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RESEARCH ARTICLE

Optical Modelling of Typical Organic Solar Cell using Transfer Matrix Model

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Abstract

Objectives: Green energy has led to a lot of development in the energy sector. The use of germanium, silicon PV technology has got major limitations of costing and engineering applications. Organic Solar Cell (OSC) is latest addition in green energy having immense application and economic potential. **Method** Computer simulation for optical modelling for OPV has been used. Efforts have been made to study the variation of Light intensity on efficiency of organic solar cells. **Findings:** Worldwide researchers are making efforts to find out ways and means of improving the efficiency of OSC's. In our case, efforts have been made to achieve optimum efficiency of OSC through optical modelling of organic solar cell Simulation of electrical parameters with the help of optical characteristic is discussed. The effect of. light intensity on the power conversion efficiency of the organic solar cell is also studied. **Novelty:** This study uses Transfer matrix model (TMM) where accuracy level is high and electric field intensity variation with light intensity is analyzed.

Keywords: Organic Solar Cell; Optical Modelling; Charge Carrier; Light Intensity; Transfer matrix model (TMM)

1 Introduction

Organic Semiconductors form the basis of Organic Solar Cells. They have alternating single & double bond conjugated structures and conduct electricity based on their chemical configurations. These materials are flexible, economic, environment friendly and may be easily designed for better optical, electrical and mechanical properties. They are broadly classified into two classes: Conjugated Polymers and Small Molecule Organic Semiconductor (SMOS). SMOS are also conjugated structured molecules but their weight is small as compared to conjugated polymers. (1)

Unlike inorganic semiconductors which work on the concept of conduction and valence band, organic semiconductors function upon Lowest Unoccupied Molecular Orbital (LUMO) analogous to conduction band and Highest Occupied Molecular Orbital (HOMO) analogous to valence band. (2) The electrons and holes when bound together by columbic forces are termed as excitons i.e. the bound electron-hole pair. The band-gap of organic semiconductors are designed and tuned to absorb maximum number of photons for achieving higher efficiency. Active layer, Buffer layer, Cathode layer and Anode layer are the four layers of the material of the PV cell as shown in

Figure 1.[3]

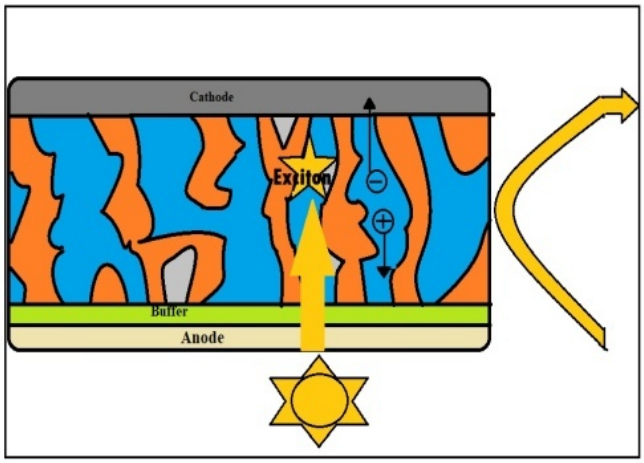

Fig 1. Operating Principle of Organic Solar Cells

2 Optical Modelling of OPV

Optical modeling of an OPV is a complex process because of varying layers along-with wavelength. In the following paras approximation for optical modeling of an OPV will be discussed. The Beer-Lambert law is generally used for understanding attenuation in photons describes the relation between properties of material and attenuation of light. Eq[1] is one of the most used practical expressions of the Beer-Lambert law which refers to the optical attenuation of a physical material. It accommodates a single attenuation species of identical concentration to the optical path length.[4] This expression is:

$$A = \varepsilon \times l \times c \tag{1}$$

Where,

- A is the absorbance
- ε is the molar attenuation coefficient
- l is the optical path length
- c is the concentration of the attenuating species.

However, as mentioned earlier, the above expression is not applicable over OPV devices due to width of the layers in the composition of this kind of PV cells deteriorates wavelength, where interference effects plays a very important role. In view of this, the following expression explains the relationship between optical electric field based on input electric field using transfer matrix model – (TMM).[5]

$$E_j(z) = \frac{S_{j,11} exp(i\zeta_j(z-d_j)) + S_{j,21} exp(i\zeta_j(d_j-z))}{M_{j,11} S_{j,11} exp(-i\zeta_j d_j) + M_{j,12} S_{j,21} exp(i\zeta_j d_j)} \tag{2}$$

Where j implies to the layer number, $E_j(z)$ is the optical electric field at the point z, ζ_j = $\frac{2\pi n_j d_j}{\lambda}$ is the wave phase change, $\bar{d}_j$ is thickness of the layer, $\bar{E}_0$ is optical electric field at the substrate and $\bar{n}_j$ is the complex index of refraction.

The effects of variation of light intensity on the generation rate of excitons and charge carriers are described below. The above Equation 1 is used to calculate the exciton generation rate for a certain position of active layer thickness.[6] The same has been done for all positions inside the organic solar cell and all wavelengths. Absorbed photon density vs position graph is shown in Figure 2 and Photon density vs energy graph is shown in Figure 3. To see the effects of all the photons, integration of all the wavelengths has been done.[7] To get exciton generation rate per unit area, which represents the number of excitons generated per unit time in the volume covering a unit area of incident-surface and length of whole active layer thickness, has been calculated for several values of light intensity.[8] The product of exciton generation rate and dissociation probability gives the charge carrier generation rate per unit area has been calculated.[9]

Figure 4, shows the generation rate per unit area versus position for both charge carriers and excitons. Both show deep ripples at lower positions and shallow ripples at higher positions. For other positions, the generation would be high as the interaction of incident and reflected light would be additive, whereas for some, the generation would be low as well as the ripple because the interaction would be subtractive. [10]

With the change of position, charge carrier is affected in two ways, i.e as the position increases, effect of exciton increases and the effect of probability is decreased. When the position value is too high, the two effects cancel each other, therefore at large position rate of increase of curve is low almost flat. [11,12]

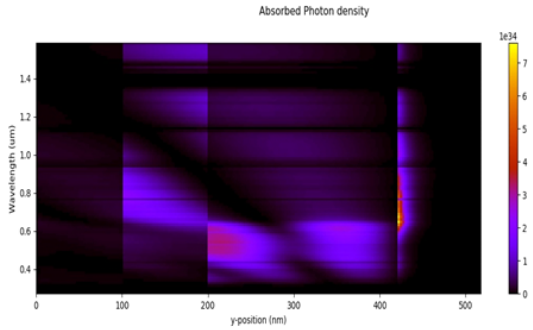

Fig 2. Absorbed Photon Density vs Wavelength vs Position in Organic Solar Cell

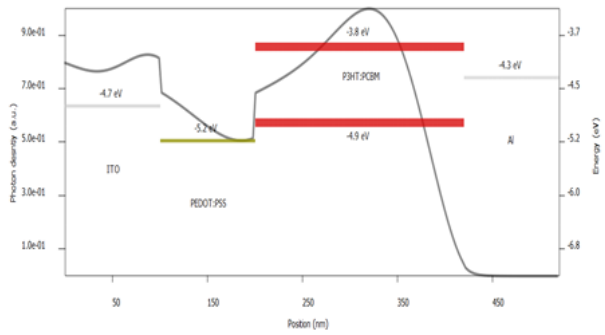

Fig 3. Photon Density vs Energy vs Position in Organic Solar Cell

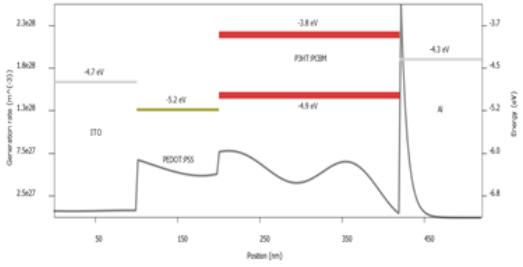

Fig 4. Generation Rate vs Energy vs Position in Organic Solar Cell

3 Simulation of Electrical Parameter from Optical Characteristics

To account for carrier trapping and recombination via trap states, Shockley-Read-Hall recombination two approaches are used. The first assumes that the trapped carrier distribution has reached equilibrium. It also assumes there are relatively few trapped charge carriers compared the number of free carriers, and thus the trapped charges do not significantly change the electrostatic potential. These assumptions are valid when the material is very ordered (i.e., GaAs) or at a push in steady state for some moderately disordered material systems.

The second method assumes trapped carriers have not reached a reached equilibrium with the free carriers. GPVDM has this non-equilibrium Shockley-Read-Hall model for solving potential and current densities in organic solar cells. The bi-polar drift-diffusion equations are solved in position space for electrons in order to describe the charge carrier transport i.e.

$$J_n = q\mu_c n\frac{\partial(-\chi - q\varphi)}{\partial x} + qD_n\frac{\partial n}{\partial x} \tag{3}$$

and for holes

$$J_p = q\mu_n p\frac{\partial(-\chi - E_g - q\varphi)}{\partial x} - qD_p\frac{\partial p}{\partial x} \tag{4}$$

Here, J_n & J_p are the current densities of electrons and holes respectively, μ_c and μ_n and the electron and hole mobilities, D_n and D_p are the diffusion coefficients of free electrons and holes. Figure 5 shows the charge density vs applied voltage graph at temperature 300⊠K and light intensity of 1.0 suns. These equations are applicable when incident light is absent. In such case, generation and recombination of new charge carriers does not occur. Even then, some charge carriers are intrinsically generated due to the existing electric field in the device and due to differential distribution of charge carrier density in bulk hetero-junction comprising of Donor and Acceptor atoms. This current is called Dark Current. It relates the current density obtained from the solar cell to the conduction gap and the free charge carrier density in the absence of incident light.

The charge carrier continuity equations for both electrons and holes given by Equation (5) and Equation (6) which is in accordance with conservation of charge carriers is forced by solving these equations. The electrical parameters were calculated for the cell at different solar insolation and the result are tabulated in Table 1 and J-V curve obtained at 300⊠K and 1 suns is shown in Figure 6.

$$\frac{\partial J_n}{\partial x} = q\left(R_n - G + \frac{\partial n}{\partial x}\right) \tag{5}$$

$$\frac{\partial J_p}{\partial x} = -q\left(R_p - G + \frac{\partial p}{\partial x}\right) \tag{6}$$

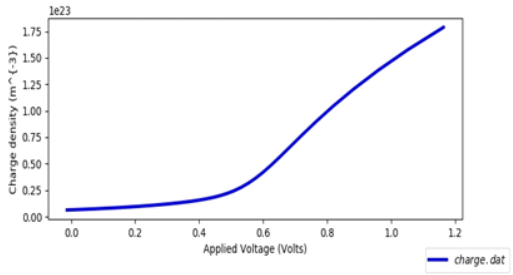

Fig 5. Charge density variations with an applied voltage at 300⊠K and 1.0 suns

Table 1. . Calculated Electrical Parameters of Organic Solar Cell

Light Intensity (Suns)	Jsc ($A.m^{-2}$)	Voc (V)	Fill Factor (%)	Power Conversion Efficiency (%)
0.005	$-5.4444x10^{-1}$	0.4033	0.3905	1.7153
0.01	-1.1069	0.4444	0.5389	2.6512
0.05	-5.6129	0.5072	0.6907	3.9331
0.1	$-1.1248x10^{-1}$	0.5304	0.7073	4.2204
0.5	$-5.6251x10^{1}$	0.5823	0.6937	4.5446
1.0	$-1.1227x10^{2}$	0.6036	0.6724	4.5575
5.0	$-5.5260x10^{2}$	0.6531	0.5757	4.1558
10.0	$-1.0851x10^{3}$	0.5007	0.5007	3.6651

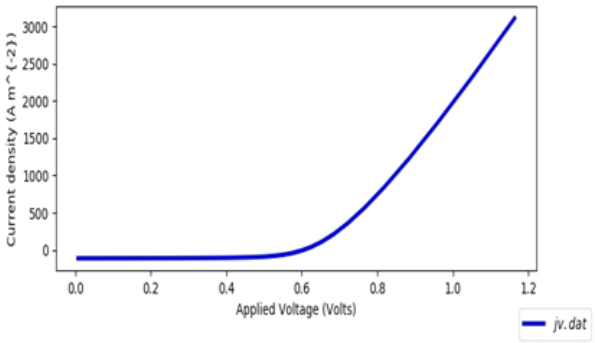

Fig 6. J-V characteristics of the organic solar cells at 300K and 1.0 Suns

4 Conclusion

Organic solar cell has been seen as one of the alternatives for energy resources because of its various advantages such as low cost and flexibility. A comprehensive model for optical as well as electrical process is discussed for organic photovoltaic cell. Transfer matrix model was used to understand optical modelling of solar cell. Generation rate vs position results for excitons and charge carriers were seen with the help of GPVDM software. Bipolar drift diffusion equations were used for electrical modelling of organic solar cell. The effect of solar intensity on the electrical property of organic solar cell such as current density, open circuit voltage, fill factor and power conversion efficiency were seen. It is seen that maximum efficiency is obtained at a light intensity of 1 Suns. The study reveals that future prospects of OPV technology is having high potential. With more concentration over suitable material identification along-with proper parametric characterisation, very high efficiency organic solar cells will be a reality very soon.

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