INFLUENCE OF LIGHT ABSORPTION PROFILE ON THE PERFORMANCE OF ORGANIC PHOTOVOLTAIC CELL USING ANALYTICAL DRIFT DIFFUSION MODEL

BY

ABDUL HALIM IKRAM BIN MOHAMED

A thesis submitted in fulfillment of the requirement for the degree of Master of Science (Electronics Engineering)

Kulliyyah of Engineering
International Islamic University Malaysia

FEBRUARY 2022

ABSTRACT

Organic photovoltaic (OPV) cell has several attractive features such as lightweight, good transparency, mechanical flexibility, and low production cost. However, their efficiencies are still relatively low to make OPV cell to be economically viable. A new approach on how to improve the efficiency of OPV cell is therefore necessary. In this thesis, how variation of light absorption at a specific position inside the active layer affects the performance of organic photovoltaic (OPV) cell, namely the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (*FF*), and power conversion efficiency (PCE), is investigated. To analyze the performance, a modified analytical current-voltage model for OPV cell is applied. The updated version allows the light absorption profile to be represented by any mathematical functions (e.g. an exponential function). It is found that light absorption profile affects the performance through the drift current. When the ratio of the mobility of the faster carrier to the mobility of the slower carrier type is less than 10^3, the PCE is maximized when the light absorption is concentrated at the center of the active layer (8.37%). When the ratio of the mobility of the faster carrier to the mobility of the slower carrier type is more than approximately 10^4, the PCE is maximized when the light absorption is concentrated near the electrode (6.65%). Therefore, the light absorption profile in an OPV cell needs to be properly tuned and adjusted in order to maximize the performance of the OPV cell.

خلاصة البحث

تحتوي الخلية (OPV) الكهروضوئية العضوية على العديد من الميزات الجذابة مثل خفيفة الوزن والشفافية الجيدة ومرونة ميكانيكية وتكلفة الإنتاج المنخفضة. ومع ذلك، لا تزال كفاءتهم منخفضة نسبيا لجعل خلية OPV لتكون قابلة للحياة اقتصاديا. لذلك من الضروري نهج جديد حول كيفية تحسين كفاءة خلية OPV. في هذه الأطروحة، ما مدى تباين من الامتصاص الخفيف في وضع محدد داخل الطبقة النشطة يؤثر على أداء خلية الكهروضوئية العضوية (OPV)، وهي كثافة الدائرة الحالية الحالية (J_{sc})، الجهد الدائريات المفتوح (V_{oc})، عامل التعبئة (FF) ، وكفاءة تحويل الطاقة (PCE)، يتم التحقيق فيها. لتحليل الأداء، يتم تطبيق نموذج التحليل التحليلي المعدل لخلايا OPV. يسمح الإصدار المحدث بتمثيل ملف تعريف امتصاص الضوء بأي وظائف رياضية (E.G. وظيفة أسية). تم العثور على أن ملف تعريف امتصاص الضوء يؤثر على الأداء من خلال التيار الانجراف. عندما تكون نسبة تنقل الناقل الأسرع إلى تنقل نوع الناقل البطيء أقل من 10^3، يتم تعظيم PCE عندما يتركز امتصاص الضوء في مركز الطبقة النشطة (8.37%). عندما تكون نسبة تنقل الناقل الأسرع إلى تنقل نوع الناقل البطيء أكثر من حوالي 10^4، تم تعظيم PCE عندما يتركز امتصاص الضوء بالقرب من القطب (6.65%). لذلك، يجب ضبط ملف تعريف امتصاص الضوء في خلية OPV بشكل صحيح وتعديله من أجل زيادة أداء خلية OPV.

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 (Electronics Engineering).

……………………………………….
Mohd Lukman Bin Inche Ibrahim
Supervisor

………………………………………..
Nurul Fadzlin Bt Hasbullah
Co-Supervisor

………………………………………..
Aisha Hassan Abdalla Hashim
Co-Supervisor

I certify that I have 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 (Electronics Engineering).

…………………………………..
Raihan Bin Othman
Internal Examiner

…………………………………..
Mohd Yusri Bin Abd. Rahman
External Examiner

This thesis was submitted to the Department of Electrical and Computer Engineering and is accepted as a fulfilment of the requirement for the degree of Master of Science (Electronics Engineering).

………………………………………..
Md. Rafiqul Islam
Head, Department of Electrical and Computer Engineering

This thesis was submitted to the Kulliyyah of Engineering and is accepted as a fulfilment of the requirement for the degree of Master of Science (Electronics Engineering).

………………………………………..
Sany Izan Ihsan
Dean, Kulliyyah of Engineering

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 other degrees at IIUM or other institutions.

Abdul Halim Ikram Bin Mohamed

Signature ……………………………………… Date ……………………..

INTERNATIONAL ISLAMIC UNIVERSITY MALAYSIA

DECLARATION OF COPYRIGHT AND AFFIRMATION OF FAIR USE OF UNPUBLISHED RESEARCH

INFLUENCE OF LIGHT ABSORPTION PROFILE ON THE PERFORMANCE OF ORGANIC PHOTOVOLTAIC CELL USING ANALYTICAL DRIFT DIFFUSION MODEL

I declare that the copyright holders of this thesis are jointly owned by the student and IIUM.

No part of this unpublished research may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording or otherwise without prior written permission of the copyright holder except as provided below

1. Any material contained in or derived from this unpublished research may only be used by others in their writing with due acknowledgement.

2. IIUM or its library will have the right to make and transmit copies (print or electronic) for institutional and academic purposes.

3. The IIUM library will have the right to make, store in a retrieval system and supply copies of this unpublished research if requested by other universities and research libraries.

By signing this form, I acknowledged that I have read and understand the IIUM Intellectual Property Right and Commercialization policy.

Affirmed by Abdul Halim Ikram Bin Mohamed

……………………….	………………..
Signature	Date

ACKNOWLEDGEMENTS

It is a great pleasure to show my gratitude to all those people who have been supporting me from beginning until the end of this master programme. First and foremost, I must acknowledge and thank to The Almighty Allah for the blessing and guiding me throughout this period. I could not have accomplished this thesis without the faith I have to the Almighty.

I express my deepest gratitude to my supervisor, Dr. Mohd Lukman Bin Inche Ibrahim for his support, motivation, constant guidance, and untiring help for me to complete my master thesis. His great knowledge on photovoltaic cells has been beneficial for me. He had given me a freedom during my research and have always been supportive. It is also my pleasure to acknowledge all my family and friend who gave motivational and inspirational supports. I will always be grateful to them for supporting me.

Finally, I would like to convey my appreciation to International Islamic Malaysia University (IIUM) for giving me a great opportunity and the facilities for me to continue and complete my study.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

CT	Charge Transfer
FF	Fill Factor
HOMO	Highest Occupied Molecular Orbital
$HOMO_a$	Highest Occupied Molecular Orbital Acceptor
$HOMO_d$	Highest Occupied Molecular Orbital Donor
LUMO	Lowest Unoccupied Molecular Orbital Lowest
$LUMO_a$	Lowest Unoccupied Molecular Orbital Lowest Acceptor
$LUMO_d$	Lowest Unoccupied Molecular Orbital Lowest Donor
MATLAB	Matrix Laboratory Software
OPVs	Organic Photovoltaic Cells
P3HT	Poly (3-Hexylthiophene)
PCBM	1-(3-methoxycarbonyl)-propyl-1-phenyl-[6,6] C61
PCE	Power Conversion Efficiency

LIST OF SYMBOLS

a	Electron-Hole Separation of CT State
C	Peak of CT State Photogeneration Rate
D_n	Electron Diffusion Coefficient
D_p	Hole Diffusion Coefficient
E_g	Effective Band Gap
E_{Fa}	Fermi Level of Anode
E_{Fc}	Fermi Level of Cathode
F	Electric Field
G_{CT}	CT State Photogeneration
$G_{CT,area}$	CT State Photogeneration per Unit Area
J	Total Current Density
J_{sc}	Short-Circuit Current Density
J_n	Electron Current Density
J_p	Hole Current Density
$J_{n,dr}$	Electron Drift Current Density
$J_{p,dr}$	Hole Drift Current Density
$J_{n,diff}$	Electron Diffusion Current Density
$J_{p,diff}$	Hole Diffusion Current Density
k_B	Boltzmann Constant
k_L	Langevin Recombination Coefficient
k_{mn}	Electron Monomolecular Recombination Coefficient
k_{mp}	Hole Monomolecular Recombination Coefficient
k_d	CT State Dissociation Rate Coefficient
k_f	CT State Decay Rate Coefficient
L	Active Layer Thickness
N_c	Effective Density of State for Electrons
N_v	Effective Density of State for Holes
n_{max}	Maximum Electron Density
n_{net}	Net Electron Density
p_{max}	Maximum Hole Density
p_{net}	Net Hole Density
P_{in}	Input Power per Unit Area of Incident Light
P_d	Dissociation Probability of CT States

R_b	Non-Geminate Bimolecular Recombination Rate
R_{mn}	Non-Geminate Monomolecular Recombination Rate per Unit Volume of Electron
R_{mp}	Non-Geminate Monomolecular Recombination Rate per Unit Volume of Hole
T	Temperature
V_{oc}	Open-Circuit Voltage
V_a	Applied Voltage
$\lvert J \rvert$	Magnitude of Total Current Density
$\lvert J_{sc} \rvert$	Magnitude of Short-Circuit Current Density
$\lvert J_n \rvert$	Magnitude of Electron Current Density
$\lvert J_p \rvert$	Magnitude of Hole Current Density
$\lvert J_{n,dr} \rvert$	Magnitude of Electron Drift Current Density
$\lvert J_{p,dr} \rvert$	Magnitude of Hole Drift Current Density
$\lvert J_{n,diff} \rvert$	Magnitude of Electron Diffusion Current Density
$\lvert J_{p,diff} \rvert$	Magnitude of Hole Diffusion Current Density
$\langle J_{n,dr} \rangle$	Average Drift Current Density
$\langle J_{n,diff} \rangle$	Average Diffusion Current Density
$\langle n_{net} \rangle$	Average Net Electron Density
γ	Bimolecular Recombination Reduction Coefficient
ε	Effective Permittivity of Active Layer
μ_{na}	Actual Electron Mobility
μ_{pa}	Actual Hole Mobility
μ_n	Electron Mobility
μ_p	Hole Mobility
φ_{pa} , φ_{nc}	Injection Barriers
λ	Donor-Acceptor Morphology Parameter
x	Position Inside OPV Active Layer

CHAPTER ONE

INTRODUCTION

1.1 INTRODUCTION

Solar cell or photovoltaic cell is a semiconductor device that converts light energy into electrical energy. It is a clean and renewable source of energy. Even though there are many sources of renewable energy in this world such as wind energy, nuclear, hydropower and geothermal energy, they could be difficult to be implemented by many applications. For example, the photovoltaic cell is the most practical source of energy for powering satellites in space. It has been subjected to extensive research since the last few decades in order to improve its efficiency and also minimise the production cost. In a conventional photovoltaic cell, the photoactive layer is made from inorganic semiconductors (e.g. silicon crystal), whereby the semiconductors are doped with n-type and p-type materials, and the layer of the two materials are stacked on top of each other creating a p-n junction. When the light strikes the semiconductors, photons are absorbed that cause free electrons and free holes to be produced. The free electrons move to n-type material while the holes move to p-type material by a driving force resulted from the electric field. The flow of the electrons and holes generates current in the active layer. The current produced is a direct current and a load that consumed low power can be used immediately by connecting it to the positive and negative terminal of the photovoltaic cell.

1.2 PROBLEM STATEMENT

The photovoltaic cell based on organic semiconductors is considered as one of the most exciting photovoltaic technologies. However, organic photovoltaic (OPV) cell suffer from a relatively low efficiency as compared to inorganic photovoltaic. In the future, it would be the most economically viable photovoltaic technology since their fabrication cost is low. Considering that an OPV cell has other advantages that inorganic photovoltaic is lacking (e.g. lightweight).

There are many factors that influence the efficiency of an OPV cell. In order to improve the efficiency of the device, it is essential to gain knowledge and understand how these factors influence its efficiency. As will be discussed in more details in the literature review section, it has been shown that light absorption profile which influences the charge carrier generation profile affects the performance of the device. Although understanding the effect of the light absorption profile is clearly important since it affects the device performance, there are still a few matters needed to be addressed for our better understanding. For example, it has been shown that a profile with high light absorption at certain position inside the active layer can improve the performance of the device (Mescher et al., 2012; Tress et al., 2013; Islam et al., 2017). However, as will be clarified later in the literature review section, there are still a few issues that need to be improvised regarding the previous studies results, especially concerning how the charge carrier mobility ratio affects the light absorption profile and consequently, influences the device performance. Furthermore, it is possible to control the light absorption profile inside the active layer to a certain extent by using several techniques that will be discussed in more detail in the literature review section.

In this thesis, the effect of the light absorption profile on the performance of an OPV cell will be investigated that includes how the charge carrier mobility ratio can influence the said effect. The output of this research is expected to enlighten the issues that concern the previous studies and improve the knowledge on how light absorption profile affects the efficiency, and this knowledge could provide an additional strategy on how the efficiency of the device could be further improved.

1.3 RESEARCH OBJECTIVE

The objective of this research as the following:

- To investigate on how the light absorption profile at different positions inside the active layer affect the photovoltaic parameters of an OPV cell at various charge carrier mobility ratios using the modified drift-diffusion model charge carrier mobility.

1.4 RESEARCH SCOPE

In this thesis, the research focusses on how light absorption profile influences the performance of an OPV cell for different cases of charge carrier mobility ratios. To achieve the objective, a parabolic light absorption profile will be used since its equation parameters can be easily changed to make the profile to have a high intensity of light absorption at different position inside the active layer. An analytical drift-diffusion model that was recently developed is used for determining the photovoltaic parameters (Ibrahim, 2018). The parabolic light absorption profile will be used as the input to the drift-diffusion model. As will be discussed in the literature review section, light absorption inside the active layer can be controlled to a certain extent by using a few available techniques such as plasmonic nanoparticles, back reflector and optical spacers. The details of how parabolic light absorption profiles with the peak absorption at different positions inside the active layer can be created and controlled are not within the scope of this thesis. Basically, the scope of the research will only involve the detail of the electrical part of an OPV cell, but not the detail of its optical part.

1.5 THESIS ORGANISATION

This thesis is divided into five chapters and organised as the following. In Chapter 1, the background of a photovoltaic cell is briefly reviewed with a proper explanation of how conventional photovoltaic cell works. After that, the problem statement, research objectives and research scope are described in Chapter 1. In Chapter 2, a literature review on the factors that can influence the performance of an OPV is presented. In Chapter 3, the methodology of this study is explained in detail. In Chapter 4, the modelling results are presented and discussed. In Chapter 5, the conclusion of the overall research findings and recommendation for future works are stated.

CHAPTER TWO

LITERATURE REVIEW

2.1 INTRODUCTION

Photovoltaic technology is growing very rapidly as it seems to be an alternative solution of a renewable source of energy to generate electricity. The release of greenhouse gases especially carbon dioxide from the non-renewable source of energy such as steam, coal, crude oil, and gas to generate electricity generating pollution that will deplete the ozone layer and causes global warming. Because of this problem, people must start looking and practicing other mechanisms to generate power supply that are more environmentally friendly so that the ecosystem can be conserved. Hence, many industries nowadays, commenced with harnessing solar energy as it has many advantages such as low maintenance cost, low electricity bill, clean and renewable energy. For example, Malaysia already built a solar farm in Cypark, Kuala Perlis that can contribute up to 5MW of power supply as shown in Figure 1.

Figure 1 Solar power plant (solar farm) in Perlis, Malaysia (Kassim et al., 2015).

2.2 PHOTOVOLTAIC CELL

Photovoltaic cell and photodiodes have the same device structures and operational principles, whereby both devices are used to convert light (i.e. electromagnetic wave) into electric current. The difference is that a photovoltaic cell is operated such that the electric current is used to store energy, while a photodiode is operated such that the electric current functions as a signal or sensor. Moreover, there are many applications of a photodiode that make people's daily life easier today in various scientific, industrial, medical, defense, and domestic applications. Therefore, since both devices are essentially the same, improving the understanding of photovoltaic cell working operation also directly improves the understanding on the working operation of photodiodes.

Nowadays, scientists are exploring several new types of photovoltaic cells. One of the photovoltaic cells that have been gaining attention is photovoltaic cell based on organic semiconductors. This is because an organic photovoltaic (OPV) cell has many advantages as compared to their inorganic counterparts such as lightweight, mechanically flexible, simple to produce, and low fabrication cost (Scharber & Sariciftci, 2013). Therefore, OPVs are viewed as an attractive alternative to supplement or probably replace the conventional photovoltaic technologies. For example, an OPV cell has a great potential to be used as an energy source for wearable devices (Scharber & Sariciftci, 2013), next generation of self-driven biomedical devices (Park et al., 2018), and off-grid devices for the Internet of Things (IoT) (Teng et al., 2018). The recorded power conversion efficiency (PCE) of an OPV cell has been improving steadily from 11% (Green et al., 2016) several years ago to 17.3% (Meng et al., 2018). Therefore, the investigation to improve the performance of OPV cell has been the focus by many researchers, persistently. The 17.3% efficiency has been achieved partly by implementing the existing knowledge on how various factors affects the device efficiency (Meng et al., 2018). This achievement has proved the importance of exploration to gain knowledge on how various factors can improve the efficiency of an OPV cell. However, the PCE of an OPV cell is still quite low as compared to other emerging photovoltaic technologies, especially the perovskite solar cell that was reported to be 19.7% efficiency (Green et al., 2016).

The active layer of an OPV cell is made of two different organic semiconductor materials that have different energy levels, namely lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO). One of the organic semiconductor material acts as an electron donating material (called donor), and the other acts as an electron accepting material (called acceptor). To maximise the performance, the OPV cell must employ bulk heterojunction design whereby the donor and the acceptor are finely mixed together. This is unlike the photovoltaic cell based on inorganic semiconductors where bilayer design is employed.

Unfortunately, organic semiconductors also have disadvantages in terms of low electrical properties as compared to inorganic semiconductors such as low charge carrier mobility and low dielectric constant (Koster et al., 2012), and it is widely known that these factors contribute to the relatively low efficiency of an OPV cell. Several studies focus on developing organic semiconductors with high electrical properties (e.g. by annealing) to improve the device performance (Mhamdi et al., 2018). In general, there are many factors that can affect the efficiency of an OPV cell, and some are not properly understood yet. A proper understanding on how these factors affect the efficiency of an OPV cell surely could contribute to a better performance. For example, it has been shown that active layer morphology is one of the important parameters that should be considered because it can also affect the device performance (Weng et al., 2020). Besides, the work function of the electrode can also influence the device performance (Lee et al., 2015; Chen et al., 2016). The studies have proven that by increasing the work function to its optimum value would increase the efficiency of an OPV cell. In fact, there are numerous studies on how the work function can be optimised so that it improved the performance of organic photovoltaics (Erray et al., 2018). This shows that it is important to discover new knowledge on how various factors could influence and enhance the performance of an OPV cell.

2.3 WORKING PRINCIPLE OF ORGANIC PHOTOVOLTAIC CELL

The fundamental distinction between the OPV cell and inorganic photovoltaic cell is the materials used to build the photoactive layer (i.e. the light absorbing layer). As the name suggests, the photoactive layer of an OPV cell is made from the combination of organic semiconductor materials that have different energy levels. One of the organic semiconductors is called donor, acting as an electron donating material, and the other is called acceptor, acting as an electron accepting material. Sometimes, a buffer layer is inserted between each electrode and the active layer (Notarianni et al., 2014). Buffer layers are used to ensure that a charge selective transport occurs that can prevent charge carriers from being extracted by the wrong electrodes that would reduce the performance of the device (electrons and holes should be extracted by the cathode and anode, respectively).

When the light is absorbed by the organic photoactive layer, excitons (strongly bound electron-hole pair) are generated. These excitons must be transported to the donor-acceptor interface in order for the excitons to be dissociated into free charge carriers (i.e. electrons and holes) before they can be extracted by the electrode (anode and cathode) to produce electricity. An OPV cell can be built using two different structures; bilayer structure and bulk heterojunction structure (see Figure 2). The excitons generated have very short lifetimes with recombination distances between 5 nm and 20 nm (Mikhnenko et al., 2015; Luhman & Holmes, 2011). If the distance between an exciton to the nearest donor-acceptor interface is too far, the exciton will recombine before it can reach the donor-acceptor interface. Hence, the difficulty for the exciton to reach donor-acceptor interface can cause free electrons and free holes which cannot be extracted, and this contributes to the decrease in the device performance. Due to this reason, bulk heterojunction design is the solution in terms of high performance because it provides a short distance for an exciton to reach the donor-acceptor interface.

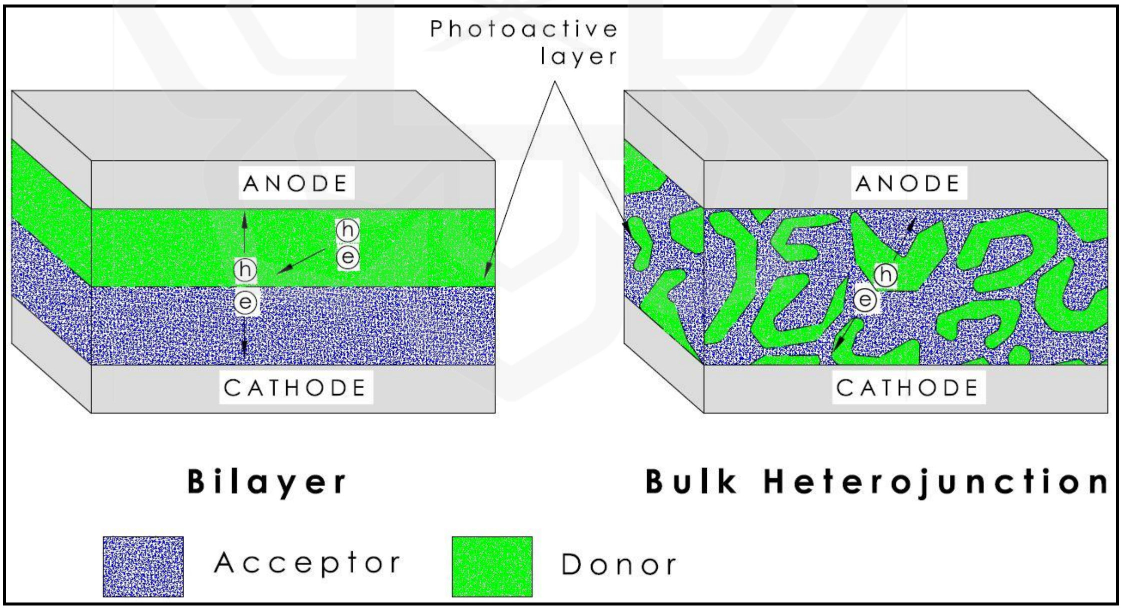

Figure 2 Illustrations of the difference between bilayer and bulk heterojunction model for organic photovoltaics. The **h** represents holes, whereas **e** represents electrons.