

Origin of the Open Circuit Voltage and Important Processes that Affect its Value in Organic Solar Cells

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Abstract—In this paper, the origin of an open circuit voltage (V_{oc}) in organic solar cells (OSCs) and processes which have a dominant impact on it were examined. The measured light current-voltage (I - V) characteristics of ITO/PEDOT:PSS/P3HT:PCBM/LiF/Al solar cells fabricated and characterized under similar conditions were collected from literature. The gathered V_{oc} data was statistically processed and 75 % of the results belonged to the range 0.52 – 0.64 V and obeyed Gaussian distribution. However, 12.5 % results had a value around 0.4 V, and another 12.5 % around 0.48 V. Three I - V curves with different V_{oc} values belonging to three observed V_{oc} ranges were simulated by the drift-diffusion model (DDM). By changing the photogeneration, transport, recombination, and extraction parameters, but with the same value of a built-in voltage (V_{bi}), which corresponds to a difference between electrodes work functions, the measured I - V curves were excellently reproduced. The experimental light I - V curves from literature of solar cells with different polymer blends used as an active layer (PTB7:PCBM, or MDMO-PPV:PCBM) but having the same electrodes and transport layers were also successfully simulated in the same way. Based on our review of published experimental results and our theoretical investigations, we confirm that the difference between electrode work functions is the source of the V_{oc} . The difference between acceptor's lowest unoccupied molecular orbital (LUMO) and donor's highest occupied molecular orbital (HOMO) affects the V_{oc} indirectly through photogeneration, transport and recombination parameters, and extraction efficiency.

Index Terms—Organic solar cells; open circuit voltage; drift-diffusion model.

INTRODUCTION

Organic solar cells (OSCs) have been getting a great deal of attention due to their potential as low-cost, simply processed and environment-friendly photovoltaic devices [1]. An improvement of OSCs is demonstrated through an increase in their power conversion efficiency (PCE), the most important performance parameter. So far, the PCE has reached value of 18 % for a single-layer OSC, 12 % for organic photovoltaic modules and even 23.6 % for perovskite/organic tandem solar cells [2–4]. Although these results are commendable, a further progress in properties of active layer blends, and an improvement of OSCs' long-term stability are seen as a path to their commercialization [5].

To reach a full potential of OSCs, we need to clarify their basic working principles. Knowledge of OSCs physics would help us to single out the basic prerequisites for an efficient photoconversion and identify loss mechanisms. However,

research so far was not focused much on elucidating physics but rather on increasing OSCs efficiency through new donor and acceptor materials to improve the photoconversion in the active layer, as well as through new transport layer materials to maximize the charge carrier collection [5,6]. The metal-semiconductor-metal (MSM) drift-diffusion model (DDM) [7] has been widely used for modeling the OSCs. This model is successful to a certain extent, but it is not able to reproduce the experimentally observed OSCs behavior to a full extent. Thus, a refinement of the DDM for OSCs has yet to be done by clarifying vague parts of it.

One of the parameters with unclear origin that directly affects the OSC's PCE is an open-circuit voltage (V_{oc}). There are many presumptions about processes that influence the V_{oc} and how they can be correlated [1]. Frequently, the V_{oc} is defined as $e \cdot V_{oc} = (E_g - 0.3) \text{ eV}$, where E_g is an active layer energy gap determined as a difference between the highest occupied molecular orbital level (HOMO) of the donor and the lowest molecular orbital level (LUMO) of the acceptor, and e is the elementary charge [8]. Trying to resolve 0.3 V voltage loss in the V_{oc} and other aspects of the V_{oc} behavior, many factors have been found that directly or indirectly have impact on it [1]. These include temperature, light intensity, active layer morphology, microstructure, recombination processes, quality and properties of donor/acceptor (D/A) interface area, density of states (DOS), electrode work functions, existence of charge transfer (CT) states, carrier density, reverse saturation current, defect states, and crystallinity [1]. All these factors are interrelated, and for a complete analysis of the V_{oc} all of them should be considered. The V_{oc} dependence on temperature and light intensity are most often researched and analyzed in the literature [9, 10]. It was found that the V_{oc} decreases as temperature increases, and for a wide temperature range that dependence is nearly linear [9]. On the other hand, the V_{oc} showed a logarithmic dependence on light intensity [10]. The reverse saturation current is one of the important parameters that influences the V_{oc} , and it was found that the V_{oc} is inversely proportional to it [11]. The influence of the charge carrier recombination on the V_{oc} was described through a correlation between the V_{oc} and the recombination rate [12] that differs for different recombination types – monomolecular, bimolecular or their combination. The monomolecular recombination implies a recombination through a recombination center or a trap state, while the bimolecular recombination indicates that holes and

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electrons are mutually recombined [12]. Higher recombination rates mean a reduced number of carriers and eventually a smaller V_{oc} [12]. A lower carrier density leads to a decreased V_{oc} . The improvement of the microstructure can minimize recombination rates, improve carrier dynamics, and benefit the V_{oc} [13]. Defect states introduce irregularities into the material structure, and thus energy disorders and a reduced crystallinity. In organic materials, these disorders are usually modelled via the Gaussian or exponential DOS, and it was shown that they degrade the performance of OSCs by degrading the V_{oc} [14]. Losses in the V_{oc} are also related to a non-radiative decay of the CT states on the D/A interface [15]. The impact of the morphology is mostly related to the quality of D/A interface (e.g., whether it is homogenous or not) [15]. In addition, it was shown that a reduction of the D/A interface area can contribute to a higher V_{oc} [16]. One of the most debatable matters is the influence of electrode work functions on the V_{oc} . It was shown that if the Fermi levels are well inside the energy gap of the active layer polymer-fullerene blend, the V_{oc} is strongly affected even by a small variation of each electrode work function [17]. However, if the anode work function is close to the donor's HOMO and the cathode work function is close to the acceptor's LUMO, the V_{oc} value reaches a plateau and is less sensitive to work functions variations [17]. In this case, the device operation is the most effective [17].

To investigate the origin of the V_{oc} and analyze important processes which affect its value, we have collected measured light current-voltage (I - V) characteristics of ITO(indium tin oxide)/PEDOT(poly(3,4-ethylene dioxythiophene):PSS(poly(styrenesulfonate)/P3HT (poly(3-hexyl-2,5-dimethylthiophene):PCBM([6,6]-phenyl-C₆₁-butyric acid methyl ester)/LiF(lithium fluoride)/Al solar cells fabricated and characterized under nearly same conditions available in the literature [19-40]. We statistically processed the collected V_{oc} data and analyzed the obtained distribution function by determining its mean value and standard deviation. Three I - V curves (each with a representative and significantly different value of V_{oc}) were selected and simulated by the DDM. Viewing the OSC as an MSM structure, the built-in voltage (V_{bi}) was taken to be the difference between the two electrode work functions. The I - V characteristics with different V_{oc} values were successfully simulated by varying the reduction factor of the Langevin bimolecular recombination rate and by changing the effective density of states (N_c, N_v) at boundaries.

To inspect the influence of E_g on V_{oc} , two more solar cells with the same electrode contacts but different active layer polymer-fullerene blends, PTB7 (poly [[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b'] dithiophene-2,6-diyl][3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-b] thiophenediyl]]):PCBM [41] and IMDMO-PPV (poly[2-methoxy-5-(30,70-dimethyloctyloxy)-1,4-phenylenevinylene]):PCBM [42] were considered. Their measured I - V characteristics obtained from literature were successfully fitted with the DDM by varying active layer transport and recombination parameters together with the N_c , and N_v at the boundaries. Based on the statistically processed experimental V_{oc} data and our DDM I - V curve simulations, we confirm that the V_{oc} originates from the difference of

electrode work functions and that the contact phenomena and the recombination losses have the greatest impact on its value.

OPEN CIRCUIT VOLTAGE IN ITO/PEDOT:PSS/POLYMER-FULLERENE BLEND/LiF/Al ORGANIC SOLAR CELLS

A. Review of Experimental Data

We started the investigation of the V_{oc} in OSCs by choosing one of the most researched device structure ITO/PEDOT:PSS/P3HT:PCBM/LiF/Al. This OSC structure is used as a reference in a large number of experimental research papers aimed at improving the OSC performance. The performance parameters for considered OSCs together with fabrication and characterization conditions are presented in Table 1. The gathered V_{oc} data are statistically processed and graphically presented in Fig. 1. The three distinct V_{oc} ranges are observed (see Fig. 1). The dominant range contains 75 % of collected data. Two smaller ranges each contain 12.5 % of the V_{oc} results. The largest number of collected V_{oc} values belongs to the 0.52–0.64 V range and the data follows the standard Gaussian distribution with the expected value $\mu = 0.58$ V and the standard deviation $\sigma = 0.024$ V. The V_{oc} values in the range of 0.46–0.48 V are mostly obtained for the devices illuminated by 3 sun (see Table 1), where 1 sun corresponds to standard illumination at AM1.5, or 1 kW/m². The V_{oc} of about 0.40 V is obtained mainly for the OSCs in which P3HT:PCBM active layer is produced from chloroform solution rather than from chlorobenzene solution (see Table 1).

According to the literature [17, 18], if injection barriers at electrode contacts are significant (i.e., rectifying junctions), the V_{oc} is defined as the difference between electrode work functions, while for optimised devices with Ohmic contacts, the V_{oc} is interpreted as the difference between the LUMO of the acceptor and the HOMO of the donor (i.e., with a mysterious loss of 0.3 V). From Fig. 1, it is clear that even for the OSCs with the same electrodes and the same D/A polymer-fullerene blend, a wide distribution of the V_{oc} values exists. This led us to the conclusion that the active layer photogeneration, transport and recombination parameters, as well as the charge extraction efficiency differ in the considered devices probably due to a different quality of the active layer, hole and electron transport layers and electrode junctions.

Additionally, the OSCs with PTB7:PCBM or MDMO-PPV:PCBM active layers with the same electrodes (ITO, Al) and transport layers (PEDOT:PSS, LiF) were examined. Although $E_g^{MDMO-PPV:PCBM} < E_g^{P3HT:PCBM}$ [35] and $E_g^{PTB7:PCBM} > E_g^{P3HT:PCBM}$ [43], the V_{oc} values obtained for these devices ($V_{oc}^{MDMO-PPV:PCBM} = 0.82$ V, and $V_{oc}^{PTB7:PCBM} = 0.75$ V) are larger than any $V_{oc}^{P3HT:PCBM}$ from Table 1. Thus, we proposed that the difference between the acceptor LUMO and the donor HOMO is not crucial for the V_{oc} , but rather the parameters of photogeneration, transport, recombination, and extraction.

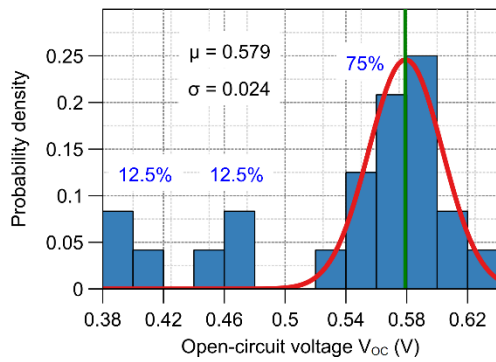


Fig. 1 Probability density obtained by statistical processing of the experimental V_{oc} data from Table 1. Gaussian function is applied to the V_{oc} data in the range 0.52 – 0.64 V (red solid curve).

TABLE I

REVIEW OF PERFORMANCE, FABRICATION AND TESTING PARAMETERS OF ITO/PEDOT:PSS/P3HT:PCBM/LiF/Al SOLAR CELLS REPORTED IN THE LITERATURE

	V_{oc} [V]	J_{sc} [$\frac{mA}{cm^2}$]	PCE [%]	Light intensity	Anneal.	Blend ratio	Solvent	Ref.
1.	0.40	9.50	1.55	1 sun	5 min at 120°C	1:1	Chloroform	[19]
2.	0.59	11.00	4.07	1 sun	10 min at 150°C	1:1	Chloroform	[20]
3.	0.40	0.70	/	1 sun	15 min at 120°C	1:1	Chlorobenzene	[21]
4.	0.59	9.70	2.64	1 sun	10 min at 120°C	1:1	Chlorobenzene	[22]
5.	0.56	8.92	3.31	1 sun	10 min at 140°C	3:2	1,2-Dichlorobenzene	[23]
6.	0.48	17.06	2.11	3 sun	5 min at 115°C	1:1	Chlorobenzene	[24]
7.	0.42	17.06	2.11	3 sun	5 min at 115°C	1:0.8	Chloroform	[25]
8.	0.57	3.64	0.62	1 sun	No anneal.	1:1	Chlorobenzene	[26]
9.	0.55	7.75	2.42	1 sun	10 min at 110°C	1:1	Chlorobenzene	
10.	0.62	13.72	2.76	1 sun	20 min at 100°C	5:3	Chlorobenzene: Chloroform (1:1)	[26]
11.	0.59	10.08	3.20	1 sun	10 min at 120°C	1:1	Dichlorobenzene	[27]
12.	0.59	14.27	2.61	1 sun	/	1:1	Chlorobenzene	[28]
13.	0.60	5.36	2.10	1 sun	15 min at 130°C	1:1	Chlorobenzene	[29]
14.	0.55	5.58	1.55	1 sun	10 min at 120°C	1:0.8	Chlorobenzene	[30]
15.	0.54	3.83	1.18	1 sun	12 min at 100°C	1:1	1,2-Dichlorobenzene	[31]
16.	0.58	4.79	1.10	/	at 120°C	1:0.8	/	[32]
17.	0.58	8.06	2.20	1 sun	10 min at 150°C	1:1	Dichlorobenzene	[33]
18.	0.58	/	/	/	15 min at 150°C	1:0.75	Ortho-dichlorobenzene	[34]
19.	0.46	6.10	1.02	1 sun	No anneal.	1:1	Chlorobenzene	[35]
20.	0.58	5.84	/	1 sun	15 min at 140°C	1:1	Chlorobenzene	[36]
21.	0.64	8.50	2.80	1 sun	30 min at 150°C	1:0.8	Chlorobenzene	[37]
22.	0.62	9.54	2.40	1 sun	10 min at 120°C	1:1	O-chlorobenzene	[38]
23.	0.48	17.06	2.11	3 sun	10 min at 120°C	1:1	Chlorobenzene	[39]
24.	0.60	9.23	1.79	1 sun	20 min at 130°C	1:1	Chlorobenzene	[40]

B. Drift-Diffusion Modeling

It has been shown that photoconductive polymer-fullerene blend placed between identical electrodes fabricated under the same environment, does not exhibit a rectifying effect and

their V_{oc} is zero [44–46]. This means that the D/A interface in polymer-fullerene blends does not contribute to the built-in voltage. Accordingly, the direct source of the V_{oc} in OSCs is the difference between the electrode work functions. The difference between the acceptor's LUMO and the donor's HOMO level influences the V_{oc} indirectly through the Fermi-level pinning [47], photogeneration, transport and recombination parameters, or extraction efficiency. In this paper, the metal-semiconductor-metal DDM was used for modeling the I - V characteristics of several OSCs. The model is based on the Poisson's equation, the hole and electron continuity equations, and the drift-diffusion transport equation for holes and electrons inside the active layer [48]. The photogeneration rate was calculated by using the transfer matrix theory and by assuming that the electric field is independent of the exciton dissociation efficiency [48]. Constant hole and electron mobilities were applied, and a reduced Langevin recombination was proposed. The Dirichlet boundary conditions were used. The solving of the equations system was done based on the finite difference discretization improved by the Scharfetter and Gummel approach and the Newton algorithm [48]. In all our calculations, a built-in voltage V_{bi} of 0.9 V as the difference between the electrode work functions was used along with the dielectric permittivity of 3.4 and the room temperature of 293.9 K.

The light I - V characteristic of three ITO/PEDOT:PSS/P3HT:PCBM/LiF/Al devices with $V_{oc} = 0.40$ V [21], $V_{oc} = 0.48$ V [24], and $V_{oc} = 0.59$ V [27] were simulated and compared with the measured ones in Fig. 2 (a), (b), and (c), respectively. The parameter values used in simulations are listed in the Insets of Fig. 2, where $\mu_{n(p)}$ is the electron (hole) mobility, $N_{c(v)}$ is the effective density of states for electrons (holes), d is the active layer thickness, g is the photoconductive gain [49], and ξ is the reduction factor of the Langevin recombination rate [50]. All three measured I - V curves are reproduced very well by the DDM, which means that the difference in the photogeneration (g), transport (μ_n, μ_p), recombination (ξ) and extraction (N_c, N_v) parameter values may explain the observed V_{oc} diversity (see Table 1, Fig. 1). The occurrence of the photoconductive gain may be explained through a volume modulation effect, where the light illumination can increase the conductive area of the cell, thus, the generated photocurrent becomes larger [51]. The N_c and N_v are used as the boundary majority charge carrier concentrations at cathode and anode, respectively, and they are the fitting parameters in the OSCs modeling of Koster et al. [7].

These parameters are representatives of contact physics in OSCs and they have a large impact on the V_{oc} . The reduction of recombination losses in OSCs quantified by ξ leads to an improvement of the V_{oc} . In most OSCs, $\xi \leq 0.2$ [52], and its higher value indicates that CT states are significant in polymer-fullerene blend and that they recombine very rapidly. The existence of CT states and their participation in the charge carrier photogeneration and recombination [7] was not considered in our DDM. Therefore, $\xi > 1$ is possible in our simulations. A higher electron mobility leads to a lower V_{oc} [53], and an increased hole mobility slightly improves the V_{oc} .

Ref. [39]. The corresponding simulation parameters are given in the Inset.

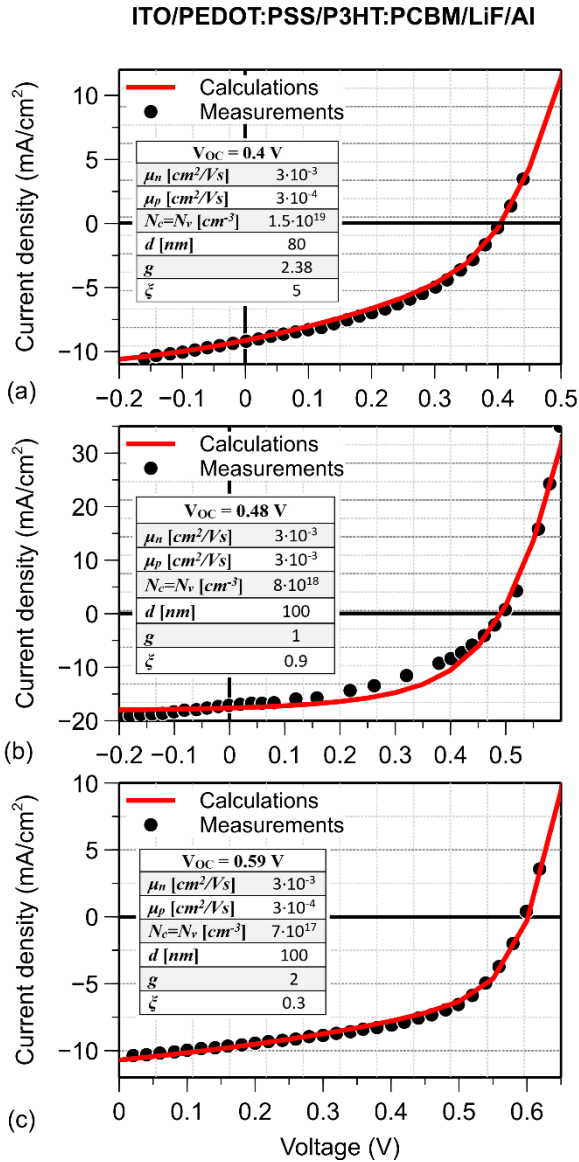


Fig 2. DDM simulated I - V curves compared to experimental ones taken from (a) Ref. [17], (b) Ref. [33], (c) Ref. [25]. The corresponding simulation parameters are given in the Insets.

In Figs. 3, and 4, calculated light I - V characteristics for the PTB7:PCBM and MDMO-PPV:PCBM based solar cells are compared with the measured ones. The simulation parameters are given in the Insets of Figs. 3, and 4.

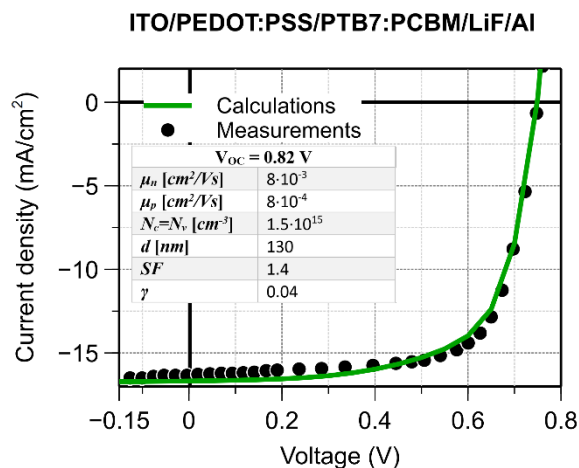


Fig. 3 DDM simulated I - V curve compared to experimental one taken from

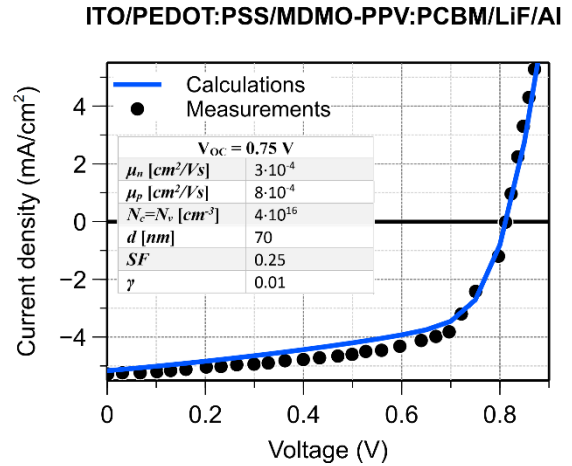


Fig.4 DDM simulated I - V curve compared to experimental one taken from Ref. [33]. The corresponding simulation parameters are given in the Inset.

Again, the experimentally obtained and theoretically predicted I - V curves coincide very well. This proves that even if a D/A polymer blend in an OSC is changed, the V_{oc} can be reproduced by tuning of parameters g , μ_n , μ_p , N_c , N_v , and ξ .

CONCLUSION

The experimental light I - V data extracted from literature showed that the V_{oc} can significantly differ for ITO/PEDOT:PSS/P3HT:PCBM/LiF/Al solar cells produced and tested under similar conditions. Three measured light I - V characteristics with $V_{oc} = 0.4$ V, $V_{oc} = 0.48$ V, and $V_{oc} = 0.59$ V were successfully reproduced by our DDM simulations by applying the same value of $V_{bi} = 0.9$ V corresponding to the difference between the LiF/Al and the ITO/PEDOT:PSS work functions, while the charge carrier photogeneration, transport, recombination, and extraction were varied. For the OSCs based on the PTB7:PCBM or MDMO-PPV:PCBM polymer-fullerene blends, our DDM simulations were, again, able to reproduce the measured I - V curves well. We concluded that the difference between the work functions of the electrodes is the source of the V_{oc} in OSCs and the difference between the acceptor's LUMO and the donor's HOMO influences the V_{oc} through charge carrier photogeneration, recombination, transport, and extraction. These processes have a significant impact on the V_{oc} value. Future work will be dedicated to research of how the LUMO and HOMO energy levels of the polymer-fullerene D/A blend as well as the CT states formed at the D/A interfaces influence the V_{oc} .

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