INFLUENCE OF ACTIVE LAYER THICKNESS ON THE PERFORMANCE OF ORGANIC PHOTOVOLTAICS WITH LIGHT TRAPPING

BY

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ABSTRACT

To maximize the performance of an organic photovoltaic device, the use of light trapping is necessary. In this thesis, the effect of active layer thickness on the performance of organic photovoltaic (OPV) cells with ideal light trapping is investigated. Although actual light trapping schemes are not ideal, this study can still be a useful guide to maximize the performance of actual OPVs with light trapping. In this study, the effect of active layer thickness on the power conversion efficiency (PCE), short-circuit current, open-circuit voltage and fill factor (FF) of OPVs with ideal light trapping is described. The analytical model for bulk heterojunction OPVs developed by Inche Ibrahim (2018) is used to calculate the current-voltage characteristics in order to determine the PCE, short-circuit current, open-circuit voltage and FF of OPVs with ideal light trapping. For a low-recombination-loss OPV with ideal light trapping, the active layer thickness weakly affects the PCE. For a high-recombination-loss OPV with ideal light trapping, the active layer thickness strongly affects the PCE. To maximize the PCE of high-recombination-loss OPV with light trapping, the active layer thickness must be very thin enough (around 10nm). This study proves that it is important for OPVs to have a low recombination loss so that the active layer thickness does not become a hindrance or an additional factor in creating highly efficient light trapping schemes that can maximize the PCE. This study also shows that it is equally (if not more) important to develop light trapping schemes that are highly efficient at very thin active layers (around 10nm) so that the PCE of any OPVs can be more or less maximized, whether the OPVs have low or high recombination losses. Finally, the use of uniform light absorption profile and non-uniform light absorption profile in modelling OPVs is being compared in this study. 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 that is roughly less than twice its average absorption. Nevertheless, the use of a uniform light absorption profile in investigating the effect of a certain parameter on the performance of OPVs should always be used with care if variations in the value of the said parameter lead to different light absorption profiles, for example when the effect of active layer thickness is investigated by varying its value.

خلاصة البحث

للحصول على اقصى اداء للجهاز العامل بالخلايا الضوئية العضوية فانه من الضروري استخدام طريقة حصر الضوء. في هذا البحث تم التحقق من تاثير سمك الطبقة الفعالة على اداء خلايا الجهازالعامل بالخلايا الضوئية العضوية مع افضل عملية حصر للضوء . وعلى الرغم من ان المخطط الحقيقي لحصر الضوء ليس الامثل, فان هذه الدراسة تبقى دليلا مفيدا لزيادة اداء الجهازالعامل بالخلايا الضوئية العضوية الى الحد الاقصى باستخدام حصر الضوء . في هذه الدراسة تم توصيف تاثير سمك الطبقة على كفاءة تحويل الطاقة ، وتوصيف تيار الدائرة القصيرة,وتوصيف فولتية الدائرة المفتوحة وعامل الملئ للجهاز العامل بالخلايا الضوئية العضوية مع عملية حصر ضوء مثالية. ان النموذج التحليلي لحجم التقاطع غير المتجانس للاجهزة العاملة بالخلايا الضوئية العضوية قد تم تطويرها من قبل انتشي ابراهيم (2018) والذي تم استخدامه لحساب خصائص فولتية التيار وذلك لغرض حساب كفاءة تحويل الطاقة وتيار الدائرة القصرة وفولتية الدائرة المفتوحة وعامل الملئ للجهاز العامل بالخلايا الضوئية العضوية مع حصر ضوء مثالية. لقد لوحظ بان تاثير سمك الطبقة الفعالة ضعيف على كفاءة تحويل الطاقة باستخدام تركيب الفقدان المنخفض للجهاز الضوئي العضوي. وعند استخدام تركيب الفقدان العالي للجهاز الضوئي العضوي باستخدام حصر الضوء المثالي وجد بان سمك الطبقة الفعالة يجب ان تكون صغيرة جدا (10 نانوميتر). ان هذه الدراسة اثبتت بانه من الاهمية بمكان للجهازالعامل بالخلايا الضوئية العضوية, فان الجهاز يجب ان يكون بخاصية تركيب الفقدان المنخض لكي لايصبح سمك الطيقة الفعالة عائقا او عاملا اضافيا لخلق مخطط حصر ضوء عالي الكفاءة والذي يؤدي الى زيادة كفاءة تحويل الطاقة الى حده الاقصى. لقد تبين ايضا و بنفس الدرجة او اكثر اهمية تطوير مخطط حصر الضوء والذي يكون فعالا جدا مع سمك طبقة صغيرة جدا (حوالي 10 نانوميتر) بحيث ان كفاءة تحويل الطاقة لاي جهازيعمل بخلايا ضوئية عضوية يمكن رفعه الى اقصى او او اقل من ذلك, بغض النظر فيما اذا كان الجهازالعامل بالخلايا الضوئية العضوية يستخدم تركيب الفقدان الادنى او تركيب الفقدان الاعلى. اخيرا تم مقارنة استخدام ملف امتصاص الضوء المنتظم وامتصاص الضوء غير المنتظم في نمذجة خلايا الجهازالعامل بالخلايا الضوئية العضوية في هذه الدراسة. ولتجنب التعقيد, فان ملف الامتصاص الضوئي يستخدم عادة عند نمذجة اجهزة عاملة بالخلايا الضوئية العضوية.ولكن , ملف امتصاص الضوء الحقيقي هو غير منتظم. لقد وجد بانه يمكن استخدام ملف امتصاص الضوء المنتظم كبديل لملف امتصاص الضوء غير المنتظم عند نمذجة الاجهزة العاملة بالخلايا الضوئية العضوية بشرط ان يكون ملف امتصاص الضوء الحقيقي داخل الجهاز العامل بالخلايا الضوئية العضوية له قمة امتصاص والتي

هي بشكل تقريبي اقل من ضعف معدل الامتصاص. ومع ذلك, فان استخدام ملف امتصاص الضوء المنتظم يجب ان يكون بعناية عند التحقق من تاثير معلمة معينة على اداء الجهاز العامل بالخلايا الضوئية العضوية اذا كانت الاختلافات في قيمة المعلمة تؤدي الى ملف امتصاص ضوء مختف , على سبيل المثال عند التحقق من فعالية طبقة السمك الفعال بتغيير قيمتها.

APPROVAL PAGE

I certify that I have supervised and read this study and that in my opinion, it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a thesis for the degree of Master of Science (Materials Engineering)

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DECLARATION

I hereby declare that this thesis is the result of my own investigations, except where otherwise stated. I also declare that it has not been previously or concurrently submitted as a whole for any degrees at IIUM or other institutions.

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LIST OF ABBREVIATIONS

AZO	Aluminum-Doped Zinc Oxide
BHJ	Bulk Heterojunction
BIPV	Building-Integrated Photovoltaic
CBLs	Cathode Buffer Layers
CT state	Charge Transfer State
FF	Fill Factor
HOMO	Highest Occupied Molecular Orbital
HOMO(a)	Highest Occupied Molecular Orbital of the Acceptor
HOMO(d)	Highest Occupied Molecular Orbital of the Donor
LUMO	Lowest Unoccupied Molecular Orbital
LUMO(a)	Lowest Unoccupied Molecular Orbital of the Acceptor
LUMO(d)	Lowest Unoccupied Molecular Orbital of the Donor
MATLAB	Matrix Laboratory
ODE	Ordinary Differential Equation
OPVs	Organic Photovoltaic Cells
P3HT	Poly(3-Hexylthiophene)
PCBM	1-(3-methoxycarbonyl)-propyl-1-phenyl-[6,6] C61
PCE	Power Conversion Efficiency
TCOs	Transparent Conductive Oxides
a-Si: H	Hydrogenated Amorphous Silicon
uc-Si: H	Hydrogenated Microcrystalline Silicon

LIST OF SYMBOLS

a	Electron-Hole Separation of the CT State
α	CT State Generation Property of the Active Layer
D_{n}	Electron Diffusion Coefficient.
D_{p}	Hole Diffusion Coefficient.
ε	Effective Permittivity of the Active Layer
ε_r	Relative Permittivity
E_{b}	Binding Energy of the CT State.
E_{g}	Effective Band Gap
E_{Fa}	Fermi Levels of the Anode
E_{Fc}	Fermi Levels of the Cathode
F	Electric Field
$\lvert F\rvert$	Magnitude of the Electric Field
G_{n}	Electron Generation Rate Per Unit Volume,
G_{p}	Hole Generation Rate Per Unit Volume
G_0	CT State Generation Property of the Active Layer
G_{CT}	CT State Generation Rate per Unit Volume due to Exciton Relaxation (Light Absorption)
$G_{\mathrm{CT,area}}$	CT State Generation Rate per Unit Area
$G_{\mathrm{CT,ave}}$	Average CT State Generation Rate per Unit Volume
I	Light Irradiance
J	Total Current Density
$\lvert J\rvert$	Magnitude of the Total Current Density
J_{n}	Electron Current Density,
J_{p}	Hole Current Density
J_{sc}	Short-Circuit Current Density
$\lvert J_{\mathrm{sc}}\rvert$	Magnitude of Short-Circuit Current Density
J_1	Bessel Function of the First Kind of Order 1
$\lvert J_{\mathrm{mp}}\rvert$	Magnitude of the Total Current Density That Produces Maximum Power Output

J_{diff}	Diffusion Current Density
$\langle J_{\mathrm{diff}} \rangle$	Average Diffusion Current Density
$J_{\mathrm{diff,\,n}}$	Electron Diffusion Current Density
$J_{\mathrm{diff,\,p}}$	Hole Diffusion Current Density
k_{B}	Boltzmann Constant
k_{d}	CT State Dissociation Rate Coefficient
k_{f}	CT State Decay Rate Coefficient
k_{L}	Langevin Recombination Coefficient
k_{mn}	Monomolecular Recombination Coefficient for Electrons
k_{mp}	Monomolecular Recombination Coefficient for Holes
L	Active Layer Thickness
n	Electron Density (Number of Free Electrons per Unit Volume)
n_{max}	Maximum Electron Density
n_{net}	Net Electron Density
N_{c}	Effective Density of States for Electrons
N_{v}	Effective Density of States for Holes
$n_{\mathrm{cont}}\big\|_{x=0}$	Density of Free Electrons at the $x=0$ Contact
$n_{\mathrm{cont}}\big\|_{x=L}$	Density of Free Electrons at the $x=L$ Contact
p	Hole Density (Number of Free Holes per Unit Volume)
p_{max}	Maximum Hole Density
p_{net}	Net Hole Density
P_{w}	Power Generated by OPV
P_{d}	CT State Dissociation Probability
P_{out}	Maximum Power Output
$p_{\mathrm{cont}}\big\|_{x=0}$	Density of Free Holes at the $x=0$ Contact
$p_{\mathrm{cont}}\big\|_{x=L}$	Density of Free Holes at the $x=L$ Contact
q	Elementary Charge
Φ_{a}	Work Functions of the Anode
Φ_{c}	Work Functions of the Cathode
φ_{nc}	Electron Injection Barrier at the Cathode
φ_{pa}	Hole Injection Barrier at the Anode
R_{b}	Non-Geminate Bimolecular Recombination Rate Per Unit Volume

R_{n}	Non-Geminate Recombination Rate Per Unit Volume for Electrons
R_{p}	Non-Geminate Recombination Rate Per Unit Volume for Holes
R_{mn}	Non-Geminate Monomolecular Recombination Rate Per Unit Volume for Electrons
R_{mp}	Non-Geminate Monomolecular Recombination Rate Per Unit Volume for Holes
$R_{\mathrm{n\text{-}g}}$	Non-Geminate Recombination Rate Per Unit Volume
$\left\langle R_{\mathrm{n\text{-}g}} \right\rangle$	Average Non-Geminate Recombination Rate Per Unit Volume
t	Time
T	Absolute Temperature
μ_{n}	Electron Mobility
μ_{p}	Hole Mobility
μ_{na}	Actual Electron Mobility
μ_{pa}	Actual Hole Mobility
V_{a}	Applied Voltage
V_{bi}	Built-in Voltage
V_{mp}	Applied Voltage That Produces Maximum Power Output
V_{oc}	Open-Circuit Voltage
x	Position Inside OPV Active Layer
γ	Bimolecular Recombination Reduction Factor
λ	Donor-Acceptor Morphology Parameter
$\Delta\psi$	Electric Potential Difference Across the Active Layer

CHAPTER 1

INTRODUCTION

1.1 INTRODUCTION

Electrical energy is one of the most important forms of energy used in our daily life activities. This form of energy is used to run most appliances such as home appliances, medical equipment, communication equipment, and even transportation. Therefore, it is important to secure the continuous supply of electrical energy in order to fulfill the growing demand of electrical energy use.

Solar energy is considered as the potential candidate to provide a continuous source of electrical energy since it has the most abundant source of energy due to the unlimited and endless supply of sunlight. It is also one of the important sources of renewable energy. Other examples of renewable energy are wind energy, hydropower, biomass, and geothermal energy. These renewable energy sources are advantageous compared to non-renewable energy sources such as oil, fossil fuels and natural gas which are limited (Campbell, 2008).

The energy output of the solar irradiation exceeds the yearly global power demand by several thousand times (Demirbaş, 2006). However, solar energy power is still not being able to be fully harvested according to global needs. Photovoltaic technologies are well-known methods that can generate electric power by converting solar energy into electrical energy. Therefore, extensive research on photovoltaic technologies has been conducted by scientists and engineers to enhance the photovoltaic cell's performance and then, make this source of renewable energy relevant for the future energy market.

1.2 RESEARCH MOTIVATION

1.2.1 Problem Statement

Organic photovoltaic cells are an emerging photovoltaic technology that possesses several unique advantages over traditional photovoltaic cells as mentioned earlier. However, the efficiency of OPVs remains significantly lower than the efficiency of traditional photovoltaics. This limitation is a major barrier for OPVs to be commercially viable in the market. Therefore, one of the main focuses in OPV research is to improve the device efficiency. To maximize the efficiency of OPVs, the use of light trapping is essential. Light trapping enhances the light absorption by the active layer through the enhancement of light confinement inside the active layer. The enhanced light absorption leads to the increase of charge carrier generation inside the active layer, and thus, increases the output electrical current.

Note that when light reaches a photovoltaic device, some of the incident light may be reflected away and some may be absorbed by the components above the active layer before the light reaches the active layer. Ideally, when light trapping schemes are employed, all the remaining photons (with energies within the absorption range of the active layer) that reach the active layer are absorbed by the active layer. Therefore, an ideal light trapping can be described here as an array of light trapping techniques that makes the active layer to absorb all the absorbable light that reaches the active layer irrespective of the active layer thickness. In other words, ideal light trapping makes the light absorption by the active layer of an OPV to be independent of the active layer thickness.

Since the use of light trapping is necessary to maximize the performance of OPVs, it is therefore necessary to understand the effect of device parameters on the performance of OPVs with light trapping. The active layer thickness is one of the most basic parameters of an OPV. The effect of active layer thickness on the performance of OPVs without light trapping has been extensively studied (Apaydın et al., 2013; Namkoong et al., 2013; Fallahpour et al., 2014; Zang et al.,2018), but, the effect of active layer thickness on the performance of OPVs with light trapping has never been investigated before.

The effect of active layer thickness on OPVs with ideal light trapping is expected to be vastly different compared with the effect of active layer thickness on OPVs without light trapping. In an OPV with ideal light trapping, the number of photons absorbed, and thus the number of excitons generated, are the same as the active layer thickness is reduced. This can be understand from the fact that the use of light trapping can help to prevent the exciton loss in OPVs when the light is absorbed (Ko et al., 2011; Nirmal et al., 2017; Novas et al., 2019). Therefore, as the active layer thickness in OPVs is varied, the number of photons absorbed and thus, the number of excitons generated inside the active layer of OPVs will be ideally the same irrespective of its active layer thickness. The exciton density keeps increasing as the active layer thickness of an OPV with ideal light trapping is reduced. However, the situation is different for an OPV without light trapping where the number of excitons generated may increase or decrease when the active layer thickness is reduced. (Apaydın et al., 2013; Namkoong et al., 2013; Fallahpour et al., 2014).

Finally, the influence of different light absorption profiles on the current-voltage characteristics of OPV will be investigated. The investigation will be carry out by comparing how the use of uniform and non-uniform light absorption profiles differ in modelling OPV. Previously, a lot of studies use a uniform light absorption profile when modelling OPV since this assumption can greatly simplify the calculation by eliminating the need to use the optical transfer matrix method (Gevaerts et al., 2011).

In (Koster et al., 2005), a device model has been developed by assuming a uniform light absorption profile. According to (Koster et al., 2005), the assumption of uniform profile while developing the model will not result to any inconsistency.

However, the actual light absorption is not uniform. Therefore, in order to make accurate predictions on the device performance, it is essential to determine how the use of a uniform light absorption differs from the use of a non-uniform light absorption profile in producing the current-voltage characteristics of OPVs. The results from this investigation provide useful information when performing OPV modelling. For example, when modelling the effect of active layer thickness on OPV performance where the value of the thickness is varied. Different active layer thickness produces different light absorption profiles (Fallahpour et al., 2014). Thus, it is important to know the effect of light absorption profiles on OPV performance when the active layer thickness is varied to make sure that there are no mistakes made when investigating the influence of active layer thickness on the OPVs performance.

1.2.2 Research Objectives

There are four main objectives in this study which are:

- To theoretically investigate the influence of active layer thickness on the performance of OPVs with ideal light trapping.
- To determine and understand how the active layer thickness influences the performance of OPVs with ideal light trapping.
- To investigate on how the use of uniform light absorption profile differs from the use of non-uniform light absorption profile in producing the current-voltage characteristics of OPVs.

- To suggest how the efficiency of actual photovoltaics with ideal light trapping can be improved using the knowledge gained from the study.

The main purpose of this study is to theoretically investigate the effect of active layer thickness on the performance of OPVs with ideal light trapping. This study aims to determine and understand how the active layer thickness influences the performance, namely the short-circuit current, the open-circuit voltage, the fill factor, and ultimately the power conversion efficiency, of OPVs with ideal light trapping. The outcomes of this study can be used as a guidance on how to maximize the performance of actual OPVs. Although actual light trapping may not be ideal, the results obtained from this study can still be used to suggest appropriate actions that can be taken so that the performance of actual OPVs can be maximized as much as possible.

Another objective of this study is to determine the accuracy of using a uniform light absorption profile in modelling OPVs. Since many studies simplify the actual light absorption profile in performing their investigations (including in this thesis where the same profile is assumed when the active layer thickness is varied), it is therefore important to know how light absorption profiles affects the modelling of OPVs.

1.2.3 Research Scopes

The details of how light is being trapped inside the active layer and the performance of various light trapping schemes are not within the scope of this thesis. Basically, the light trapping will be simply assumed as ideal as defined earlier in section 1.2.1 without detailing what light trapping schemes are being used. Therefore, scope of research will only involve the electrical characteristics of OPVs but not the details of the optical part.

1.3 THESIS ORGANIZATION

This thesis is organized as follows. In chapter 2, the literature reviews of the study will be provided including the background of photovoltaic technologies, the working operations of OPVs and the light trapping. In chapter 3, the methodology in carrying out this study is described, where the basic equations that govern the charge carriers in OPVs, the analytical modelling used to calculate the current-voltage characteristics and the procedures of calculation are described. In chapter 4, the results of the influence of the active layer thickness on the performance of OPVs with ideal light trapping, namely the short-circuit current, open-circuit voltage, fill factor, and power conversion efficiency, are presented, discussed, and summarized. In chapter 5, the results between the use of uniform and non-uniform light absorption profiles in modelling OPVs are compared, discussed, and summarized. In chapter 6, the thesis is concluded, and possible future works are suggested.

CHAPTER 2

LITERATURE REVIEW

2.1 INTRODUCTION

Photovoltaic cells are electronic devices that capture the electromagnetic waves (including sunlight) and turn it directly into electricity. Instead of generating electricity from chemicals (e.g. battery cell), photovoltaic cells generate power from light absorption to create electrical energy. The development of photovoltaic devices is preliminarily based on inorganic material (e.g. crystalline silicon) (Miles, Zoppi, & Forbes, 2007). The crystalline silicon photovoltaic cells have been the most efficient devices to convert the light irradiation into electrical energy. However, there are some limitations of these photovoltaic devices that hinder them from being used in large scales such as high manufacturing cost (Tao, 2008) and inflexible design. Figure 2.1 and 2.2 show the examples of the current application of typical photovoltaic cells in the industry.

Figure 2.1 The 40 kWp facade of the Northumberland building at Northumbria University, United Kingdom, which uses the crystalline silicon solar modules manufactured by BP Solar (Saturn modules) (Miles, Zoppi, & Forbes, 2007).