Simulation Study on Organic Solar Cell consist of SWCNT in presence of Stone Wall Defect

Ankit Mishra

Abstract— In this paper, we study the Organic solar cell property by introducing the stone wall defect in CNT. We use Graphene/ PEDOT: PSS / Perovskite / PCBM+CNT/Al as base structure. PEDOT: PSS and PCBM are used as Hole transportation layer and Electron transportation layer whereas Graphene is used as Transparent Electrode material in anode side and Aluminum in Cathode side. Electrical properties, Defects and Fermi level are discussed in detail. For the relative realistic study, we use ATLAS device simulator with intra-band and trap-assisted tunneling models in order to provide experimental guidance. We have also used Atomistix tool kit (ATK) to analysis the fill factor, Bandstructure, wavelength, and efficiency. Density functional theory (DFT) and Extended Huckel approximation method are used to analysis the work function, band gap and Density of state. The simulation results also indicate the difference between the efficiency in presence of Stone Wall defect and without the defect in CNT.

Index Terms— ATK Quantumwise, Graphene, Perovskite, Stone Wall Defect, , Silvaco TCAD, SWCNT

1 INTRODUCTION

The increase in the technology in this era wills demands the increase of power. Low cost with high-efficiency devices is required to produce power through sunlight to fulfill the energy demands. For converting solar energy to electrical power researchers are work a lot on both bulk –Heterojunction solar cell and dye-sensitized solar cell (DSC) in this last two decades [1]. Recently, researchers are started massive work on the organic solar cell (OSC). Use of PCBM, PEDOT: PSS, PPV, P3HT and other polymer based material are profoundly used in Organic photovoltaic's depend on Hole transportation layer and Electron Transportation layer. In this HTL and ETL, the researcher is added other materials to increase the efficiency of the device. In this paper we used,Graphene/ PEDOT: PSS / Perovskite/ PCBM+CNT/ Al as ANODE LAYER/ HTL/ ACTIVE LAYER/ ETL/ CATHODE LAYER based structure [2]. The size of the structure is 1mm X 1mm. Perovskite is an organic-inorganic material with a polycrystalline structure "ABX3". AB and X3 are the two parts of the perovskite structure. AB is the cation and X3 are the anion part (situated at face centers). A is existing at the eight positions of the cube whereas B is placed at body center confined by 6 X- anions. The chemical formula of Perovskite is

CH3NH3PbX3 where X can be (Br, Cl, I or can be the combination of them). This organic-inorganic lead halide material shows high charge carrier mobility, diffusion length and due to high absorption coefficient [3].

Phenyl-C61-butyric acid methyl ester (PCBM) is rich Electron transport layer whereas PEDOT: PSS is Hole transport layer. PCBM is the fullerene derivative of the C60 buckyball. In this PCBM, Single-Walled Carbon Nanotube (SWCNT) is added as a buffer layer which will increase the efficiency of polymer photovoltaic [4]. Graphene, PCBM, and PEDOT: PSS and Perovskite are the chemical solution which can be deposited by the spin coating. The work of Carbon Nanotube in PCBM is to pass the electron from one side to another [5]. As an anode material Graphene has honeycomb arrangement bound with 2D covalent atoms. As a 2D molecule, it holds some of the useful characteristic properties in electronics, chemical, mechanical, optical and as well as in thermal stability.It is used as a transparent electrode layer in anode part [6]. The aim of this paper is to analysis the solar cell structure in presence of stone wall defect and without it.

2 Overview On CNT

Carbon Nanotube (CNTs) are cylindrical tube shaped hexagonally oriented carbon atoms and allotrope of carbon material. The Carbon Nanotube is 16 times stronger then stainless steel. The structural bond of CNT is sp2 hybridized which enhance the unique strength [7]. When the graphene sheet is rolled in some manner then it became CNT.

The single graphene sheet is rolled into the cylinder then it's called Single-walled Carbon Nanotube.In fig (1) the

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single-walled carbon Nanotube is shown, whereas more than one graphene sheet rolled into the cylinder then it is called multi-walled carbon Nanotube [8].

The indices, n, and m will denote the unit vectors. The rolling of graphene sheet in different angle will give different properties. There are some accepted modals for MWCNT are Russian doll model and parchment. These two models are mostly used for the formation of CNTs [9].

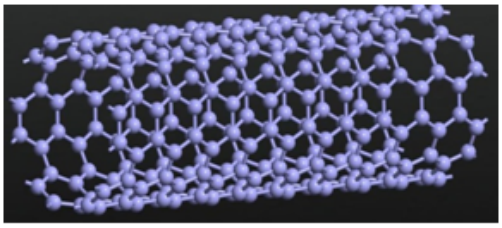

Fig (1): SWCNT in ATK Simulation Tool

2.1 Stone Wall Defect

In CNT, when the pair of atoms rotates which cause the stretch and twist in the structure of CNT with axial change is known as Stone wall defect [10]. Due to the stretching and twisting of atoms, there will be a change in the energy which leads to the failure of the structure. The confinement property of carbon nano tube will be the change [11].
The energy will be lost which causes the low-efficiency rate of the structure.

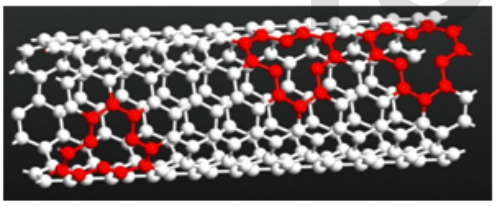

Fig (2): Stone Wall Defect in SWNT using ATK Simulation Tool

3 Simulation Devices

ATOMISTIX TOOL KIT (ATK) and SILVACO TCAD are used for simulating the device structure of organic photovoltaic cell [12]. ATK is used to create Single-walled Carbon Nanotube and set up a defect in the Carbon Nanotube. SILVACO TCAD helps to simulate the Graphene/PEDOT: PSS / Perovskite /PCBM+CNT/Al base structure and obtained the electrical and optical properties of it [13].

3.1 Atomistix Tool Kit

ATOMISTIX TOOL KIT (ATK) helps to calculate and simulate the electronic transport property of atomic structure of CNT acquires the required results.

In ATK the electronic structure of the system is defined in Density functional theory by one-electron Kohn-Sham Hamiltonian

$$\boldsymbol{H_{1el} = -\frac{\hbar}{2m}\nabla^2 + V^{eff}[n](r)} \qquad \textbf{(1)}$$

$\frac{\hbar}{2m}\nabla^2$ Is the kinetic energy of electron and $\boldsymbol{V^{eff}[n](r)}$ is potential energy.
Eigenstates of one-electron Kohn-Sham Hamiltonian is defined by one-electron Schrödinger equation

$$\boldsymbol{H_{1el}\Psi(r) = \varepsilon_\alpha \Psi_\alpha(r)} \qquad \textbf{(2)}$$

Solving this differential part, the above wave function should be expanding

.

$$\boldsymbol{\psi_\alpha(r) = \sum_i \alpha\, \phi_i(r)} \qquad \textbf{(3)}$$

After solving this differential part into matrix equation the equation will be

$$\boldsymbol{\sum_j H_{ij} C_{j\alpha} = \varepsilon_\alpha \sum_j S_{ijCaj}} \qquad \textbf{(4)}$$

The total energy of DFT is given by

$$\boldsymbol{E[n] = T[n] + E^{xc}[n] + E^{H}[n] + E^{ext}[n]} \qquad \textbf{(5)}$$

Where $\boldsymbol{T[n]}$ is Kinetic energy, $\boldsymbol{E^{xc}[n]}$ is exchange-correlation energy, $\boldsymbol{E^{H}[n]}$ is Hartree energy and $\boldsymbol{E^{ext}[n]}$ is interaction energy.

The other method used in ATK is Extended Huckel approximation method, which is the semi-empirical tight-binding simulation. This method is suitable for calculating inorganic atom structures [14].

3.2 Silvaco TCAD

In this paper, we also use SILVCO TCAD simulation research tool to obtained electrical and optical property of the base structure. This tool is used to simulate both organic and inorganic material, in the case of inorganic semiconductors we can use CVT, SRH models but for the organic semiconductors, we have to use Langevin model. Langevin gives the theory that how the hole can capture the electron in slow mobility rate. In recombination, this model shows exacts behavior of electron-hole pairs or exaction

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$$\boldsymbol{E_c = \frac{e^2}{4\pi\varepsilon\varepsilon_0(R_E + R_H)}} \qquad \textbf{(6)}$$

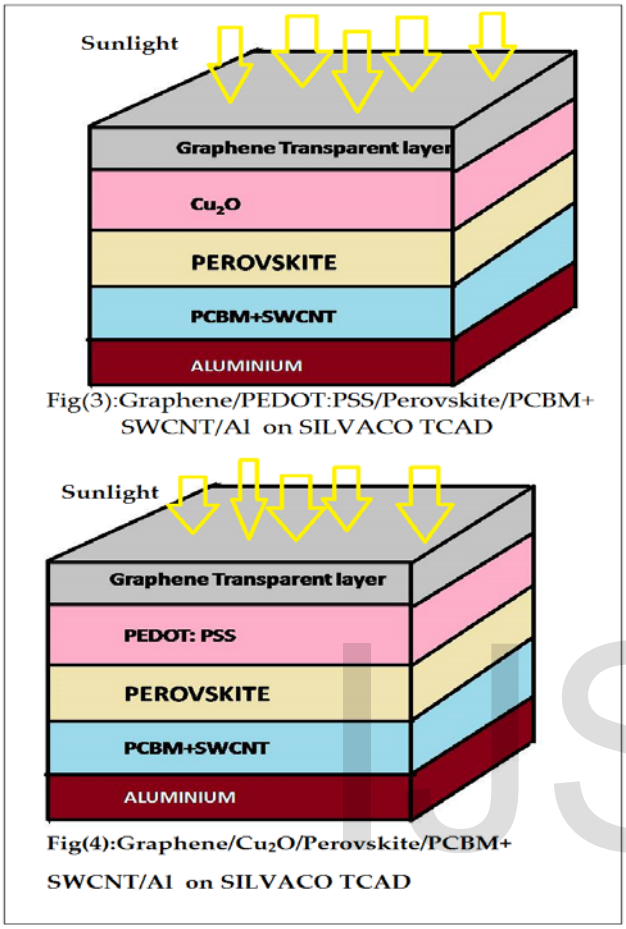
Where R_E and R_H are the wave function of the electron and hole.

$$\boldsymbol{Rn,p = \frac{qnp}{\epsilon\epsilon o}(\mu n(E) + \mu p(E))} \qquad \textbf{(7)}$$

Rn,p shows recombination rate occur inside the structure [15].

The perovskite solar cell consist of cuprous oxide as hole transporting layer of 50 nm and electron transport layer as PCBM of 100 nm, the constructed film stacked of PSC is graphene/PEDOT:PSS/CH3NH3PbI3Clx/PCBM+SWCNT /Al, FTO and Al is used as the electrode, we have also used PPV as HTL and graphene transparent layer as active electrode with the thickness 50 nm and 0.43 nm respectively [16].

4 FIGURE



Fig(3):Graphene/PEDOT:PSS/Perovskite/PCBM+ SWCNT/Al on SILVACO TCAD

Fig(4):Graphene/Cu_2O/Perovskite/PCBM+ SWCNT/Al on SILVACO TCAD

Parameters	Cu_2O	Perovskite	PCBM	Multilayer Graphene
Eg (eV)	2.22 [20]	1.5	2 [22]	0
Mun($cm^2v^{-1}s^{-1}$)	30 [20]	14	0.2 [22]	1-1x10^9 [7]
Mup($cm^2v^{-1}s^{-1}$)	30 [19]	14	0.2 [22]	10 [8]
Nc (cm^{-3})	1 x10^{19} [18]	2.5 x 10^{20}	2 x 10^{21} [21]	3x10^9 [7]
Nv (cm^{-3})	1 x10^{19} [18]	2.5 x 10^{20}	2 x 10^{21} [21]	3x10^9 [7]
Affinity X (eV)	3.4 [17]	3.96	3.9 [21]	3.4-4.8 [8]
Permittivity (Er)	7.5 [17]	30	3.9 [21]	10-20 [8]
Thickness (nm)	50	500	100	10

4.1 TABLE 1

PARAMETERS USED IN SILVACO TCAD TOOL

5 RESULTS

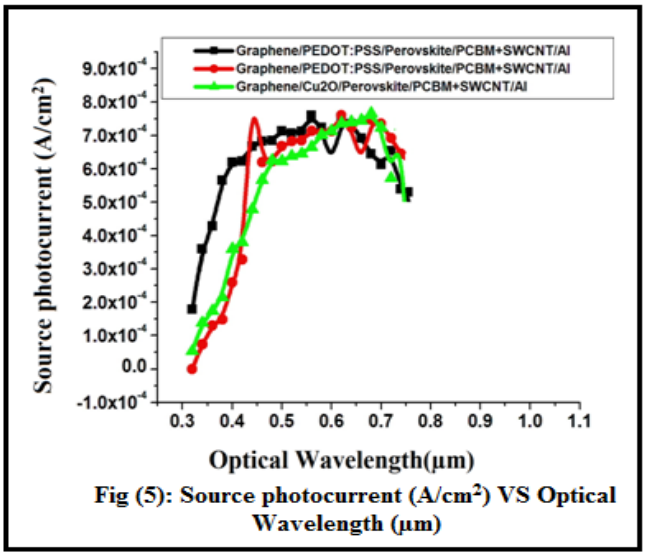


Fig (5): Source photocurrent (A/cm²) VS Optical Wavelength (µm)

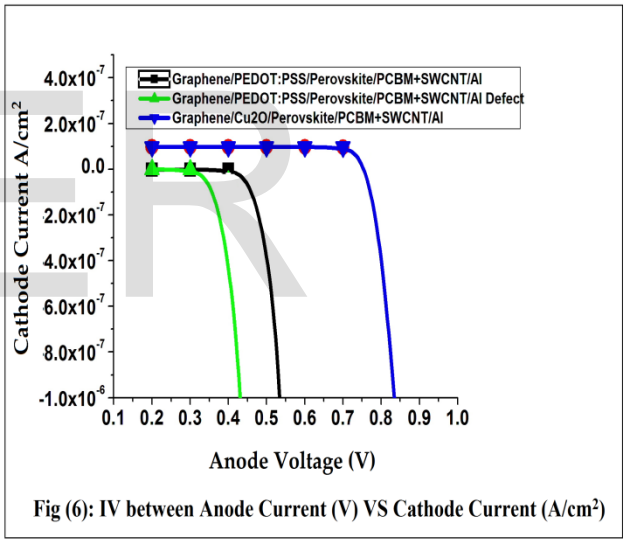


Fig (6): IV between Anode Current (V) VS Cathode Current (A/cm²)

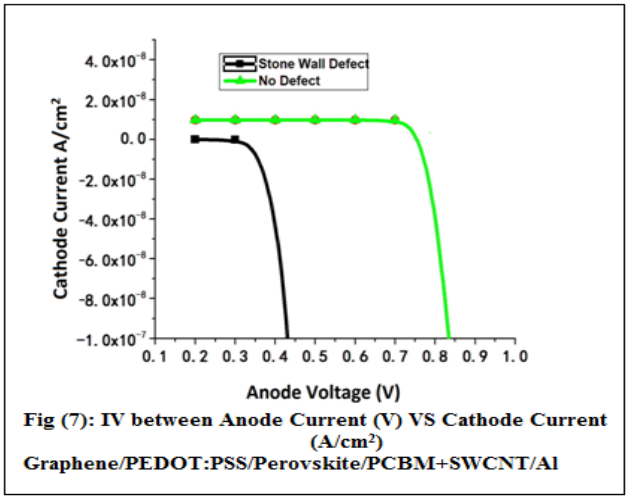


Fig (7): IV between Anode Current (V) VS Cathode Current (A/cm²) Graphene/PEDOT:PSS/Perovskite/PCBM+SWCNT/Al

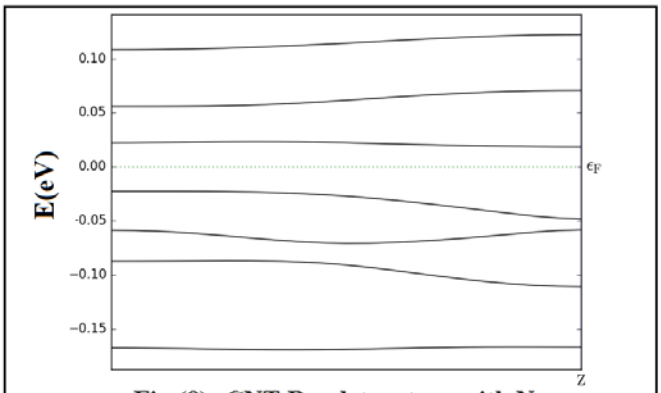


Fig (8): CNT Bandstructure with No Defect

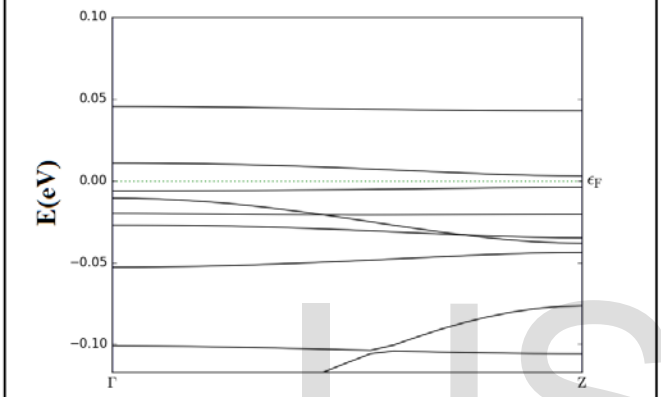


Fig (9): CNT Bandstructure with Stone Wall Defect

6 DISCUSSION

The two structures are simulated under AM 1.5 illumination that are Graphene / PEDOT:PSS/Perovskite / PCBM + SWCNT /Al and Graphene/Cu2O / Perovskite / PCBM+ SWCNT /Al. SWCNT play important role in the base structure [23]. The short circuit current (Jsc), the open- circuit voltage (Voc), power conversion efficiency (η) are plotted in the figure (6). By adding the SWCNT it is clear that it shows the strong influence on the structure [24].

The Jsc of the Graphene / PEDOT: PSS/Perovskite / PCBM + SWCNT /Al is 4.9 mAcm-2 without introducing the defect in the SWCNT whereas when the stone wall defect is introduced the Jsc is 3.5 mA cm-2. The Voc without defect is 0.85 V and with stone wall defect it shows 0.44 V. The same simulation is carried out with the Graphene/ Cu2O / Perovskite / PCBM+ SWCNT /Al. SWCNT structure. The Jsc is 5.1 mAcm-2, Voc is 0.88 V and with stone wall defect the Jsc is 4.6 mAcm-2. The Voc is 0.8 V [25].

The Fill Factor of solar cell can be obtained by using following formula

$$FF = \frac{V_{max} I_{max}}{V_{oc} I_{sc}} \quad (8)$$

Where V_{max} and I_{max} is the Voltage and current density which shows the maximum product of I-V in the fourth quadrant [26].

The efficiency can be obtained by

$$\eta = \frac{V_{oc} I_{sc} FF}{P_{in}} \quad (9)$$

In Fig (6), we simulate Graphene /Cu2O /Perovskite / PCBM + SWCNT / Al and Graphene /PEDOT: PSS /Perovskite /PCBM+SWCNT/Al with no defect and with stone wall defect [27]. The figure consist of three wave in which black and red wave denotes the stone wall defect, green wave is without defect in CNTs.

The green wave absorbs more light and transfers electron from Electron transport layer to active layer as compared to black and red wave. Due to stone wall defect, the confinement of CNTs changes which causes the energy lost in the CNTs.

Figure 8 and 9 shows the bandstructure of SWCNT simulated in ATK research tool with the help of DFT. In defect CNT there will be distortion in the band gap whereas in no defect CNT the direct and indirect gap is same momentum. The bandstructure is obtained by DFT calculation.

Table 2: Photovoltaic performance of the investigated photovoltaic device

Structure	Jsc	Voc	FF	η
Graphene/PEDOT:PSS/Perovskite /PCBM+SWCNT/Al	4.9	0.82	0.51	2.4
Graphene/PEDOT:PSS/Perovskite/PCBM +SWCNT/Al (Defect)	3.5	0.44	0.48	1.8
Graphene/Cu_2O/Perovskite/PCBM +SWCNT/Al	5.5	0.85	0.64	3.9
Graphene/Cu_2O/Perovskite/PCBM +SWCNT/Al (Defect)	4.4	0.54	0.5	3.3

7 CONCLUSION

In summary, we studied the simulation result of two structures with the defect and no defect in CNTs. Graphene/ PEDOT:PSS/ Perovskite/ PCBM+SWCNT/ Al shows efficiency 2.4 whereas Graphene/ Cu_2O/ Perovskite/ PCBM+SWCNT/ Al show efficiency 3.9. We conclude that using of Cu_2O will give higher efficiency. While when the stone wall defect is introduced the efficiency will be less. This is because of lost of energy. The calculation is carried in ATK tool and Silvaco TCAD tool. We use ATK to find out the electrical parameters of CNT. Whereas Silvaco TCAD is used to obtained I-V characteristics of the solar cell.

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