Materials Research Express

PAPER

Electrical simulation of the function of tungsten oxide in polymeric solar cells

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Keywords: polymeric solar cells, SCAPS, AMPS, buffer layers

Abstract

In this research, polymeric solar cells (PSCs) are numerically simulated using SCAPS and AMPS. The study deals with the effects of the thickness of active and buffer layers, defect densities of active layers, and temperature on open-circuit voltage (VOC), fill factor (FF), short-circuit current density (JSC), and performance (PCE). Also, J-V characteristics and quantum efficiency are plotted in two types of buffer layers (i.e. PEDOT:PSS and WO3). The results show an optimal value for the absorber and the buffer layer thickness. Also, an increase in the defect densities of the absorber layer is found to cause a decrease in the efficiency of the PSCs. According to the findings, it is possible to use WO3 for the higher conversion efficiency of buffer layers.

1. Introduction

Polymer solar cells (PSCs), serving as a means of obtaining renewable energy, have recently become a subject of universal interest. Their attraction is due to certain advantages such as low cost, simple fabrication, light weight, and flexibility [1–3].

A combination of the active layers of an electron-donating material and an electron-accepting material makes it possible to absorb light and generate excitons [4–7]. Holes and electrons can then be separated from each other. Finally, an interpenetrating network of electron donors and electron acceptors is formed on a nanometer scale within the active layer [8–13]. It is to be mentioned that a simple structure that includes an active layer between the two electrodes (i.e. anode and cathode) is just not adequate for this scenario.

The charge collection at the interface between the active layer and the electrodes is of low efficiency [6]. This problem is often solved by introducing an interfacial layer, such as a composite of poly_3,4 ethylenedioxythiophene:poly_styrenesulfonate (PEDOT:PSS), between the active layer and the anode. This leads to the enhancement of the open-circuit voltage (VOC) and the improvement of the charge carrier collection [7].

However, due to its electrical non-homogeneities and corrosion of indium tin oxide (ITO), PEDOT:PSS is considered to have an adverse effect on the performance of PSCs [14–18]. To deal with the problem, certain materials that can serve as interfacial layers are used to improve the performance of PSCs. Recently, vanadium oxide (V2O5), molybdenum oxide (MoO3), and nickel oxide (NiO) have been proposed as appropriate alternatives for PEDOT:PSS and as buffer layers in PSCs [19–22]. Also, tungsten oxide (WO3), as an electron extraction layer, is used in inverted PSCs [23–27]. Tungsten oxide has advantages of being nontoxic, low-cost and easily evaporable. In this study, the basic factors that can affect the function and efficiency of PSCs are investigated with reference to the structures of glass/ITO/buffer layers/P3HT:PCBM/Ag. The buffer layers are WO3 and PEDOT:PSS. The calculations are done by using the AMPS and SCAPS software programs.

2. Materials and methods

2.1. Program explanation

SCAPS-1D and AMPS are two simulation software programs developed at the Universities of Gent and Pennsylvania. SCAPS is commonly used to simulate solar cells and calculate steady-state band diagrams,
recombination profiles, and carrier transport in one dimension. It functions on the basis of the Poisson equation along with hole and electron continuity equations. Recombination currents are calculated with the Shockley-Read-Hall (SRH) model for bulk defects, but an extension of that SRH model is applied to interface defects. To keep the model as simple as possible, only one type of single-level defects is introduced in each layer. These defects are all compensating ones positioned at the intrinsic level close to the mid-gap. The SCAPS-1D software, which was modeled under an AM 1.5 light spectrum and a power of 1000(\text{W m}^{-2}), can describe layers of PSCs with different properties [28]. The software can also simulate several common measurements including C–V, C–f, I–V, and QE [29]. As for the AMPS simulation software, it transports the carriers on the basis of the continuity equations devised for holes and electrons and can solve three basic kinds of equations including Poisson’s equation, continuity equations, and transport equations [30]. The expertly engineering of the software has made it a very general and versatile computer simulation tool for analyzing device physics and device designs. AMPS has been intended to teach how material properties (e.g., band gap, doping, affinity, mobility, and gap state defect distributions in the bulk and at interfaces) join the device design/structure to control the device physics and, thereby, the device response to temperature, light, and impressed voltage. This software allows users to learn the ‘whys and wherefores’ of the response of a device to a given situation (i.e., light bias, voltage bias, and temperature). The insight is provided through exploration and comparison of band diagrams, current components, recombination and generation patterns as well as electric field plots. The parameters, made available and analyzed by AMPS, are, indeed, the functions of light intensity, voltage, temperature, and position.

2.2. Cell structure
The overall efficiency of organic photovoltaic cells is affected by the device structure. The so-called ‘direct structure’ is the mostly used stack of layers on glassy ITO/hole transport layer (HTL)/P3HT:PCBM/electrodes. HTL, which also serves as an hole transport layer, is typically made of a solution-processed conducting polymer such as PEDOT-PSS. In a direct structure, the top electrode (anode) must consist of a relatively low work-function metal such as Ag, Ca, or Al.

Beside direct structures, inverted structures, too, have been favored owing to their air stability. A basic inverted structure can be found in an ITO/electron-transport layer (ETL)/P3HT:PCBM/HTL/electrode. An ETL is a semi-permeable membrane that serves to prevent hole transport to the bottom of the electrode. The materials generally used in ETLs are metal oxides such as TiO2, TiOx, WO3 or ZnO. PSCs have been simulated with two input layers including P3HT:PCBM as an absorber layer and PEDOT:PSS and WO3 as buffer layers [31]. Also, as shown in figure 1, silver (Ag) has been used for the back contact while Indium tin oxide (ITO) has served as an electrode for the front contact.

2.3. Input parameters
Due to their various layers and the influence of the material parameters involved, PSCs are considered as complex structures. This structural complexity often results in some particular mechanisms [32]. Software can be utilized to wisely evaluate the possible values and to explain the mensuration of PSC structures. Simulation software programs can be of benefit in the analysis of how the variation of layer parameters affects the achievement of optimal values to provide highly efficient PSCs. This analysis can be conducted on the variation of the individual properties involved, the presence or absence of particular properties, or the existence of a range of values. Device manufacturers should be trained as how to modify their production modes to raise the product performance. So far, to simulate the application of PSCs, different software programs, such as ASA, SCAPS-1D, AMPS-1D, OPVDM, and AFORS-HET, have been introduced. Before the discussion of such simulation programs, the materials which are used to fabricate the structures should be described [33–35]. As presented in table 1, the parameters used for the simulations of standard PSCs have been ITO, PEDOT:PSS, WO3, P3HT:PCBM, Ag, and Au [36–38]. Here, $\chi$ is the electron affinity (eV), $N_D$ is the donor concentration (cm$^{-3}$), $N_A$ represents the acceptor concentration (cm$^{-3}$), $\varepsilon_r$ denotes the relative permittivity, $E_g$ stands for the band gap energy (eV), $\mu_e$ is the electron mobility (cm$^2$/Vs), $N_E$ represents the band effective density of states (1/cm$^3$), $N_V$ refers to the valence band effective density of states (1/cm$^3$), $V_h$ is the electron thermal velocity (cm/s), $u_p$ stands for the hole thermal velocity (cm/s), and $u_p$ is the hole mobility (cm$^2$/Vs) [23, 29].

3. Results and discussion

3.1. Effect of the active layer thickness
As plotted in figure 2, the thickness of the active layer varied from 40 to 140 nm in correspondence to $J_{SC}$, $V_{OC}$, PCE, and FF. The optimization of the active layer value was carried out with two types of buffer layers as reported in table 2. Values of about 80–100 nm emerged to be optimal for the buffer layers and 90–110 nm for the
absorber layer. It is to be mentioned that these values were sentient to the mobility of the carrier. The dependence of the saturation current ($I_0$) of the software values on the active layer thickness is demonstrated in figure 3. This dependence may be best realized on the basis of the following equation [39]:

Figure 1. Schematic structure of the PSCs.

Figure 2. Absorbance of WO$_3$, PEDOT:PSS and P$_3$HT:PCBM.
where \( T \) is the working temperature, \( J_{SC} \) denotes the short-circuit current density, \( k \) represents Boltzmann’s constant, and \( J_0 \) is the saturation current density.

### 3.2. Effect of the thickness of the buffer layer

The optimized values of the active layer were applied to calculate the optimum thickness of the buffer layers. For this purpose, the buffer layer thickness was changed from 40 to 140 nm in correspondence to \( J_{SC}, V_{OC}, PCE, \) and \( FF \). The simulation plot is presented in figure 4. Also, the optimized values for each of the two layers are presented in table 2. As it was observed, an increase in the buffer layer thickness made no sensible change in the

![Graph showing the effect of buffer layer thickness on various photovoltaic parameters](image-url)

**Figure 3.** Effect of the buffer layers thickness on (a) \( V_{OC} \), (b) \( J_{SC} \), (c) \( FF \) and (d) \( PCE \).
values of \( V_{OC} \) and FF, and they remained almost fixed. However, the value of \( J_{SC} \) gradually decreased due to a reduction in the light absorption. This is while the value of PCE at first increased and then decreased from thickness of 80 nm for WO\(_3\) and 100 nm for PEDOT:PSS. The PN junction model can help to conclude this phenomenon, which is explained by the following equation [39]:

\[
J_0 = A q n_i^2 \left( \frac{D_e}{L_e N_A} + \frac{D_h}{L_h N_D} \right)
\]

where \( N_A \) is the acceptor doping concentration, \( N_D \) denotes the donor doping concentrations, \( L \) stands for the diffusion length, \( q \) is the electronic charge, \( n_i \) refers to the intrinsic concentration, \( D \) represents the diffusion coefficient, and \( A \) is the quality factor of the diode. The subscript \( e \) refers to electrons, and \( h \) refers to holes. When the absorber carrier density, \( N_A \), is increased, the saturation current density, \( J_0 \), is reduced, which results in an increase in the \( V_{OC} \). However, the short-circuit current density decreases as the carrier density increases. These changes, which occur according to equations (1) and (2), are mainly due to the fact that higher carrier densities enhance the recombination process and reduce the chance of the photon-generated electrons to be collected, and the quantum efficiency of the long-wavelength photons is also reduced. Since these photons are absorbed deeply in the active layer, the collected efficiency of the generated electrons is more dependent on the diffusion effect.

Figure 4. Effect of the absorber thickness on (a) \( V_{OC} \), (b) \( J_{SC} \), (c) FF, and (d) PCE with two buffer layers.
3.3. Effect of the absorber layer defect density with different buffer layers
Defect density plays a crucial role in the function of PSCs. Its influence on the efficiency of PSCs was investigated in the range of $10^7 \text{ cm}^{-3}$ to $10^{14} \text{ cm}^{-3}$ according to the PV parameters with different buffer layers. The simulation results are presented in figure 5. As it can be seen, the PV parameters were reduced once the defect density rose to a value higher than $10^{11}$ for both buffer layers, i.e. WO$_3$ and PEDOT:PSS.

3.4. Effect of temperature on PSCs
Temperature plays a key role in the function of PSCs. Since solar cell panels are installed outdoors, PSCs have to operate at a temperature higher than 300 K. The influence of temperature on the PSCs performance was investigated with two buffer layers. The temperature was given a variation from 300 K to 440 K in accordance with $J_{SC}$, $V_{OC}$, PCE, and FF. The simulation results, plotted in figure 6, suggest that PSCs efficiency would rise by a rise in the temperature. Also, parameters such as hole and electron density concentration as well as hole and electron mobility were found affected at a higher temperature, which, in turn, affected the cell efficiency. As for the FF, it rose at a higher temperature. However, the open-circuit voltage firstly increased at temperatures up to 400 k but then decreased at higher temperatures.
3.5. Effect of the back contact on PSCs

In the optimum simulation format, the values of active thickness, the buffer layers, and the optimum temperature were applied to make a \(J-V\) plot in terms of the following structures. Figure 7 shows the simulated \(J-V\) plot in AM1.5 illumination conditions (100 mW cm\(^{-2}\)). Table 3 presents the comparative simulation of solar cells with all the PV parameters (i.e. \(J_{SC}\), PCE, \(V_{OC}\), and FF) included.

A: ITO/PEDOT:PSS/P\(_3\)HT:PCBM/Ag
B: ITO/PEDOT:PSS/P\(_3\)HT:PCBM/Au
C: ITO/WO\(_3\)/P\(_3\)HT:PCBM/Ag
D: ITO/WO\(_3\)/P\(_3\)HT:PCBM/Au

According to the results in table 3, structure C has a higher performance.

3.6. Quantum efficiency simulation

It is possible to calculate the quantum efficiency by measuring the current response at a zero voltage and normalizing the current to the flux density of the incident light. The calculation is performed through the following equation [40]:

\[
\text{Quantum Efficiency} = \frac{J}{\Phi} \times 100
\]

\(J\) is the current density, and \(\Phi\) is the flux density of the incident light.
where $f$ is the flux density of the total monochromatic optical light. At the peak of the quantum efficiency, the wavelength starts to vary within the spectrum of the solar cells. Since it is an empirical simulation, it is usually $j = 10$ to be used. Also, the relationship between the short-circuit current density and QE can be expressed by equation (3) [41]:

$$J_{SC} = q \int F(\lambda).QE(\lambda) d\lambda$$

where $F$ is the flux density in a single wavelength.

Table 3. Summary of the performance characteristics of the solar cells simulated in this study.

| Cells configuration | $V_{OC}$ (V) | $J_{SC}$ (mA cm$^{-2}$) | FF (%) | PCE (%) |
|---------------------|-------------|-------------------------|--------|---------|
|                     | SCAPS       | AMPS                    | SCAPS  | AMPS    | SCAPS  | AMPS    | SCAPS  | AMPS    |
| A: ITO/PEDOT:PSS/P3HT:PCBM/Ag | 0.62 | 0.66 | 13.44 | 12.71 | 67.51 | 69.23 | 5.21 | 5.56 |
| B: ITO/PEDOT:PSS/P3HT:PCBM/Au | 0.67 | 0.69 | 12.83 | 12.28 | 65.43 | 64.32 | 4.83 | 5.02 |
| C: ITO/WO3/P3HT:PCBM/Ag | 0.61 | 0.62 | 15.65 | 14.58 | 72.04 | 72.28 | 8.67 | 9.58 |
| D: ITO/WO3/P3HT:PCBM/Au | 0.72 | 0.70 | 14.36 | 13.96 | 70.23 | 68.96 | 8.48 | 8.95 |

Figure 7. Effect of temperature with two buffer layers on (a) $V_{OC}$ (b) $J_{SC}$ (c) FF and (d) PCE.

Figure 8. Current–voltage characteristics under AM1.5 illumination with different structures.
The choice of buffer layers can also be characterized by the plot of QE, as shown in figure 8. The results suggest that PSCs with WO3 and PEDOT:PSS buffer layers show an increased spectral response that reaches a maximum of 79% and 68% from the wavelength of 460 nm to 560 nm respectively.

4. Conclusion

In this paper, we studied the performance of PSCs and the effect of two buffer layers, including WO3 and PEDOT:PSS, on the efficiency of those cells. An analysis of the outcomes showed that the optimum thickness of WO3 and PEDOT:PSS was 80 and 100 nm respectively. Also, the optimal active layer thickness was 100 nm, and the optimum temperature and the defect density of the active layer were 420 K and 1011. The optimum parameters were calculated by using $V_{OC}$, $FF$, $J_{SC}$ and PCE obtained with the buffer layers of PEDOT:PSS, WO3, back contact Ag, and Au. We compared the results of simulating PSCs with different buffer layers and back contacts. It was indicated that the conversion of type-C solar cells, which contains a WO3 buffer layer and the back contact Ag, leads to an enhancement of the cell performance up to 13.77%. This makes the cells a potential substitute for other cells.

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