related to the structure of a single-junction solar cell. These layers eventually comprise a P-N connection that whose task is to create a discharge zone and a photovoltaic process similar to the original solar cell protocol. The characteristics of the employed layers are given in Table 3.

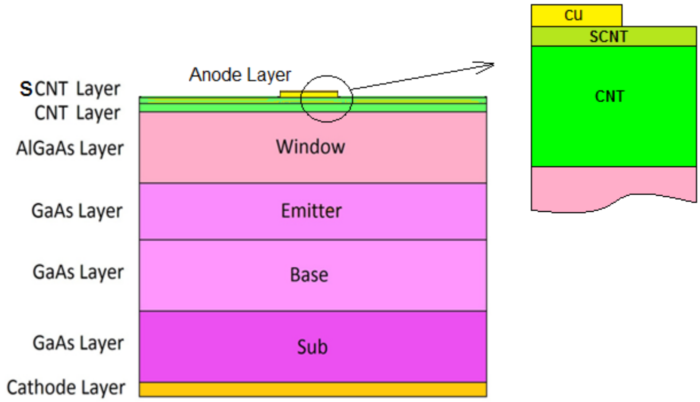

Fig. 2. Proposed model with a SCNT layer on the top CNT layer

TABLE 3

Characteristics of the employed layers for GaAs solar cell

Layer	Depth(nm)	Material	Doping	Type
Anode	10	Copper	-	-
Improver	10	SCNT	-	10% strain
Improver	90	CNT	-	-
Window	500	AlGaAs	1e+18	p.type
Emitter	400	GaAs	1e+18	p.type
Base	8000	GaAs	1e+17	n.type
Substrate	10000	GaAs	5e+17	n.type
Cathode	10	Copper	-	-

Fig. 3 shows a schematic view of the simulated model. This figure shows the layer arrangement in single junction GaAs solar cell. As shown in the enlarged part of this figure, the total thickness of the two CNT surface-enhancing layers is 100 nm, which is divided into two strained and non-strained sections. The thickness of the strained layer is much less than that of the other layer. The main source of the ohmic resistance is the connection. Because the current density must pass through the CNTs, they should have low ohmic resistance. However, the ohmic resistance of the strained CNTs is large. For this reason, the narrow strained layer is only used to absorb more photons.

GaAs solar cells can be made by chemical etching. The nanoparticles produced in the heat process are used by the etch method to produce an emitter surface and other layers. It is also possible to create an absorbent layer of nanotubes structures capable of trapping light on the surface of the structure. The application of nanotubes structures on GaAs solar cells as an anti-reflection layer enhances the photovoltaic properties of the cells [52].

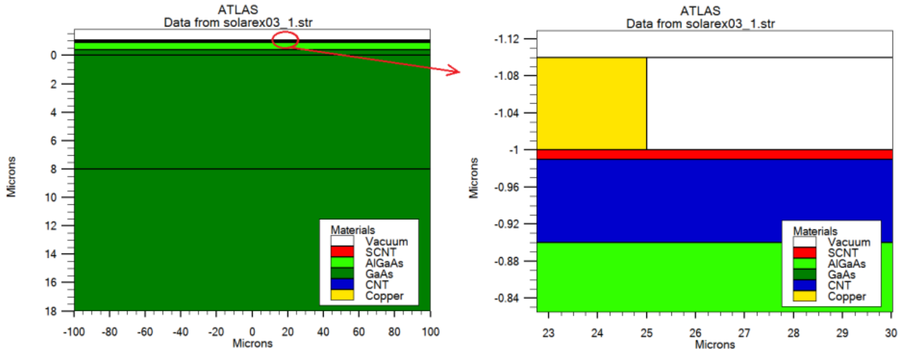

Fig. 3. Schematics of the investigated model

Fig. 4 shows the meshing image used in the simulation process. The simulation process is performed here using Silvaco Atlas software module. As it can be seen in this figure, to have more accurate results it is necessary to look more closely at some areas of the cell. For this reason, the elements are finer in these areas. Besides, the continuity should be considered in the meshing.

In order to obtain the accurate results which are close to real, meshing settings are crucial. One of the most important outputs used for the solar cells is the current-voltage curve related to the standard light spectrum. However, in order to investigate the behavior of the device with more details, other parameters such as photovoltaic conversion process, the current density absorption pathway, and the photon absorption rate should be determined. In the next section, these parameters would be obtained and discussed.

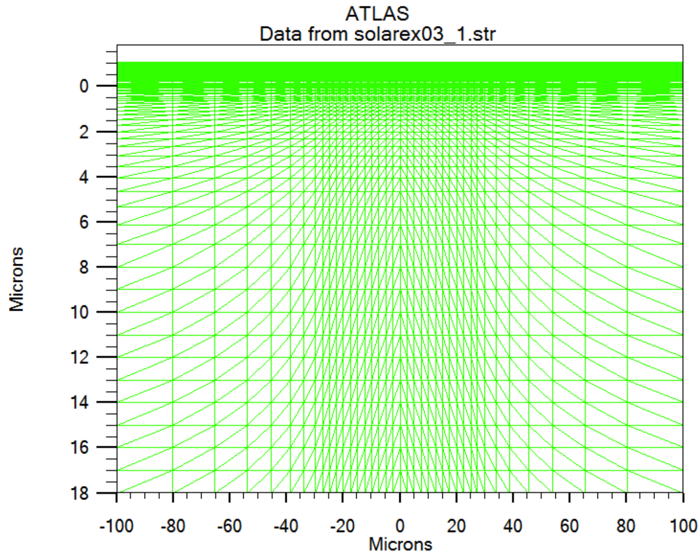

Fig. 4. Meshing image of the model used in the simulation process

The number of photons imported into the cell can be increased by using the SCNT as the surface enhancer layer on the solar cell surface instead of CNT layer. But it should be noted that the ohmic resistance of the section that collects the solar cell's surface current should be as small as the original model. Hence, both CNT and SCNT layers are used to cover these two demands. In other words, the top SCNT layer, which is under 10% strain, is applied absorb more light into the solar cell. Besides, the below CNT layer with smaller ohmic resistance helps to absorb more electrical current. The simulations are performed by Silvaco software. The input parameters of the pure and SCNT are given in Table 4.

TABLE 4

Input parameters of the pure and SCNT in Silvaco software

Layer Characteristic	ATLAS Symbol	CNT	SCNT (10%)	AlGaAs	GaAs
Band gap Eg (eV)	EG	2.29	1.58	1.5487	1.42
Electron affinity Xe (eV)	Affinity	5.8	5.8	3.96	4.07
Relative permittivity εr (F cm^{-1})	Permittivity	5.4	5.4	12.616	13.5
Electron mobility μn (cm2/Vs)	MUN	13889	42565	2000	8800
Hole mobility μp (cm2/Vs)	MUP	13889	42565	138	400
Conduction band effective density of states Nc (cm^{-3})	NC300	3×10^{17}	3×10^{17}	1.39×10^{18}	4.7×10^{17}
Valence band effective density of states Nv (cm^{-3})	NV300	3×10^{17}	3×10^{17}	9.78×10^{18}	7×10^{18}

Now, based on the data collected to evaluate the performance of the solar cell with the desired conditions, it is possible to analyze the amount of variation of its efficiency.

3. Results

Here, the research suggests that the performance of solar cells with dual layers of surface enhancers can be examined in detail.

One of the most important parameters for measuring and evaluating the performance of solar cell is the simulation of the standard light beam. Here, the performance of sunlight exposure to the surface of the solar cell is analyzed based on the AM1.5G standard. In Fig. 5, the standard AM1.5G beam is displayed before and after passing through the semi-transparent CNT layer.

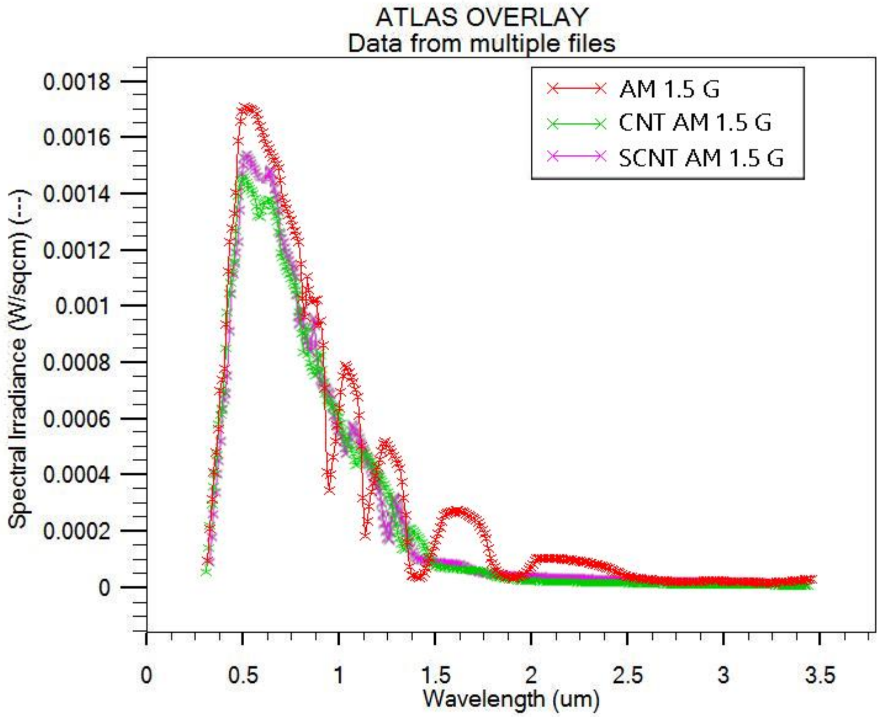

Fig. 5. Standard AM1.5G beam before and after passing through the semi-transparent CNT and SCNT layer

The AM1.5G standard beam is used to provide identical solar cell conditions and have comparable results. The power of the spectrum of light emitted to the surface of the solar cell is maximized in the absence of any barrier to light. But if any material is applied on the surface of the solar cell, it is possible to reduce this energy level. However, if the applied layer is semi-transparent, the transmitted energy loss would be further reduced. If the transparency of the applied surface layer is increased, more energy levels would be incorporated into the photovoltaic process of the solar cell.

As shown in Fig. 6, the energy level of the beam passing through the CNT layer is slightly reduced. This reduction is due to the use of semi-transparent nanotubes. The fully transparent nanotube provides good light transmittance (Fig. 6), but cannot be a good electrode for the solar cell due to its high junction resistance. For this reason, the current-voltage diagram of a solar cell represents its performance changes. By comparing the diagrams shown in Fig. 6, one can compare the difference in the current-voltage value of the solar cell. Here, the current-voltage curve of the model with a sole SCNT layer, sole CNT layer and no CNT over the GaAs solar cell are compared.

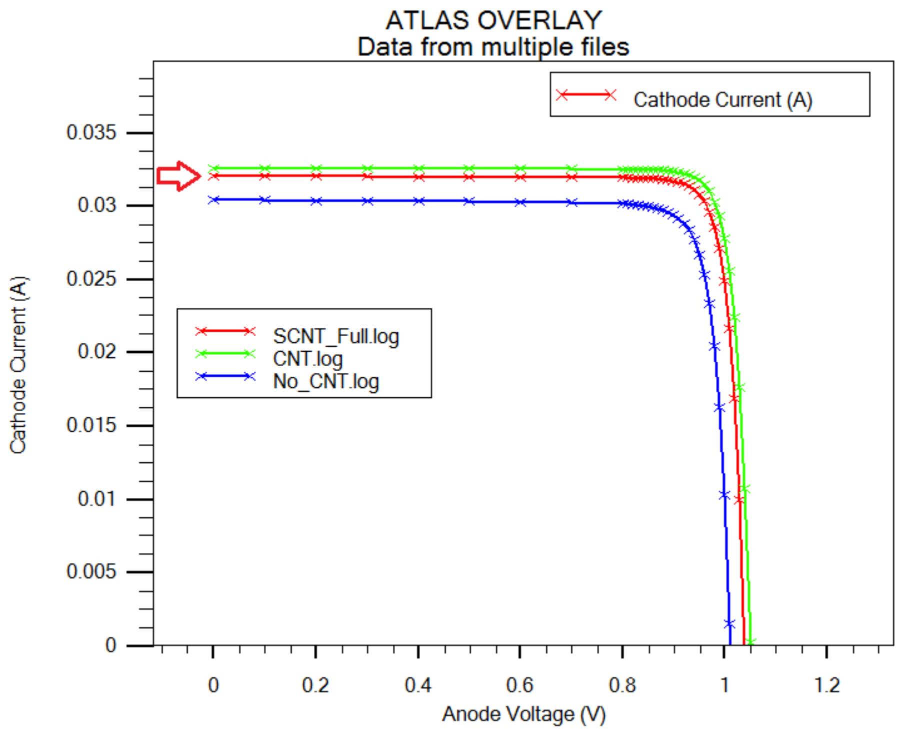

Fig. 6. Comparison the current-voltage curve of the model with a sole SCNT layer, sole CNT layer and no CNT

As shown in Fig. 7, the current-voltage curve is minimal when the solar cell have no surface-enhancing layer. By adding the CNT layer to the surface of the solar cell, the value of the current-voltage curve increases. However, with the application of sole transparent strained CNT, the value of the current-voltage curve decreases. Thus it can be said that adding only the strained CNT not only does not improve the efficiency of the curves, but a slight reduction in the current-voltage curve occurs.

By analyzing the two processes examined so far, it can be concluded that the existence of a strained CNT surface-enhancing layer can reduce the scattering of light beam but its ohmic resistance has increased. This increase in ohmic resistance could justify the reason for reduction in solar cell efficiency. In other words, the increased amount of photons absorbed in the cell is not sufficient to change the ohmic resistance of CNT as the charge collector. It should be noted here that the main idea behind the application of CNT on the surface of the solar cell was to absorb the surface currents produced in the cell. This means that a low-ohmic conductor with the ability to be transparent is needed to enhance the efficiency of the solar cell. This is illustrated in Fig. 7 in which it is represented that how the path of the current flux density changes.

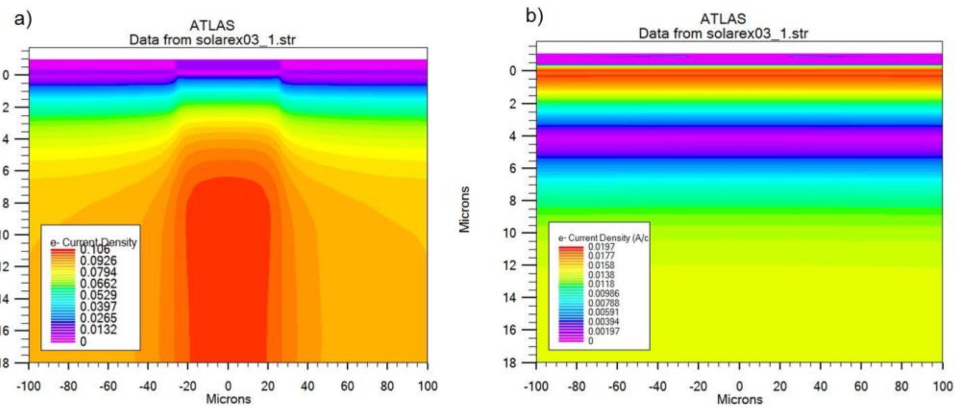

Fig. 7. The path change of the current flux density using the CNT as the charge collector (a: Before & b: After CNT layer)

As it is seen, by a CNT adding to the cell surface, the surface current is uniformly absorbed from the entire cell surface. This is suitable for increasing solar cell efficiency. However, by decreasing the ohmic resistance of the surface CNT, its performance as a charge-collecting electrode is impaired and prevents increasing the efficiency of the cell.

Therefore, to have a combination of the advantages of both two layers, the improving double layer method is used. In other words, the low-ohmic CNTs are used on the surface of the solar cell to absorb surface currents as the first layer. Then a SCNT layer is used over the previous layer to absorb more photons and prevent the scattering of the photons emitted on the solar cell surface. With this technique, the advantages of both of the mentioned layers are employed.

Also, the efficiency improvement in this structure is due to two contributing factors. In other words, the efficiency is increased due to the formation of a two-layer structure one of which of absorbs more photons and the other collects the surface current. The latter layer can equalize the usage of the entire solar cell structure by creating a surface-enhancing layer and using the environment around the cell as well as its middle part for the photovoltaic process.

The model proposed here uses 90% to 10% hybrid structure. In other words, a low resistance CNT layer with the thickness of 90 nm is used on the surface of the solar cell to transmit surface current. Moreover, to improve the photon absorption a (10,10) SCNT layer under 10% strain with the thickness of 10 nm is used. The total thickness of two layers is equal to 100 nm. The influence of the thickness of surface CNT layers on the solar cell efficiency is given in Fig. 8.

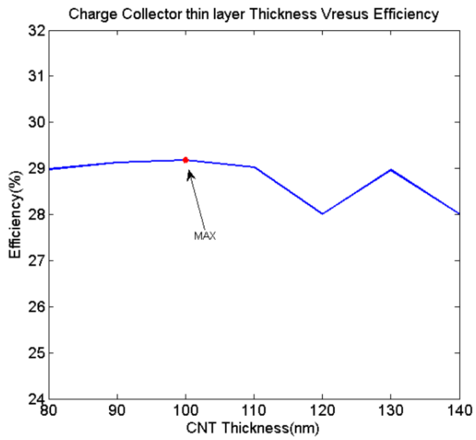

Fig. 8. Efficiency of the solar cell against the thickness of the surface CNT layers [46]

As shown in this figure, the maximum efficiency of the solar cell happens at the thickness of 100nm. Therefore, based on this figure and considering other simulations, this thickness is used as the best conditions for increasing solar cell efficiency. Using the described method, it can be anticipated that the performance of the solar cell increases. In Fig. 9 the current-voltage curve of the model with a hybrid surface-improvement layer is compared with the previous models. In this figure, SCNT-CNT shows the hybrid layer mode. While, CNT shows the results associated with the model having only pure CNT.

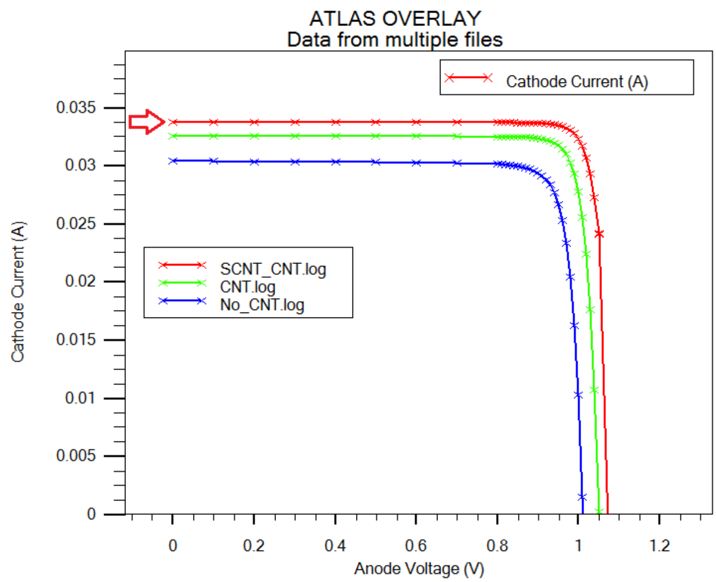

Fig. 9. Comparison the current-voltage curve of the model with a hybrid surface-improvement layer with the previous models

As it was predicted, the improvement of solar cell performance is clearly observed. This increase in the current-voltage curve of the device also increases its efficiency. In Table 5 the efficiencies of the solar cells discussed here are compared.

TABLE 5

Comparing the efficiency of the proposed model for the solar cell with the previously reported results

Authors	Year	Layers	Structure	Isc (mA/cm^2)	Voc (V)	FF	Eff(%)
Tatavarti et al. [53]	2008	InGaP/GaAs/AlGaAs	n-on-p	24.57	1.01	85.25	21.11
Wu et al. [54]	2014	InGaP/GaAs	n-on-p	19.61	1.00	81.48	15.98
Lee et al. [55]	2014	AlGaAs/GaAs	p-on-n	24.21	0.98	76.40	18.10
Moon et al. [56]	2016	InGaP/GaAs	n-on-p	27.06	0.98	83.35	22.08
K.J.Singh et al. [45]	2017	AlGaAs/GaAs	p-on-n	28.80	1.03	87.02	26.04
K.J.Singh et al. [46]	2017	CNT/AlGaAs/GaAs	p-on-n	33.23	1.04	86.43	29.18
Current work	2019	SCNT/CNT/AlGaAs/GaAs	p-on-n	33.59	1.064	89.66	31.04

As can be seen from this table, the efficiency of the solar cell with the hybrid SCNT-CNT layer has been increase by about 2%. This can be associated with the reducing the scattering of light beam. The rate of photon absorption for the utilized unit cell with the hybrid SCNT-CNT surface layers is shown in Fig. 10. According to this figure, a uniform absorption rate is observed in different layers of the solar cell.

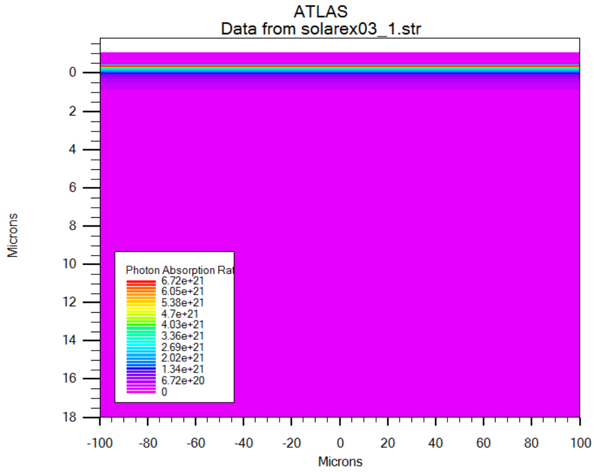

Fig. 10. Rate of photon absorption for the utilized unit cell with the hybrid SCNT-CNT surface layers

The final comparison of the current-voltage curves obtained for different configurations studied in this paper is given in Fig. 11. It is seen that the SCNT-CNT configuration gives the largest efficiency.

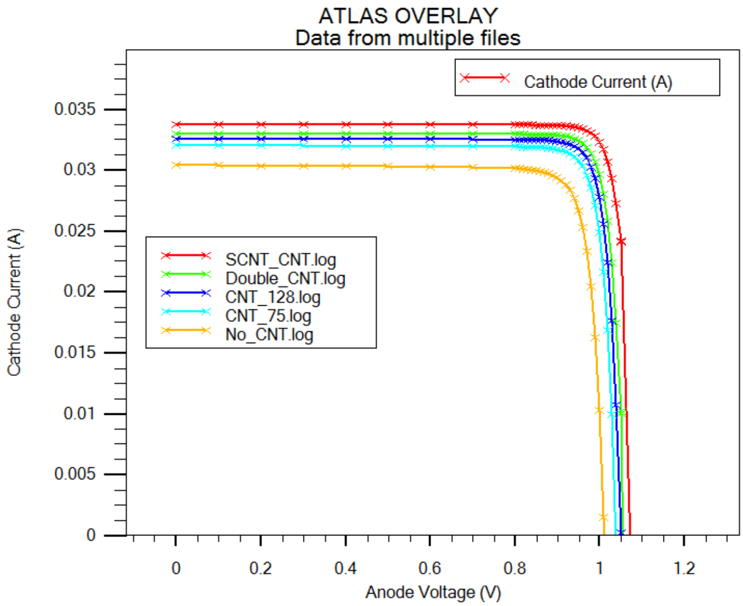

Fig. 11. Final comparison of the current-voltage curves obtained for different configurations studied in this paper

4. Conclusion

In this paper, the influence of adding a strained CNT surface-enhancing layer a GaAs solar cell on its performance was investigated. Considering the reported results in the literature, due to the least amount of light scattering, a (10,10) armchair nanotube layer under the strain of 10% was selected. However, as the junction resistance is also increases by applying the sole SCNT layer, the hybrid layer model was used which composed of a strained CNT layer over a pure CNT layer. One of these layers is responsible for collecting the surface current as the electrode whose thickness is larger than the other layer. The second layer, i.e. SCNT, which was placed on the top surface of the solar cell has smaller thickness and was used to absorb more photons and prevent the scattering of the photons emitted on the solar cell surface. The addition of the SCNT layer lead to improvement the efficiency of the solar cell by the percentage of about 2% over the solar cell without the CNT layer. In other words, using this technique, the efficiency of 31% was observed for the single-junction GaAs solar cell.

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