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Simulation of Organic Solar Cells Using AMPS-1D Program

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Abstract: The analysis of microelectronic and photonic structure in one dimension program [AMPS-1D] program has been successfully used to study inorganic solar cells. In this work the program has been used to optimize the performance of the organic solar cells. The cells considered consist of poly(2-methoxy-5-(3,7-dimethyloctyloxy)-1,4-phenylenevinylene) [MDMO-PPV]] as electron donors, and (6,6)-phenyl-c_{61}-butyric acid methyl ester [PCBM] as electron acceptor, (MDOM-PPV/PCBM) is used as photo - active material, sandwiched between a transparent indium tin oxide (ITO)and layer of poly(3,4-ethylenedioxythiophene)/poly(styrenesulfonate)(PEDOT/PSS) on top of the ITO electrode and an AL backside contact . The results are found to be in a good agreement with the experimental results, obtained from the literature. The results have shown that the optimum thickness of the solar cell is about 120 nm, the optimum energy difference between the lowest unoccupied molecular orbital of the electron donor and the electron acceptor is about 0.5 eV, and the maximum efficiency for the organic solar cell is about 9%. The results have also shown that the open circuit voltage decreases with temperature at a rate of about 0.55 mV/^{0}K.

Key words: AMPS-1D program, bulk heterojunction, efficiency, open circuit voltage, organic solar cells, thickness

INTRODUCTION

Organic solar cells based on conjugated polymers are promising candidates for a cheap and flexible alternative to inorganic devices. The most recent and efficient polymer solar cells fabricated today are based on the concept of bulk heterojunction.

Photo-excitations in organic materials do not lead directly to free charge carriers, as in inorganic materials, but to bound electron-hole pairs (excitons). The excitons can be dissociated at interfaces of materials with different electron affinities. Usually the polymer, electron donor, is blended with the electron acceptor, [6, 6]-phenyl-C_{61}-butyric acid methyl ester (PCBM), which has high electron affinity. After dissociation, a pair of a hole in the donor and an electron in the acceptor is formed across the interface. The internal electric field separates the pair into free charge carriers. The free hole and the free electron are then transported through the donor and acceptor to the electrodes. The lifetime of the separated charges in such blend has to be sufficiently long in order to be transported to the electrodes.

The power efficiency, η, is given by:

$$\eta = FF\, I_{sc}\, V_{oc}/\mathrm{P} \quad (1)$$

where FF is the fill factor, I_{sc} is the short circuit current, V_{oc} is the open circuit voltage, and P is the solar power incident on the cell.

The short circuit current is determined by the photon absorption and the internal conversion efficiency. The amount of absorbed photons can be increased by increasing the thickness. As the thickness increases, the possibility of recombination losses increases, due to the low charge mobility. The recombination losses decrease the fill factor.

The AMPS-1D program (Analysis of microelectronic and photonic structure-one dimension) has been used, successfully, to study the efficiency of inorganic multi-junction solar cell (Pennsylvania State University, 1997). In this work the program was used to study the optimum performance of organic solar cells.

Organic solar cells: Organic solar cells mainly consist of two organic materials one of which is a donor and the other is an acceptor. Conjugated polymers, generally, are used as donors and fullerenes as acceptors, in organic solar cells. One of the main differences between inorganic and organic semiconductors (here conjugated polymers) is the magnitude of exciton binding energy. An exciton is defined as a bound electron-hole pair created upon

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excitation of the semiconductor across the band gap. For most inorganic semiconductors, the exciton binding energy is small compared to the thermal energy at room temperature (kT~0.025eV). Therefore, free charges are generated under ambient conditions. Organic semiconductors, on the other hand, typically have exciton binding energies exceeding kT by more than an order of magnitude (Mihailetchi, 2005). As a consequence, excitons are formed upon excitation instead of free charges. Organic solar cells need an additional mechanism to dissociate the excitons. If an exciton is created in the donor and reaches the donor/acceptor interface, the electron will be transferred to the acceptor material and the hole will recede in the donor material. Similarly, a hole will be injected in the donor material after excitation of the acceptor material.

An exciton created in either the donor or acceptor will reach the interface within its lifetime only if it is created within a slab of material around the interface with a thickness less than the exciton diffusion length. The thickness is limited to about 10 nm for organic semiconductors. In order to solve this dilemma, efficient polymer solar cells require a nano-scale interpenetration of a continuous network of donor and acceptor materials, within the whole photoactive layer, to ensure an efficient dissociation of photo-generated excitons, and transport of the charges to the electrodes. This is called a Bulk Hetero-Junction (BHJ) solar cell (Wang *et al.,* 2008).

For generation of electrical power by absorption of photons, it is necessary to separate the Electron-Hole Pair (E.H.P), generated in the primary absorption process, before recombination takes place. In an organic solar cell, the stabilization of the Photo-excited Pair (P.E.P) can be achieved by blending the polymer (donor) with an acceptor molecule, having an electron affinity that is larger than the electron affinity of the polymer, but still smaller than its ionization potential. Under these conditions, photo-induced electron transfer from the conjugated polymer (donor) to the acceptor molecule is generally favorable (Lemahu, 1996). The primary process of photo current generation is by the generation of excitonsafter absorption of light, either by the donor or by the acceptor. The excitons then diffuse in either of the domains towards the polymer-fullerene (donor - acceptor) interface and dissociate via ultra fast electron transfer (Goh and Gehee, 2005). After dissociation, a pair of a hole at the donor and an electron at the acceptor is formed.

AMPS-1D program: The computer models can be used as a method that leads to a better device design. Device modelling involves the numerical solution of a set of equations, which form a mathematical model for device operation. The usefulness of the simulation results strongly depends on the reliability of the input parameters that are required by the internal numerical models. By using simulation programs it is possible to examine the influence of model parameters, which cannot be determined experimentally.

The one-dimensional device simulation program AMPS solves Poisson equation and the electron and hole continuity equations by using the method of finite differences and the Newton-Raphson technique (Pennsylvania State University, 1997).

RESULTS AND DISCUSSION

The open circuit voltage: The open circuit voltage V_{oc} of bulk hetero-junction solar cells based on [6, 6]-phenyI C_{61} -butyric acid methyI ester PCBM as electron acceptor and poly (2-methoxy-5 - (3, 7-dimethloctyloxy)-1, 4-phenylene [vinylene] MDMO-PPV as an electron donor has been investigated extensively in the literature. It was demonstrated that (Mihailetchi *et al*., 2003), the V_{oc} is governed by the $LUMO_A$ and $HOMO_D$ levels of the acceptor and donor, respectively, which pin the Fermi levels of the cathode and anode.

The AMPS program has been used to study the effect of the $HOMO_D$-$LUMO_A$ offset on the open circuit voltage. The input values for the work function of PEDOT: PSS, thickness of the blend, temperature, and the $HOMO_D$ level of MDMO-PPV were taken to be 5.2 eV, 100 nm, 300 ºK and 5.3 eV, respectively (Mihailetchi *et al*., 2003). The $LUMO_A$ level of PCBM is increased from a value of 3.7eV to 4.5 eV. The relationship between the open circuit voltage and $HOMO_D$ -$LUMO_A$ offset is shown in Fig. 1. It is noticed that the relationship is linear and the slope of the line is equal to 1.0. This relation can be described by the equation,

$$qv_{oc} = (0.97\pm0.01)\,(H_D - L_A) - (0.05\pm 0.02) \qquad (2)$$

This can be approximately written:

$$qv_{oc} = (H_D - L_A) - 0.05$$

where, q is the electronic charge and H_D , L_A is the $HOMO_D$ and is the $LUMO_A$.

The relationship for the V_{oc} obtained from experiments, (Lemahu, 1996), has the form:

$$qV_{oc} = (H_D - L_A) - 0.2$$

The effect of temperature: The temperature dependence of the open circuit voltage V_{oc} has been studied, using AMPS program. The input was the work function of PEDOT: PSS, the thickness of the blend, the $HOMO_D$ level of MDMO-PPV, and the $LUMO_A$ level of PCBM. The temperature was changed from 150 to 350ºK.The results are shown in Fig. 2.

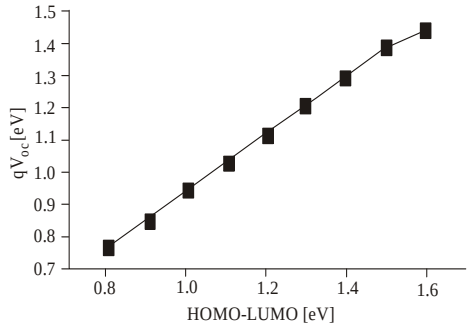


Fig 1: Variatiotheopen circuit voltage with HOMOD - LUMOA offset

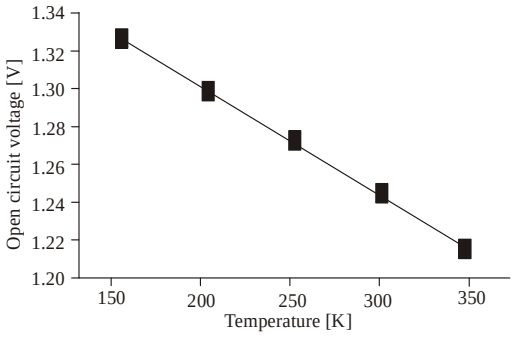


Fig. 2: Variation of the open circuit voltage with temperature

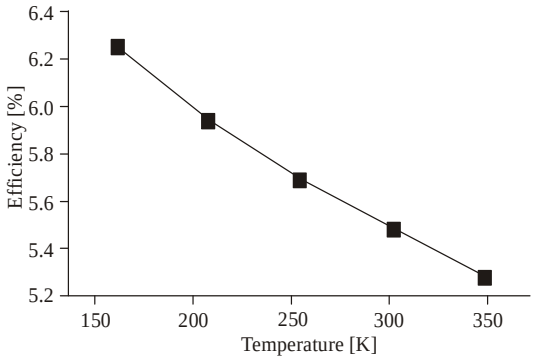


Fig. 3: Variation of the efficiency with temperature

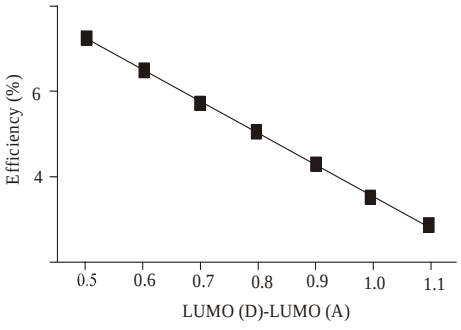


Fig.4: Variation of the efficiency with LUMO (A)-LUMO (D)

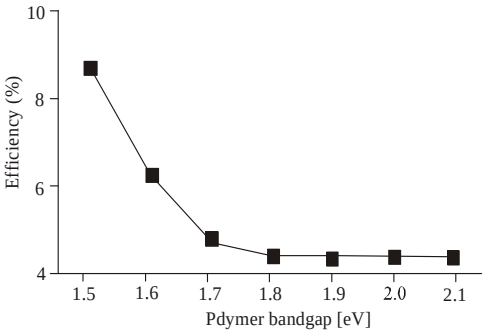


Fig. 5: Variation of the efficiency with polymer band gap

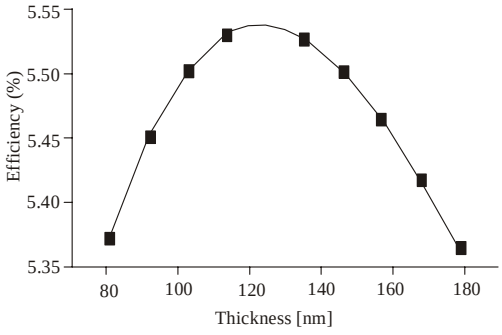


Fig. 6: Vriation of the efficiency with the thickness, MDM0PPVand PCBM solar cell

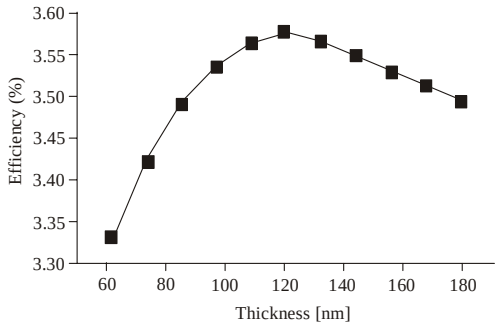
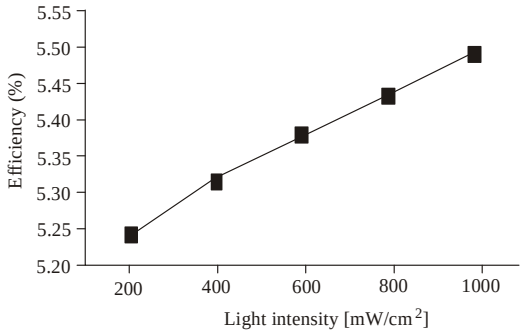


Fig. 7: Variation of the efficiency with the thickness, P3HTand PCBM solar cell



F ig. 8: Variation of the efficiency with light intensity

The open circuit voltage V_{oc} decreases with the temperature by -0.55 mV per degree .The relationship is given by:

$$V_{oc} = (1.4 \pm 0.001) + (-5.5x10^{-4} \pm 6.83x\ 10^{-6})\ T \quad (3)$$

$$dV_{oc}/dT = -5.5x10^{-4}\ V/^{0}K \cong 0.55\ mV/^{o}K \quad (4)$$

It has been reported that the open circuit voltage of an inorganic solar cell decreases with increase in temperature at a rate of 2.3 mV/ºK (Messenger and Ventre, 2004). It appears that the effect of temperature is more significant on inorganic solar cells than in organic solar cells.

The efficiency is calculated as the temperature is changed from 150 to 350ºK. The relation between the efficiency and the temperature can be described by the Eq. (5):

$$\eta = (7.08\pm0.07) + (-0.0050\pm3.0x10^{-4})\ T \quad (5)$$

The results are shown in Fig. 3.

The effect of the $LUMO_D$ - $LUMO_A$ offset on the efficiency: Figure 4 shows the change in the efficiency as the $LUMO_A$- $LUMO_D$ offset is changed. An increase of the offset by 1.0 eV, decreases the efficiency by about 5 %. As the exciton dissociation energy is in the range of 0.3-0.5 eV (Bassler *et al*., 2003; Mihailetchi *et al.*, 2003), the minimum value for the offset has to be about 0.5 eV. This gives a maximum value of 6.5% for the efficiency as shown by Eq. (6):

$$\eta = (8.96\pm0.009) - (4.92\pm0.011)\ (L_D - L_A) \quad (6)$$

$L_{D,}$ L_A is the $LUMO_D$ and $LUMO_A$

Eq. (6) predicts a maximum efficiency of about 9%.

In order to generate an electron-hole pair, the photon energy has to be greater than the band-gap. If the band-gap is decreased, photons of lower energy can be utilized, and hence the current will be increased. Since the open circuit voltage is proportional to the band-gap, the voltage decreases when the band-gap is decreased. The band-gap has to be optimized according to the spectral distribution of solar radiation.

It has been shown that, at air mass one and 300º K temperature, the optimum band-gap is about 1.5 eV (Sze, 1985). The efficiency of a BHJ solar cell with 1.5 eV band-gaps is about 1.5 times that with band-gap of 2.1 eV.

The AMPS-1D program is used to calculate the efficiency when the band gap is 1.5 eV and the $LUMO_D$ - $LUMO_A$ offset is 0.5 eV. The efficiency increased to a value of 8.7%, Fig. 5. The optimum theoretical efficiency reported in the literature is about 8% (Koster *et al*., 2006).

The optimum thickness: The efficiency was calculated as the thickness of the blend was changed from 70 to 170 nm. The results are shown in Fig. 6 and 7. The results show that the optimum efficiency for both MDMO-PPV /PCBM solar cell and P3HT/PCBM solar cell is at 120 nm thickness. The experimental results give an optimum thickness of about 100 nm (Popescu, 2008).

The relationship between the light intensity and the efficiency of the solar cell: The efficiency was calculated as the light intensity was changed from 200 to 1000 W/m^2. The result is shown in Fig. 8. We notice that the efficiency increases with the increase of light intensity and can be described by the relationship:

$$\eta = (5.19\pm0.007)+(3.26x10^{-4} \pm1.17x10^{-5}) \quad (7)$$

where, I is the light intensity in W/m^2. The efficiency increases by about 0.3 % for an increase in the intensity of 1.0 W/m^{-2}.

CONCLUSION

The polymer used in this study consist of a blend of poly (2-methoxy-5-(3,7-dimethloctyloxy)-1,4-phenylene [vinylene] MDMO-PPV, poly(3-hexylthiophene) P3HT as electrons donor and 6,6-phenyl C_{61}-butyric acid methyl ester (PCBM) as the electrons acceptor, sandwiched between Indium Tin Oxide (ITO), and an evaporated aluminum(Al), top electrode.

The dependence of the efficiency on different parameters has been studied. The parameters considered included $HOMO_D$- $LUMO_A$ offset temperature, thickness, and incident light.

The results obtained by the AMPS-1D program are in good agreement with the experimental results.

The results show that the optimum organic cell needs to have a thickness of about 120 nm and a $LUMO_D$-$LUMO_A$ offset of about 0.5 eV, and band-gap of about 1.5 eV. The maximum efficiency which could be achieved is about 9%. The results also show that the open circuit voltage decreases with increase in temperature at a rate of about 0.55 mV per degree.

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