Comparison between the use of uniform and non-uniform light absorption profiles in modelling organic photovoltaics

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Comparison between the use of uniform and non-uniform light absorption profiles in modelling organic photovoltaics

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Abstract. To avoid complexity, a uniform light absorption profile is usually used when modelling organic photovoltaic cells (OPVs). However, the actual light absorption profile is not uniform. It is found that a uniform light absorption profile can be used as a replacement for the actual non-uniform light absorption profile in modelling an OPV provided that the actual light absorption profile inside the OPV has a peak absorption value that is roughly less than twice its average absorption value. Nevertheless, the use of a uniform light absorption profile in investigating the effect of a certain parameter (e.g. the active layer thickness) on the performance of OPVs should still be used with care if variations in the value of the said parameter lead to different light absorption profiles.

1. Introduction

Organic photovoltaic cells (OPVs) have unique advantages compared with traditional photovoltaic cells such as high mechanical flexibility, low production cost, ease of mechanical integration on various shapes, high transparency, and lightweight [1]. Therefore, OPVs could be an attractive power source for existing applications. This is partly due to the prospect of a high ratio of the power output to the production cost. OPVs are also being explored as power sources for new applications, for example, for powering next-generation self-driven biomedical devices [2] and off-grid devices for Internet of Things [3].

Light absorption inside the active layer of OPVs is not uniform [4–8]. However, it is convenient to use a uniform light absorption profile when calculating the current-voltage (J-V) characteristics since this assumption greatly simplifies the calculations by eliminating the need to use the optical transfer matrix method to determine the actual light absorption profile. Therefore, many previous studies simply used uniform light absorption profiles [9,10] or approximately uniform light absorption profiles [11,12] in calculating the J-V characteristics.

To attain better performing OPVs, it is important to be able to make accurate predictions on the device performance. In this study, we will investigate how the use of a uniform light absorption profile differs from the use of a non-uniform light absorption profile in predicting the J-V characteristics of OPVs. It is hoped that this study can clarify whether a uniform light absorption profile can be used as a replacement for the actual non-uniform light absorption profile in modelling OPVs.

2. Method

To calculate the current-voltage characteristics, the analytical model for bulk heterojunction OPVs developed by Ref. [11] is used. Light absorption by the active layer generates excitons (strongly bound electron-hole pairs). When the excitons reach the donor-acceptor interface, they may be converted into charge-transfer (CT) states. Due to the bulk heterojunction design of OPVs, CT states are generated at approximately the same location where the excitons are generated. Hence, the shape of the light absorption profile can be assumed to be the same as the shape of the profile of the CT states generated due to the light absorption. The CT state photogeneration rate per unit volume in the model by Ref. [11] is given by

$$G_{\mathrm{CT}} = G_0 \exp(-\alpha x)\,, \tag{1}$$

where G_0 and α are the CT state photogeneration properties and x is the position inside the active layer. The CT state photogeneration rate per unit area of the active layer is therefore given by

$$G_{\mathrm{CT,area}} = \int_0^L G_{\mathrm{CT}}\,dx = \frac{G_0[1-\exp(-\alpha L)]}{\alpha}\,, \tag{2}$$

where L is the active layer thickness. In the model by Ref. [11], the interface between the anode and the active layer is located at $x = 0$ whereas the interface between the cathode and the active layer is located at $x = L$ (see Figure 1).

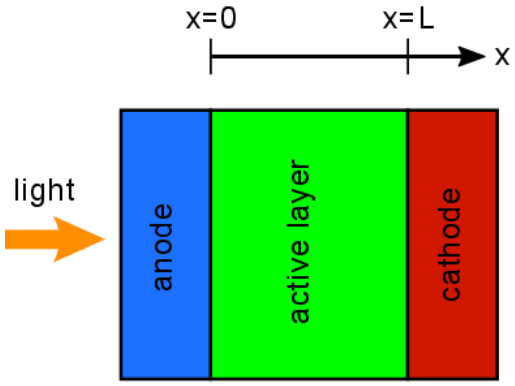

Figure 1. A simple illustration of the device structure.

To minimize the device degradation, anode is typically made as the top electrode (meaning that light enters the active layer from the anode as shown in Figure 1). According to the Beer-Lambert law, light absorption in a material decreases exponentially from the entrance point. In this work, we will compare and clarify how the use of a uniform light absorption profile differs from the use of a non-uniform light absorption profile that decreases exponentially from the anode to cathode in modelling OPVs. Although the actual light absorption profile in the active layer may not be exponentially decreasing from the anode to cathode (i.e. may have other non-uniform profiles due to the reflection and interference effects [4–8]), this study can still give an idea on how a uniform light absorption profile could differ from the actual light absorption profile (which is non-uniform) in modelling OPVs.

To simulate a uniform light absorption profile, which automatically means a uniform G_{CT} profile, equation (1) must have a very low value of α (note that $\alpha = 0$ cannot be used as explained in Ref. [11]). Here we use $\alpha = 1$ m^{-1}, which is low enough to make the profile virtually constant across the active layer. To produce a light absorption profile that decreases exponentially from anode to cathode, a sufficiently large value of positive α needs to be used [11].

To make an appropriate comparison, it is important that each of the studied profile is examined using an OPV with same properties and dimensions. Furthermore, we must ensure that the total light absorption rate (and hence the total CT state photogeneration rate too) produced by each of the studied

profile is the same. Hence, the average CT state photogeneration rate per unit volume $G_{\mathrm{CT,ave}}$ produced by each of the studied profile must also be the same for a fair comparison. The average CT state photogeneration rate per unit volume is

$$G_{\mathrm{CT,ave}} = \frac{G_{\mathrm{CT,area}}}{L}. \tag{3}$$

Since L is fixed for a fair comparison, the value of $G_{\mathrm{CT,area}}$ for each of the studied profile must also be the same. Therefore, from equation (2), the value of G_0 that should be used in each calculation is given by

$$G_0 = \frac{\alpha G_{\mathrm{CT,area}}}{1-\exp(-\alpha L)}. \tag{4}$$

where the values of $G_{\mathrm{CT,area}}$ and L in equation (4) above are fixed. Table 1 shows the values of the parameters used in this study. The values are typical for OPVs as used in previous studies [10–12]. Figure 2 illustrates the profiles of the CT state photogeneration rate per unit volume G_{CT} that are being compared in this study. As can be seen in Figure 2, the peak G_{CT} for the profile with $\alpha = 2\times10^{7}\ \mathrm{m^{-1}}$ is roughly twice its $G_{\mathrm{CT,ave}}$ whereas the peak G_{CT} for the profile with $\alpha = 5\times10^{7}\ \mathrm{m^{-1}}$ is about five times its $G_{\mathrm{CT,ave}}$. Note that $G_{\mathrm{CT,ave}}$ for all three profiles shown in Figure 2 is the same which is $1\times10^{28}\ \mathrm{m^{-3}s^{-1}}$.

Table 1. Parameter values used in the calculations unless otherwise specified. The symbols used here are the same as the ones used in Ref. [11] unless otherwise specified.

Parameter (Symbol)	Value
Effective band gap (E_{g})	1.1 eV
Density of states (N_{c}, N_{v})	$2\times10^{26}\ \mathrm{m^{-3}}$
Electron mobility (μ_{n})	$2\times10^{-7}\ \mathrm{m^2V^{-1}s^{-1}}$
Hole mobility (μ_{p})	$3\times10^{-8}\ \mathrm{m^2V^{-1}s^{-1}}$
Actual electron mobility (μ_{na})	$4\times10^{-5}\ \mathrm{m^2V^{-1}s^{-1}}$
Actual hole mobility (μ_{pa})	$6\times10^{-6}\ \mathrm{m^2V^{-1}s^{-1}}$
Effective permittivity of the active layer (ε)	$3\times10^{-11}\ \mathrm{F\cdot m^{-1}}$
Injection barriers (φ_{pa}, φ_{nc})	0.05 eV
CT state decay rate coefficient (k_{f})	$1\times10^{8}\ \mathrm{s^{-1}}$
Electron-hole separation of the CT state (a)	1.8×10^{-9} m
Temperature (T)	300 K
Donor-acceptor morphology parameter (λ)	0.15
CT state photogeneration rate per unit area ($G_{\mathrm{CT,area}}$)	$1\times10^{21}\ \mathrm{m^{-2}s^{-1}}$
Active layer thickness (L)	100 nm
Bimolecular recombination reduction coefficient (γ)	0.001
Monomolecular recombination coefficient for electrons (k_{mn})	$100\ \mathrm{s^{-1}}$

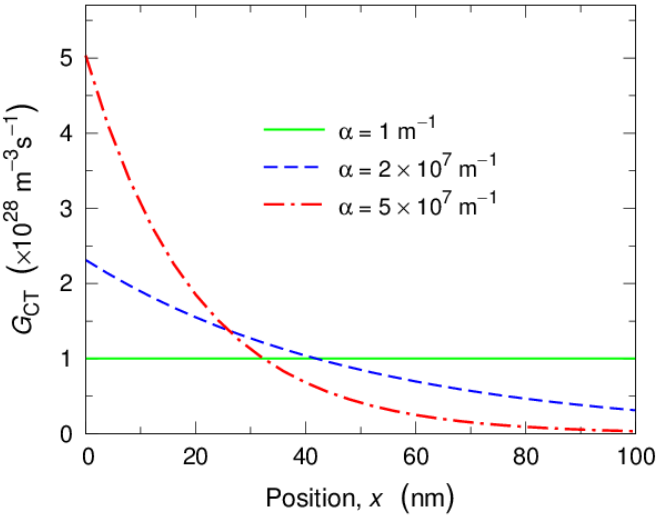

Figure 2. Profiles of the CT state photogeneration rate per unit volume G_{CT} that are used in this study [see equation (1)]. The values of G_0 used to obtain the profiles are as given by equation (4). Note that the light absorption profile is assumed to have the same equivalent shape as the G_{CT} profile.

3. Results and discussions

Figure 3 shows the current-voltage (J-V) characteristics calculated using the studied G_{CT} profiles. It can be deduced from Figure 3 that as the light absorption (or the CT state photogeneration) becomes more concentrated at the anode (or becomes more non-uniform), the J-V characteristic calculated using the non-uniform profile will deviate further from the J-V characteristic calculated using the equivalent uniform profile. Basically, the J-V characteristic produced by the uniform profile overestimates the J-V characteristic produced by the non-uniform profile.

To reduce the above-mentioned overestimation, one could use a lower $G_{CT,area}$ (or a lower $G_{CT,ave}$) when using a uniform profile as compared with the $G_{CT,area}$ of the non-uniform profile. However, the use of a lower $G_{CT,area}$ would underestimate the short-circuit current but overestimate the fill factor. For example, as shown in Figure 3, the uniform profile ($\alpha = 1$ m^{-1}) with $G_{CT,area} = 0.9\times10^{21}$ m^{-2}s^{-1} gives a short-circuit current density of -128.66 Am^{-2} and a fill factor of 0.7362, whereas the non-uniform profile with $\alpha = 5\times10^{7}$ m^{-1} and $G_{CT,area} = 1\times10^{21}$ m^{-2}s^{-1} gives a short-circuit current density of -133.26 Am^{-2} and a fill factor of 0.6804. Table 2 summarizes the J-V characteristics shown in Figure 3.

It is important to note that the solid line in Figure 3 ($\alpha = 1$m^{-1} with $G_{CT,area} = 1\times10^{21}$ m^{-2}s^{-1}) has approximately the same shape as the dashed line in Figure 3 ($\alpha = 2\times10^{7}$ m^{-1} with $G_{CT,area} = 1\times10^{21}$ m^{-2}s^{-1}). In other words, if we use a lower value of $G_{CT,area}$ for the solid line as compared with the value of $G_{CT,area}$ for the dashed line, we could easily make the solid line to be approximately the same as the dashed line. Therefore, if the level of non-uniformity of a non-uniform G_{CT} profile is not high (such that the peak value for the non-uniform profile is roughly less than twice its average value), then a uniform G_{CT} profile can be used as a replacement for the non-uniform G_{CT} profile provided that the value of $G_{CT,area}$ for the uniform profile is adjusted accordingly (slightly lowered) compared with the

value of $G_{CT,area}$ for the non-uniform profile. From the results here, it also means that the use of a uniform G_{CT} profile when investigating the effect of a certain parameter on the performance of OPVs has to be used with care if different G_{CT} profiles are produced when the value of that parameter is varied. For example, as we vary the active layer thickness, different light absorption profiles (and thus G_{CT} profiles) are produced [7]. For a certain active layer thickness, the light absorption profile can be approximately uniform, but for another active layer thickness the light absorption profile can be highly non-uniform. Therefore, to compare the effect of different active thicknesses on the performance of OPVs by using a uniform light absorption profile for all active layer thicknesses could lead to somewhat unfair comparison and inaccurate conclusion.

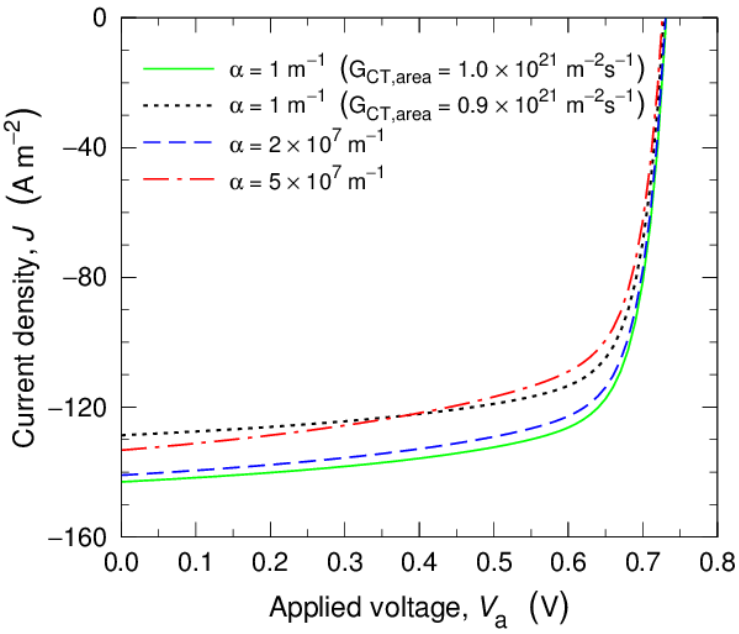

Figure 3. Current-voltage (J-V) characteristics calculated using different G_{CT} profiles. All J-V characteristics are calculated using $G_{CT,area} = 1\times10^{21}$ $m^{-2}s^{-1}$ except the J-V characteristic denoted by the dotted line, which is calculated using $G_{CT,area} = 0.9\times10^{21}$ $m^{-2}s^{-1}$. The values of other parameters are as given in Table 1.

Table 2. Short-circuit current density J_{sc}, open-circuit voltage V_{oc}, and fill factor (FF) for each J-V characteristic shown in Figure 3.

$G_{CT,area}$ ($m^{-2}s^{-1}$)	α (m^{-1})	J_{sc} (Am^{-2})	V_{oc} (V)	FF
1×10^{21}	1	−143.02	0.7313	0.7360
0.9×10^{21}	1	−128.66	0.7284	0.7362
1×10^{21}	2×10^{7}	−140.97	0.7305	0.7259
1×10^{21}	5×10^{7}	−133.26	0.7265	0.6804

4. Conclusion

A comparison between the use of uniform and non-uniform light absorption profiles in modelling OPVs has been made. It is found that by making a simple adjustment to the value of $G_{\mathrm{CT,area}}$, a uniform G_{CT} (or light absorption) profile can produce a J-V characteristic that is approximately the same as the J-V characteristic produced by a non-uniform G_{CT} profile provided that the non-uniform profile has a peak value that is roughly less than twice its average value. Therefore, this study suggests that a uniform light absorption profile can be used in modelling an OPV provided that the actual light absorption profile inside the OPV has a peak absorption that is roughly less than twice its average absorption. However, the use a uniform light absorption profile when investigating the effect of a certain parameter on the performance of OPVs must still be used with care if variations in the value of the said parameter lead to different light absorption profiles.

Acknowledgments

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