High-efficiency perovskite –nanowire-based organic-inorganic solar cell

Ankit Mishra

Dept. of Electrical
Amity University Chhattisgarh

Abstract

In this paper we have simulate the Perovskite solar cell based structure and find the best possible structure to fabricate. The PSC consists of Nanowires with Perovskite which absorbs the incident light and provide channel path for photo-generate electron and hole. We use first principle technique for calculating electrical, chemical and optical properties of structure. Here we use Silvaco TCAD research tool and ATK-quantum wise to design the PSC structure. We get 14.21% efficiency.

Keywords— Perovskite, Nanowire, Graphene, LANGEVIN model

I. INTRODUCTION

The rise in energy demand will rise the new way of methods to generate electricity. The solar cell is the most promising way to create free energy. Now a day's researcher is working on the organic-inorganic based structure which is low cost with high efficiency. Most of the researchers in the world are working on the Perovskite based structure for its high absorption capability, tunable band gap and high efficiency [1]. A Perovskite is an exceptional crystal structure, consisting of formamidinium with multiple cations and mix halide anions. The perovskite chemical formula is ABX_3 where AB and X_3 are the two parts of the perovskite structure. AB is the cation and X_3 are the anion part (located at face centers). A is at the eight corners of the cube whereas B is at the body centre surrounded by six X- anions ($A = \text{ions or molecules}$, $B = \text{Ge, Sn, Pb, and } X = \text{I, Br, Cl}$). Recent studies show that Perovskite based structure shows 22.1 % efficiency.[2] This organic-inorganic lead halide is used as the absorber layer in the structure. For the better improvement of the structure efficiency, we use graphene as the transparent active layer. Addition of graphene in the based structure will also increase the electrical, electronic and optical properties of the PSC. This novel graphene material is chemically stable and due to the high electrical conductivity, this material is a most promising material which is highly used nowadays [6]. To get better efficiency we also used other polymer materials like PEDOT: PSS, PCBM, P3HT as hole transport layer and electron transport layer. The recent efficiency of Perovskite is mentioned 22.1 % [4]. In this paper, we use Silvaco Tcad simulation research tool and ATK Quantum wise to analysis different base structures of polymer and to obtain electrical, electronics, chemical and optical properties of the structure. Apart from this we also analyzed the change in Fermi level energy band gap of the structure [7]. The purpose of present work is to stimulate $\text{Cu}_2\text{O}/\text{CH}_3\text{NH}_3\text{PbI}_3\text{Cl}_x+\text{NW}/\text{PCBM}$ structure with transparent layers graphene; we also use different HTL materials like PPV and Cu_2O to check the efficiency variation in the model. Cu_2O is good p-type material; PCBM is rich electron acceptor and can be used as an n-type semiconductor [11], perovskite is used as the active layer in solar cell model structure. Apart from this two interesting materials i.e. graphene and perovskite, researchers are also using semiconductor Nanowires (NW) to enhance the transportation property of electron and hole in the structure. NW have the advantage of light trapping, strain relaxation ability, separation of charge mechanism, least filling ratio and enhancement the absorption of light [14].

II. DEVICE SIMULATION

We take the base structure Anode/HTL/CH₃NH₃PBI₃ +NW / ETL/Cathode, where we use different polymer materials HTL and ETL for increasing the efficiency of the device [15]. We design the structure in computer aided Silvaco Tcad research tool. In this paper we tend to use the organic and inorganic material, just in case of inorganic semiconductors we will use CVT, SRH models except for the organic semiconductors we've to use Langevin model [16]. Langevin offer the idea that however hole will capture the electron in slow quality rate. In recombination this model shows exacts behavior of electron-hole pairs or exactions. In the device simulation light is implementing by the Beam command which is equal to standard AM 1.5 spectrum [19].

LANGEVIN model depends on the rate of exciton recombination,

$$P_E > W_0 \exp\left(-\frac{E_B}{kT}\right) \quad (1)$$

$$E_B > kT \ln\left(\frac{W_0}{P_E}\right) \quad (2)$$

P_E is thermal ionization, When this condition is not satisfy then the Langevin model is not used, due to which recombination rate is small. For applying the LANGEVIN model, excitation energy should be large [21].

$$E_c = \frac{e^2}{4\pi\epsilon\epsilon_0(R_E + R_H)} \quad (3)$$

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

$$Rn, p = \frac{qnp}{\epsilon\epsilon_0} (\mu n(E) + \mu p(E)) \quad (4)$$

Electron and hole current can be written as,

$$\frac{\partial n}{\partial t} - \frac{1}{q} \nabla J_n = G_n - R_n \quad (5)$$

$$\frac{\partial n}{\partial t} + \frac{1}{q} \nabla J_p = G_n - R_n \quad (6)$$

Poisson's equation is used to employ for the potential within the model electrodes. It helps to investigate performance, efficiency and how to improve them. This equation gives the basic relationship between charge and electric field [23].

$$\text{div}(\epsilon \nabla \phi) = -\rho \quad (7)$$

III. FIGURE

Fig (1): Graphene/PEDOT:PSS/ Perovskite +NW/PCBM/AL

Fig (2): Graphene/PPV/ Perovskite +NW/PCBM/AL

Fig (3): Graphene/Cu₂O/ Perovskite +NW/PCBM/AL

Fig (4): Graphene/P3HT/ Perovskite +NW/PCBM/AL

IV. Parameter Table

Parameters	Cu ₂ O	Multilayer Graphene	Perovskite	PCBM
E _g (eV)	2.22 (7)	0	1.5 (5)	2 (8)
M _n (cm ² v ⁻¹ s ⁻¹)	30 (5)	1x10 ⁹ (7)	14 (5)	0.2 (8)
M _p (cm ² v ⁻¹ s ⁻¹)	30 (5)	10(15)	14 (6)	0.2
N _c (cm ⁻³)	1x10 ¹⁹ (5)	3x10 ⁹ (15)	2.5 x 10 ²⁰ (6)	2 x 10 ²¹ (8)
N _v (cm ⁻³)	1x10 ¹⁹ (5)	3x10 ⁹ (10)	2.5 x 10 ²⁰ (6)	2 x 10 ²¹
Affinity X (eV)	3.4 (5)	3.4-4.8 (9)	3.96 (6)	3.9
Permittivity E _r	7.5 (5)	10-20 (7)	30 (6)	3.9 (8)
Thickness (nm)	50 (5)	10 (9)	200 (6)	100 (8)

V. RESULTS

Fig (5): AM1.5 spectrum

Fig (6): Voltage VS Current Density

Fig (7): Potential VS Wavelength

Fig (8):Anode Voltage VS Cathode Current

VI. DISCUSSION

We use Silvaco Tcad and ATK *research tool* quantum wise *research tool* simulated under AM 1.5 illuminations. We have obtained the electrical, optical and chemical property of the structure. We use ATK quantum wise to determine the material electrical, optical and chemical parameters. We design the base structure Anode/HTL/CH₃NH₃PbI₃ +NW / ETL/Cathode in TCAD Silvaco research tool. Addition of Nanowire in the base structure provides higher efficiency[24]. The main aim of the work is to add Nanowire material in the base structure with change in hole transportation layer. The open- circuit voltage (Voc) and the short circuit current (Jsc) are plotted in Fig (6). Here

we also obtain the wavelength and optical efficiency graph. The fill factor of solar cell can be obtained by using the 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.

The efficiency can be obtained by[26],

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

Table 2: Photovoltaic performance of the investigated photovoltaic device

Structure	Current Density (mA/cm ²)	FF	η %
1) Graphene/Cu ₂ O/ Perovskite +NW/PCBM/AL (50nmperovskite)	-16.98	0.6	12.21
2) Graphene/ Cu ₂ O/Perovskite +NW/PCBM/AL (100 nm perovskite)	-17.28	0.68	12.79
3) Graphene/Cu ₂ O/Perovskite +NW/PCBM/AL (200 nm perovskite)	-18.96	0.72	14.21
4) Graphene/PPV/ Perovskite + NW /PCBM/AL	-13.27	0.41	9.9
5)Graphene/ PEDOT:PSS / Perovskite +NW /PCBM/AL	-14.78	0.47	10.87
6) Graphene/ P3HT Perovskite + NW /PCBM/AL	-13.98	0.42	10.21

VII. CONCLUSION

In summary, we have simulated different structures with different hole transportation layer and we obtain higher efficiency while using Graphene/Cu₂O/CH₃NH₃PbI₃Cl_x +NW /PCBM/AL (200 nm perovskite) structure. We also investigate by changing the size of perovskite layer and we obtain higher efficiency in 200 nm. The purpose of this simulation is to design low cost, high efficiency

and use of organic- inorganic material in the structure. All the results are carried out in Sivaco TCAD research tool. The efficiency we obtain is 14.21 %.

REFERENCE

- [1] A. Kojima, K. Teshima, Y. Shirai, T. Miyasaka "Organometal halide perovskites as visible-light sensitizers for photovoltaic cells." J. Am. Chem. Soc. 2009, 131, 6050
- [2] Yixin Zhao and Kai Zhu "Charge Transport and Recombination in Perovskite (CH₃NH₃) PbI₃ Sensitized TiO₂ Solar Cells." J. Phys. Chem. Lett. 2013, 4, 2880–2884
- [3] Edoardo Mosconi, Anna Amat, Mohammad Khaja Nazeeruddin, Michael Grätzel, and Filippo De Angelis "First Principles Modeling of Mixed Halide Organometal Perovskites for Photovoltaic Applications" J. Phys. Chem. 2013, 117 (27), pp 13902–13913
- [4] Chog Barugkin, Jinjin Cong, The Duong, Shakir Rahman, Hieu T. Nguyen, Daniel Macdonald, Thomas P. White, and Kylie R. Catchpole "Ultralow Absorption Coefficient and Temperature Dependence of Radiative Recombination of CH₃NH₃PbI₃ Perovskite from Photoluminescence" 2015 J. Phys. Chem. Lett., 6, 767–772
- [5] Robertson J and Clark S J 2011 Limits to doping in oxides Phys. Rev. B 83 075205
- [6] Malinkiewicz O, Yella A, Lee Y H, Espallargas G M, Graetzel M, Nazeeruddin M K and Bolink H J 2013 Perovskite solar cells employing organic charge-transport layers Nat. Photonics 8 128–32
- [7] Mrowec S and Grzesik Z 2004 Oxidation of nickel and transport properties of nickel oxide J. Phys. Chem. Solids 65 1651–7
- [8] Bi C, Shao Y, Yuan Y, Xiao Z, Wang C, Gao Y and Huang J upstanding the formation and evolution of interdiffusion grown organ lead halide perovskite thin films by thermal annealing J. Mater. Chem. A 2 18508–14
- [9] Newman R and Chrenko R M 1959 Optical properties of nickel oxide Phys. Rev. 114 1507–13
- [10] Wehrenfennig C, Liu M, Snaith H J, Johnston M B and Herz L M 2014 Charge-carrier dynamics in vapour-deposited films of the organolead halide perovskite CH₃NH₃PbI₃-xCl_x Energy Environ. Sci. 7 2269–75
- [11] Wehrenfennig C, Eperon G E, Johnston M B, Snaith H J and Herz L M 2014 High charge carrier mobilities and lifetimes in organolead trihalide perovskites Adv. Mater. 26 1584–9
- [12] Hu L et al 2014 Sequential deposition of CH₃NH₃PbI₃ on planar NiO film for efficient planar perovskite solar cells ACS Photonics 1 547–53
- [13] Eperon G E, Burlakov V M, Docampo P, Goriely A and Snaith H J 2014 Morphological control for high performance, solution-processed planar heterojunction perovskite solar cells Adv. Funct. Mater. 24 151–7
- [14] Saha S K, Guchhait A and Pal A J 2012 Cu₂ZnSnS₄ (CZTS) nanoparticle based nontoxic and earth-abundant hybrid pn junction solar cells phys. Chem. Chem. Phys. 14 8090–6
- [15] Blom P W M, De J M J M and Munster M G V 1997 Electric field and temperature dependence of the hole mobility in poly(p-phenylenevinylene) Phys. Rev. B 55 656–9
- [16] Deuermeier J, Gassmann J, Brötz J, Klein A and Bro J 2011 Reactive magnetron sputtering of Cu₂O: dependence on oxygen pressure and interface formation with indium tin oxide J. Appl. Phys. 109 113704
- [17] Matsuzaki K, Nomura K, Yanagi H, Kamiya T, Hirano M and Hosono H 2008 Epitaxial growth of high mobility Cu₂O thin films and application to p-channel thin film transistor epitaxial growth of high mobility Cu₂O thin films and application to p-channel thin film transistor appl. Phys. Lett. 93 202107
- [18] Shi J et al 2014 Hole-conductor-free perovskite organic lead iodide heterojunction thin-film solar cells: high efficiency and junction property appl. Phys. Lett. 104 063901

- [19] Meyer B K et al 2012 Binary copper oxide semiconductors: from materials towards devices *Phys. Status Solidi* 249 1487–509
- [20] Conwell E and Weisskopf V F 1950 Theory of impurity scattering in semiconductors *Phys. Rev.* 77 388–90
- [21] Halme J, Vahermaa P, Miettunen K and Lund P 2010 Device physics of dye solar cells *Adv. Mater.* 22 210–34
- [22] Wang K, Shen P, Li M, Chen S, Lin M, Chen P and Guo T 2014 Low-temperature sputtered nickel oxide compact thin film as effective electron blocking layer for mesoscopic NiO/CH₃NH₃PbI₃ perovskite heterojunction solar cells *ACS Appl. Mater. Interfaces* 6 11851–8
- [23] Xing G, Mathews N, Lim S S, Yantara N, Liu X, Sabba D, Grätzel M, Mhaisalkar S and Sum T C 2014 Low temperature solution-processed wavelength-tunable perovskite for lasing *Nat. Mater.* 13 476–80
- [24] Jung J W, Williams S T and Jen A K-Y 2014 Low-temperature processed high-performance flexible perovskite solar cells via rationally optimized solvent washing treatment *R. Soc. Chem. Adv.* 4 62971–7
- [25] Abate A, Saliba M, Hollman D J, Stranks S D, Wojciechowski K, Avolio R, Grancini G, Petrozza A and Snaith H J 2014 Supramolecular halogen bond passivation of organic–inorganic halide perovskite solar cells *Nano Lett.* 14 3247–54
- [26] Noel N K, Abate A, Stranks S D, Parrott E, Burlakov V, Goriely A and Snaith H J 2014 Enhanced photoluminescence and solar cell performance via lewis base passivation of organic–inorganic lead halide perovskites *ACS Nano* 8 9815–217 *Semicond. Sci. Technol.* 30 (2015) 054004 Y Wang et al