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Modeling and simulation of Organic solar cell consisting of Nanoscale Layers and Films by Using Silvaco ATLAS Software

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Abstract

An organic photovoltaic device (OPV) with poly (3-hexylthiophene) (P3HT) absorber layer was designed and simulated using SILVACO ATLAS software. The effective area of the cell was 6 mm^2. Langevin recombination, a.singlet and s.binding models were used to simulate this device. Under an illumination of one Sun (AM 1.5G, 100 mW/cm^2), the simulated cell showed an open-circuit voltage of 0.32 V, a short-circuit current density of 0.07 mA/cm^2 and a fill factor of 29.5%, resulting to a power conversion efficiency of 0.005%.

Keywords: Organic Photovoltaic, Simulation, Silvaco, ATLAS.

Introduction

Third generation solar cells (Organic and Quantum dot sensitized solar cells) are the most promising field of photovoltaic solar cell research. A solar cell (photovoltaic system) directly converts sunlight energy into electricity power. When photon of appropriate energy strikes the active area of solar cell, an electron by acquiring energy from incident photon moves from one layer to another and consequently generates electricity. Advanced technologies are using this phenomenon to synthesize solar cells, but low efficiency and high cost are major challenges for them. Simulation of this type of devices is an important strategy to design the considered structures and to predict the effect of physical changes on the cell performance. Different solar cell models have been developed to describe their electrical behavior.

The fundamental parameters open circuit voltage (V_{OC}), short circuit current density (J_{SC}), fill factor (FF) and power conversion efficiency (η), can be used for quality control during production or to provide insights into the operation of solar cells, thereby leading to improvement in devices.

Silvaco ATLAS software is a physically-based two and three dimensional device simulator that predicts the electrical behavior of semiconductor devices at specified bias conditions. This software is also a suitable simulation tool, which considers the different mathematical models, solves them, gives the simulated structural design and the desired parameters as output result.

In this work, a solar cell with ITO/ZnO/P3HT/Ag structure is designed using Silvaco ATLAS software. The materials are chosen on the basis of their band gap. We select the AM1.5 source as the light source, the Fermi statistics as carrier statistics, the langevin recombination, field dependent mobility, and the photo-generation models[1]. Then we will compare these simulation outcomes to our experimental results.

Device Simulation

Generally, a solar cell or photovoltaic (PV) device directly converts electromagnetic radiation of solar energy to electricity power through photovoltaic effect.

An organic photovoltaic (OPV) cell consists of an active layer (organic material) placed between two electrodes with different work functions (WFs). This difference of WFs sets up an electric field (potential slope) in the organic layer.

When exposed to sunlight, the active layer absorbs light (the photons having energy greater than the band-gap energy of the material could be absorbed); some electron-hole pairs or excitons will be generated. The potential created by the different work functions helps to separate the excitons, pulling electrons to the positive electrode and holes to the negative electrode; therefore, a photocurrent is created[2].

Here we simulate an organic solar cell. The base materials used for this simulation work are ITO, ZnO thin film, P3HT and Silver with thicknesses of 200, 70, 100 and 100 nm, respectively. The OPV structure used for simulation is depicted in Figure-1.

For the source of light, the Air Mass 1.5 Global (AM1.5 G) spectrum is most often used for non-concentration solar cells in theoretical analysis. AM1.5G spectrum has an integrated power of 1000 W/m^2 (100 mw/cm^2), and its plot is shown in Figure-2.

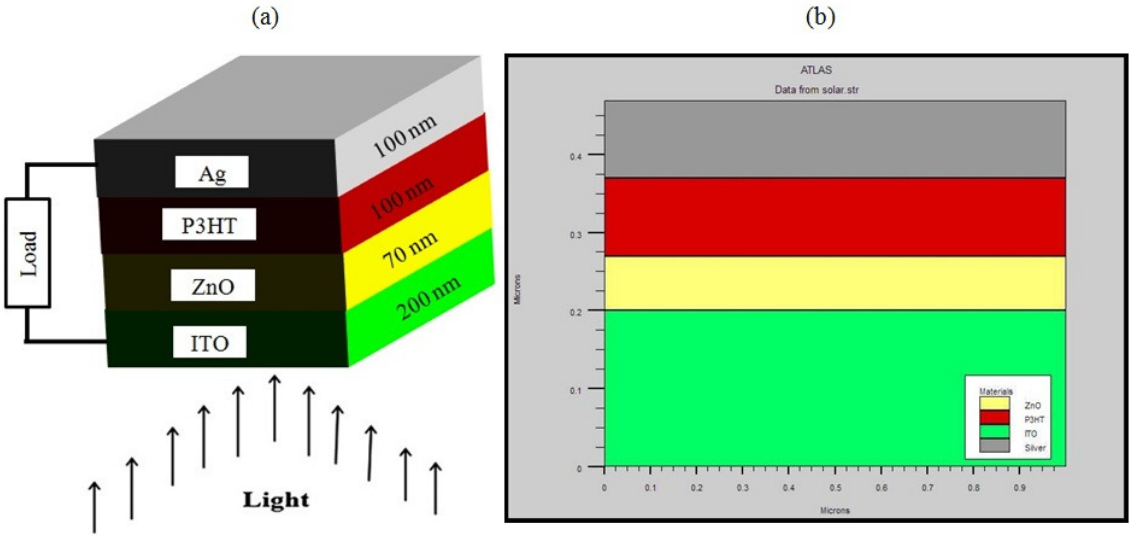

Figure-1
(a) Schematic diagram of designed structure, (b) OPV structure designed in ATLAS

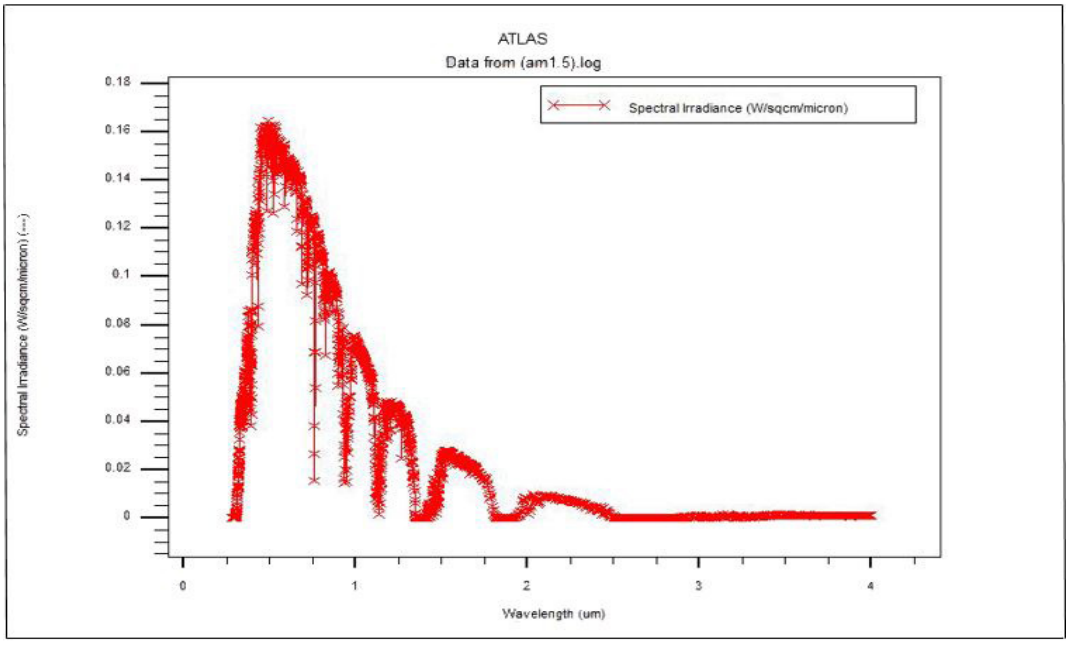

Figure-2
Standard Solar Spectrum (AM1.5G) used as source of light (Wave Length vs. Intensity in AM1.5G)

In this device, incident light generates excitons in P3HT. These photo generated excitons can become dissociated with electrons moving to ZnO (then to ITO electrode) and holes are extracted by Ag electrode.

The optical transmission spectrum of P3HT is depicted in figure 3. In order to determine the optical band gap energy (E_g) of P3HT, the standard relationship of $(\alpha h\nu)^2=A(h\nu-E_g)$ was used in which α, t and hν are absorption coefficient , thickness of layer and the photon energy, respectively. The absorption coefficient (α) determines the particular distance that a specific wavelength penetrates into a material before it is absorbed, and is calculated by following equation:

$$\alpha = \frac{1}{t}\ln\left(\frac{1}{T}\right)$$

Therefore, the band gap energy of P3HT was obtained by extrapolating the linear and sharply increasing portion of the curve and intercepting to the *hν* axis (Figure-3)[3,4].

The energy level situations, an exciton generation, electron and hole dissociation and recombination path of designed cell is shown in Figure-4.

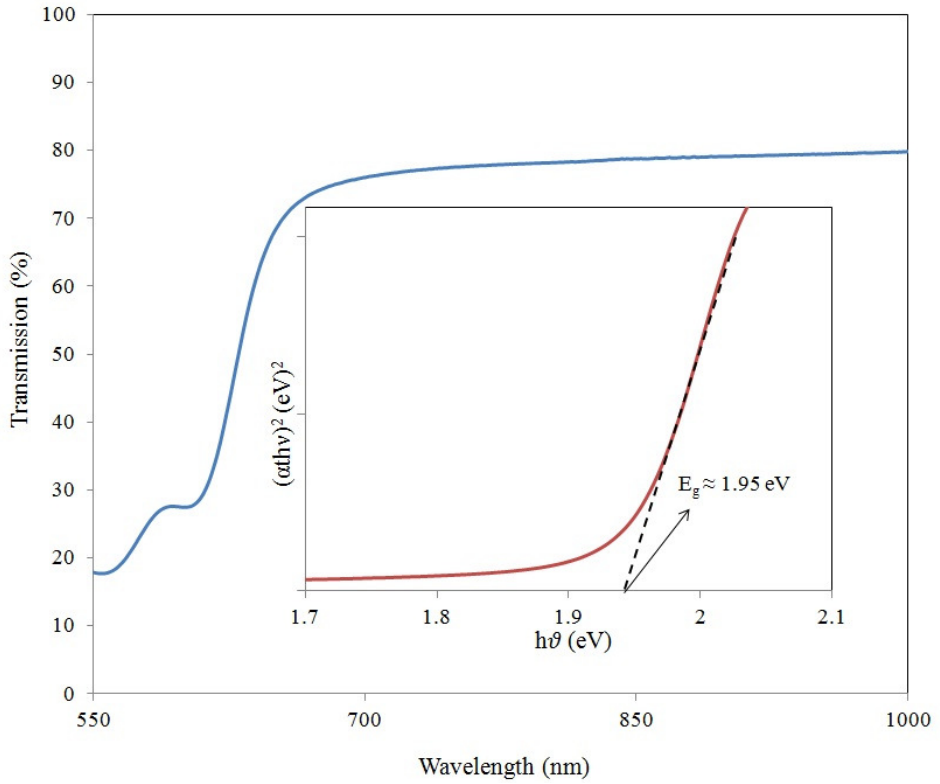

Figure-3

Optical transmission spectrum of P3HT. The inset shows the typical absorption spectrum by plotting $(\alpha th\nu)^2$ versus hν

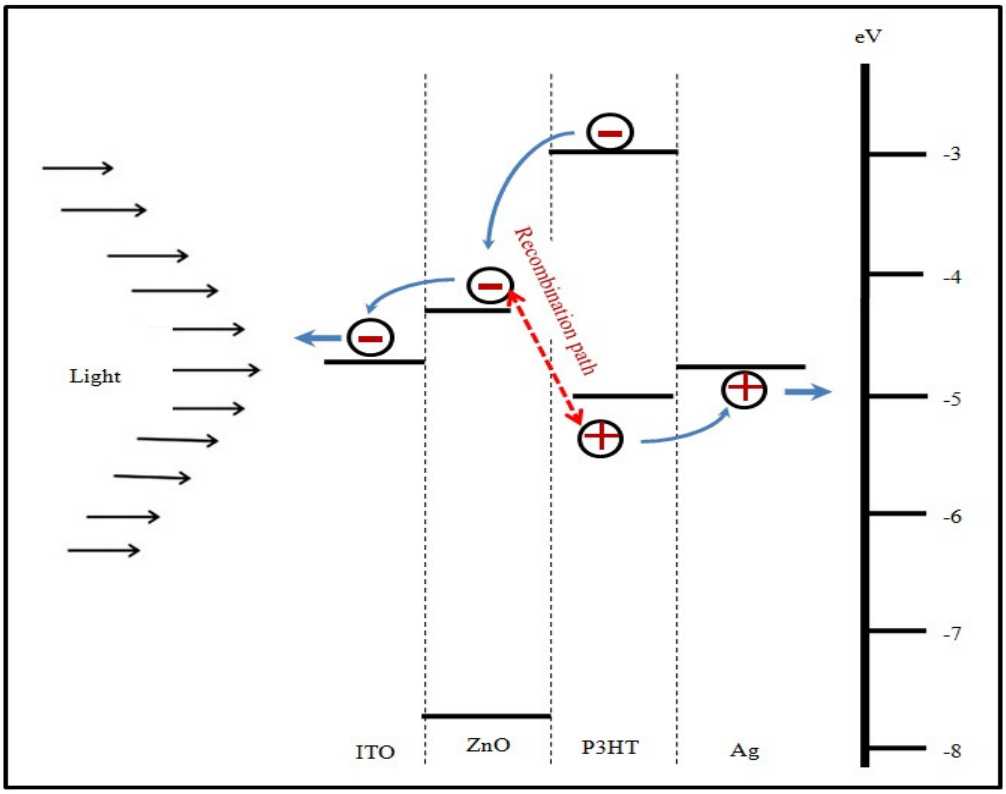

Figure-4

Energy level position, electron–hole pair generation, dissociation and recombination path of simulated device

Results and Discussion

This simulation was performed using physical Langevin recombination model. The Langevin recombination is dominant in organic solar cells. Organic materials are characterized by low mobility. Charge carriers (electrons and holes) in low mobility semiconductors move slowly. Therefore, the recombination of an electron with a hole will be probable. Langevin describes the theory of such process.

The physical parameters used in modeling of OPV consisting of band gap energy E_g, electron affinity χ, relative permittivity ε_r, effective density of states in conduction N_c and valence band N_v (at 300K), mobility of electrons μ_e and holes μ_h for the active layer (P3HT) and work function of electrodes is listed in Table-1[5-8].

Table-1
Simulated OPV specifications

Parameter	Value
E_g (eV) of P3HT	1.95
N_C (1/cm^3)	2×10^{21}
N_V (1/cm^3)	2×10^{21}
μ_e (cm^2 V^{-1} S^{-1})	10^{-6}
μ_h (cm^2 V^{-1} S^{-1})	1.2×10^{-3}
ε_r	3
χ (eV)	3.2
a.singlet	1.9
s.binding	0.28
Work Function of ITO (modified by ZnO) (eV)	4.3
Work Function of silver (eV)	4.7

The a.singlet and s.binding parameters used in material statement, represent the electron and hole separation distance and the singlet exciton binding energy, respectively.

Combining the absorption of the sample at the excitation wavelength with the number of incident photons, determines the number of photons absorbed, which is the equivalent to the number of excitations. To calculate the volume of excitation, the sample thickness and the area of the laser spot should be used. The thickness of the samples could be calculated from the absorption using Beer's Law. The singlet exciton density is shown in Figure-5.

Consider an (exciton) electron-hole pair bound by Coulomb interaction in crystal with dielectric ε_r constant. The wave-function of this exciton motion $\Psi(r)$ could be obtained from the Schrodinger equation:

$$\frac{\hbar^2}{2\mu}\nabla^2\Psi(r) + E\Psi(r) = -\frac{e^2}{\varepsilon r}\Psi(r)$$

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\mu = \frac{m_e m_h}{m_e + m_h}$$

$$r = \sqrt{x^2 + y^2 + z^2}$$

Where: ∇^2, μ and r are Laplacian operator, reduced (effective) mass of electron and hole, and the distance between electron and hole, respectively. The binding energy of the ground exciton state is:

$$E_B = \frac{\mu e^4}{2\hbar^2\varepsilon^2} = \frac{\hbar^2}{2\mu a_B^2}$$

$$a_B = \frac{\hbar^2\varepsilon}{\mu e^2}$$

Where: a_B is the Bohr radius.

The current density-voltage (J-V) curve of the simulated device is shown in Figure-6.

Open-circuit voltage (V_{OC}), Short circuit current density (J_{SC}), Maximum power (P_{max}), maximum voltage (V_{max}), Fill Factor (FF) and Power Conversion Efficiency (η) values obtained from the simulation are listed in Table-2 and compared to experimental measurement data.

Table-2
PV parameters obtained for simulated and fabricated OPV device with ITO/ZnO/P3HT/Ag structure

PV Parameter	Value (Simulation)	Value (Experimental)
V_{OC} (V)	0.32	0.3
J_{SC} (mA/cm^2)	0.07	0.09
P_m (W)	0.004	0.004
FF (%)	29.5	28.2
η (%)	0.005	0.007

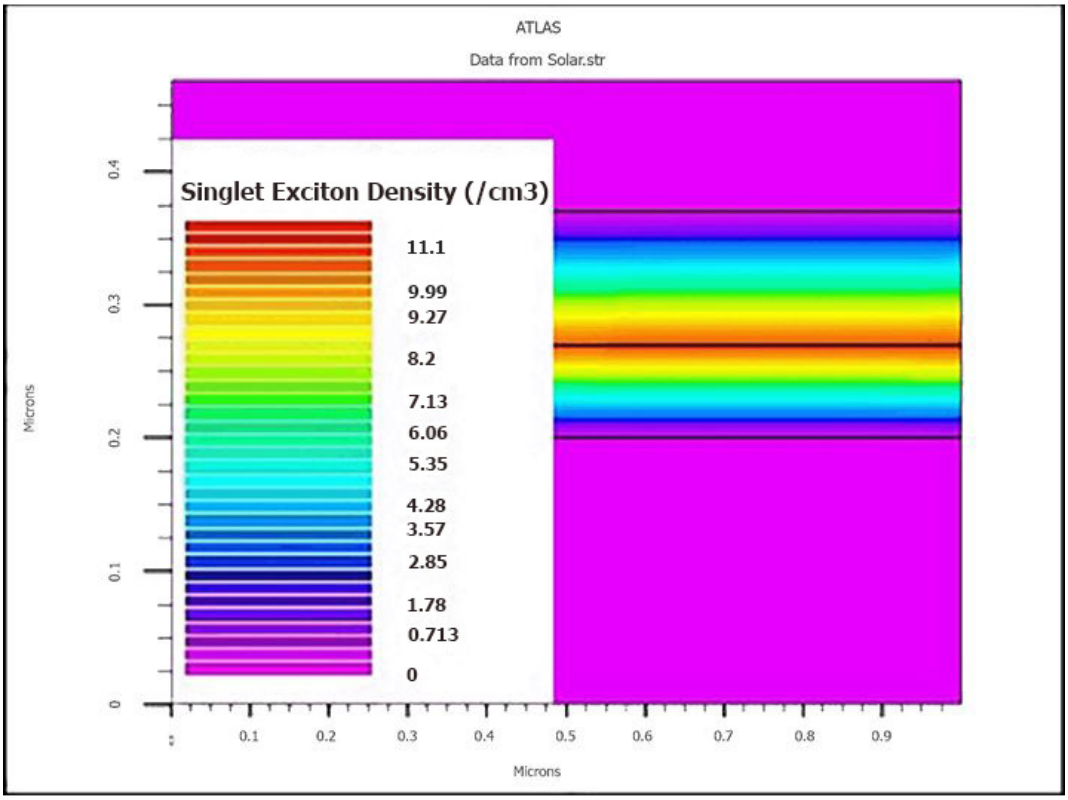

Figure-5
The density of singlet exciton obtained in Silvaco ATLAS simulation software

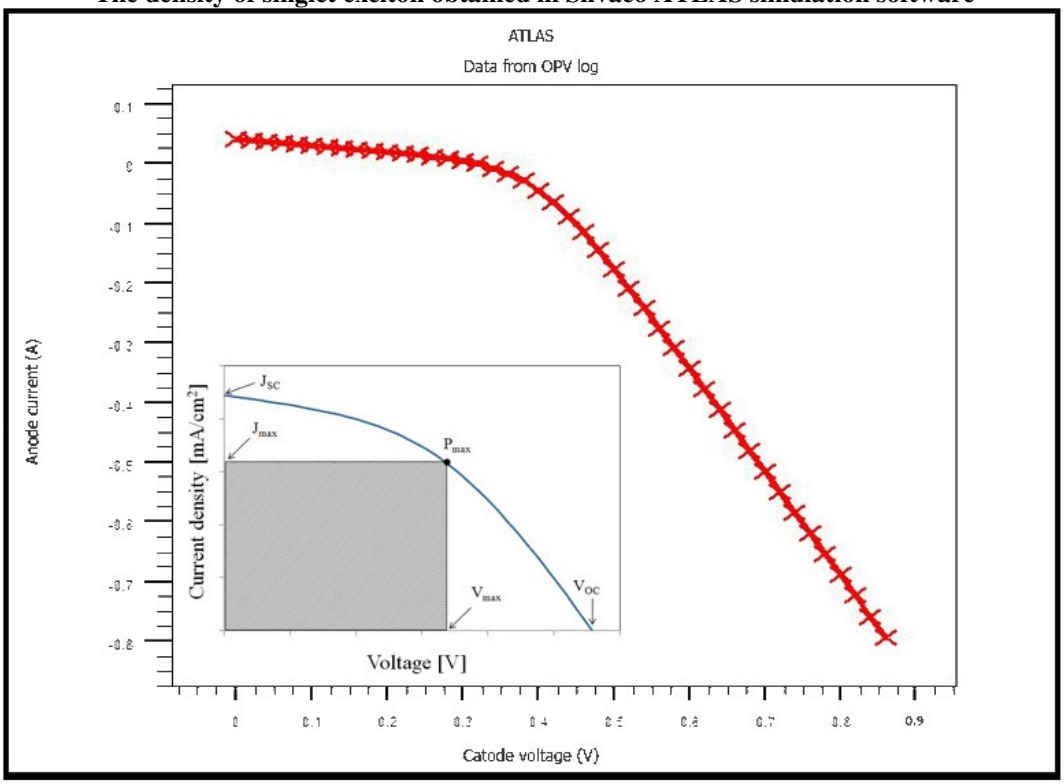

Figure-6
Current density-voltage curve of the OPV simulated device. The inset shows J–V curve and cell parameters of solar cells

The fill factor (FF) is determined from measurement of the J-V curve and is defined as the maximum power divided by the product of $J_{SC} \times V_{oc}$ (following equation):

$$FF = \frac{J_m \times V_m}{J_{SC} \times V_{OC}}$$

where the product of J_m and V_m is calculated from the J–V curve. The energy conversion efficiency (η) is calculated using the ratio of the electric power output of the device at the maximum power point (P_{max}) to the incident optical power (Plight) and is defined as:

$$\eta = \frac{FF \times J_{SC} \times V_{OC}}{P_{light}}$$

Several factors affect a cell's conversion efficiency value, including its reflectance efficiency, thermodynamic efficiency, charge carrier separation efficiency, and conduction efficiency values. Because these parameters can be difficult to measure directly, other parameters are measured instead, including quantum efficiency, V_{OC} ratio, and fill factor.

Conclusion

In this work we have successfully designed and simulated an organic photovoltaic device with ITO/ZnO/P3HT/Ag structure using Silvaco ATLAS software. In simulated OPV device, the efficiency of 0.005%, fill factor of 29.5%, short-circuit current density (Jsc) of 0.07 mA/cm^2 and open-circuit voltage (V_{oc}) of 0.32 V was obtained. These simulation results are completely coincided with the results of experimental measurement data.

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