ESTIMATION OF PEROVSKITE SOLAR CELL PERFORMANCE BASED ON OGHMANANO AND COMSOL MULTIPHYSICS MODELLING SIMULATION

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MASTER OF SCIENCE IN ELECTRICAL ENGINEERING

2025

Faculty of Electrical Technology and Engineering

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A thesis submitted
in fulfillment of the requirements for the degree of
Master of Science in Electrical Engineering

Faculty of Electrical Technology and Engineering

UNIVERSITI TEKNIKAL MALAYSIA MELAKA

2025

DECLARATION

I declare that this thesis entitled “Estimation of Perovskite Solar Cell Performance Based on Oghmanano and Comsol Multiphysics Modelling Simulation” is the result of my own research except as cited in the references. The thesis has not been accepted for any degree and is not concurrently submitted in candidature of any other degree.

Signature :.....

Name : Lee Jin Yao

Date : 30/6/2025

APPROVAL

I hereby declare that I have read this thesis and in my opinion this thesis is sufficient in terms of scope and quality for the award of Master of Science in Electrical Engineering.

Signature : .....

Supervisor Name : Dr. Rahifa binri Ranom

Date : 30/6/2025

DEDICATION

To my beloved mother and father.

ABSTRACT

Perovskite Solar Cell (PSC) is one of the third-generation solar cells with advanced materials, intelligent properties, and high potential performance. The PSC is made up of 5 layers, the active layers consist of an absorber layer (AL) sandwiched between a hole transport layer (HTL) and an electron transport layer (ETL), these active layers are sandwiched between transparent conductive oxide (TCO) as cathode and conductive metal as anode. Due to the multiple layers involved in the operation mechanism of PSC, the performance of PSC becomes unpredictable especially when the material is altered in the PSC's layers. Therefore, to prevent the wastage of precious rare materials and time of manufacture, design and modelling the PSC in a simulation is important to predict the performance of PSC. The PSC's AL contains lead which is harmful to the environment and a serious health hazard. However, the PSC with the lead-free perovskite layer has lower stability in terms of its performance. Therefore, the lead-free PSC cell performance is evaluated in this research for the potential to replace the lead PSC and the optimization for the performances of lead-free PSC is conducted. This research uses electrochemical modelling by drift-diffusion equations to model the dynamic operations in PSC in OghmaNano and COMSOL Multiphysics semiconductor modelling simulation software. The properties of each layer in PSC are extracted from the drift-diffusion equations which are defined in the semiconductor modelling simulation software before computation. The complex drift-diffusion equations are solved in semiconductor modelling simulation software with the finite element method (FEM) numerical scheme to generate the JV curve as its output. The defined problems are discretized into the various elements with the mesh number that is set and solved by using a multiple defined equations. The output JV curves generated from semiconductor modelling simulation software are dependent on the layer properties of the PSC. These properties include the layer's thickness, electron affinity, energy bandgap, relative permittivity, conduction band density, valence band density, doping density, mobility of electrons, and mobility of holes. The performance of PSC can be abstracted and calculated from the resulting JV curves. These PSC's performance includes short circuit current (JSC), open circuit voltage (VOC), fill factor (FF), and power conversion efficiency (PCE). For validation purposes, the PSC performance obtained from the simulation with the same PSC properties used in the work is validated against the results from SCAPS. The PSC's PCE showed a good agreement with the results from SCAPS, the other PSC performance's value (JSC, VOC, and FF) difference is only less than 6% under the same comparison. In the subsequent works, the results of PSC's PCE with the different cell layer properties variations are discussed in this research. A set of PSC layers properties' optimum values have been determined from the analysis. The PSC performance is computed with the optimum value of cell layer properties showing that the PSC's PCE increased by 16.14% and 9.05% in OghmaNano and COMSOL Multiphysics respectively. However, in the evaluation of the performance between lead and lead-free PSC, the simulation results show that the PSC's PCE decreased by 18.33% and 18.67% in OghmaNano and COMSOL Multiphysics respectively after replacing the lead AL of PSC with lead-free AL. The lead-free PSC's PCE also increased by 1.52% after optimizing its AL properties' value.

ANGGARAN PRESTASI SEL SOLAR PEROVSKITE BERDASARKAN SIMULASI PEMODELAN OGHMANANO DAN COMSOL MULTIPHYSICS

ABSTRAK

Sel solar perovskite (PSC) ialah salah satu daripada sel solar generasi ketiga dengan bahan termaju, sifat pintar dan prestasi berpotensi tinggi. PSC terdiri daripada 5 lapisan, lapisan aktif terdiri daripada lapisan penyerap (AL) yang diapit di antara lapisan pengangkutan lubang (HTL) dan lapisan pengangkutan elektron (ETL), lapisan aktif ini diapit antara oksida pengalir lutsinar (TCO) sebagai katod dan logam pengalir sebagai anod. Disebabkan oleh pelbagai lapisan yang terlibat dalam mekanisme operasi PSC, prestasi PSC menjadi tidak dapat diramalkan terutamanya apabila bahan diubah dalam lapisan PSC. Oleh itu, untuk mengelakkan pembaziran bahan nadir berharga dan masa pembuatan, reka bentuk dan pemodelan PSC dalam simulasi adalah penting untuk meramalkan prestasi PSC. AL PSC mengandungi plumbum yang berbahaya kepada alam sekitar dan bahaya kesihatan yang serius. Walau bagaimanapun, PSC dengan lapisan perovskite bukan plumbum mempunyai kestabilan yang lebih rendah dari segi prestasinya. Oleh itu, prestasi sel PSC bukan plumbum dinilai dalam penyelidikan ini untuk potensi menggantikan PSC plumbum dan pengoptimuman untuk prestasi PSC bukan plumbum dijalankan. Penyelidikan ini menggunakan pemodelan elektrokimia secara persamaan drift-difusi untuk memodelkan operasi dinamik dalam PSC dalam perisian simulasi pemodelan semikonduktor OghmaNano dan COMSOL Multiphysics. Sifat setiap lapisan dalam PSC diekstrak daripada persamaan drift-difusi yang ditakrifkan dalam perisian simulasi pemodelan semikonduktor sebelum pengiraan. Persamaan drift-difusi yang kompleks diselesaikan dalam perisian simulasi pemodelan semikonduktor dengan skema berangka kaedah unsur terhingga (FEM) untuk menjana lengkung JV sebagai keluarannya. Masalah yang ditakrifkan didiskrisikan ke dalam pelbagai elemen dengan nombor mesh yang ditetapkan dan diselesaikan dengan menggunakan persamaan berbilang yang ditakrifkan. Lengkung JV keluaran yang dihasilkan daripada perisian simulasi pemodelan semikonduktor adalah bergantung kepada sifat lapisan PSC. Sifat ini termasuk ketebalan lapisan, pertalian elektron, celah jalur tenaga, ketelusan relatif, ketumpatan jalur pengaliran, ketumpatan jalur valens, ketumpatan doping, mobiliti elektron dan mobiliti lubang. Prestasi PSC boleh diabstrak dan dikira daripada lengkung JV yang terhasil. Prestasi PSC ini termasuk arus litar pintas (Jsc), voltan litar terbuka (Voc), faktor isian (FF), dan kecekapan penukaran kuasa (PCE). Untuk tujuan pengesahan, prestasi PSC yang diperoleh daripada simulasi dengan sifat PSC yang sama digunakan dalam kerja disahkan terhadap data daripada SCAPS. PCE PSC menunjukkan persetujuan yang baik dengan SCAPS, perbezaan nilai prestasi PSC yang lain (Jsc, Voc, dan FF) hanya kurang daripada 6% di bawah perbandingan yang sama. Dalam kerja-kerja seterusnya, keputusan PCE PSC dengan variasi sifat lapisan sel yang berbeza dibincangkan dalam penyelidikan ini. Satu set nilai optimum sifat lapisan PSC telah ditentukan daripada analisis. Prestasi PSC dikira dengan nilai optimum sifat lapisan sel yang menunjukkan bahawa PCE PSC masing-masing meningkat sebanyak 16.14% dan 9.05% dalam OghmaNano dan COMSOL Multiphysics. Walau bagaimanapun, dalam penilaian prestasi antara PSC plumbum dan bukan plumbum, keputusan simulasi menunjukkan bahawa PCE PSC menurun sebanyak 18.33% dan 18.67% masing-masing dalam OghmaNano dan COMSOL Multiphysics selepas menggantikan AL

plumbum PSC dengan AL bukan plumbum. PCE PSC bukan plumbum juga meningkat sebanyak 1.52% selepas mengoptimumkan nilai sifat ALnya.

ACKNOWLEDGEMENT

First and foremost, I would like to express my deep and sincere gratitude to my research supervisor, Dr. Rahifa binti Ranom and my co-supervisor, Dr. Kyairul Azmi bin Baharin for their guidance, advice, and motivation. Because of their invaluable guidance with patience, several new skills were unlocked for me, and I believe the knowledge that I gained is a stepping stone for my career in future. It was a great privilege and honour to work and study under their guidance. Without their support, this research cannot be done completely.

A deep heartfelt thanks to my parents Mr. Lee Chee Min and Mrs. Boon Kam Lan for their love, prayers, caring and sacrifices for educating and preparing me for my future. Because of them, I can reach this stage of my life, without their foster after born, I am nothing. Family is always the backbone and haven for my whole life, they provide love, care, and support to me at all times.

Particularly, I would also like to express my deepest thanks to the Ministry of Higher Education Malaysia for the funding under FRGS/1/2020/FKE-CERIA/F00414 and also a special thanks to Universiti Teknikal Malaysia Melaka (UTeM) for allowing conducting the study and research works.

Special thanks to my soul mate, Ms. Nasio Sihombing for her kindness and support in physically and mentally to cross over the bottleneck along the progress of the research. Lastly, I am extending my thanks to all my friends and seniors. The views and tips from them are useful indeed, they are willing to help each other and glow together.

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LIST OF ABBREVIATIONS

UTeM	-	Universiti Teknikal Malaysia Melaka
PSC	-	Perovskite Solar Cell
AL	-	Absorber Layer
HTL	-	Hole Transport Layer
ETL	-	Electron Transport Layer
TCO	-	Transparent Conductive Oxide
FEM	-	Finite Element Method
PCE	-	Power Conversion Efficiency
TWH	-	Tera-Watt-Hour
SRH	-	Shockley–Read–Hall
CPU	-	Central Processing Unit
RAM	-	Random Access Memory
NREL	-	National Renewable Energy Laboratory
DSSC	-	Dye-Sensitized Solar Cell
QDSC	-	Quantum Dots Solar Cell
ETM	-	Electron Transporting Material
HTM	-	Hole Transporting Material
LUMO	-	Lowest Unoccupied Molecular Orbital
HOMO	-	Highest Occupied Molecular Orbital
NTU	-	Nanyang Technological University
R&D	-	Research and Development
PDE	-	Partial Differential Equation

ARC	-	Anti-Reflective Coating
DETL	-	Double Electron Transport Layer
DHTL	-	Double Hole Transport Layer
DAL	-	Double Absorber Layer
1D	-	1 Dimension
2D	-	2 Dimension
3D	-	3 Dimension
OFET	-	Organic Field Effect Transistor
OLED	-	Organic Light Emitting Diode
CIGS	-	Copper Indium Gallium Selenide
CdTe	-	Cadmium Telluride
α-Si	-	Amorphous Silicon
CELIV	-	Charge Extraction by Linearly Increasing Voltage
TPC	-	Transient Photocurrent
TPV	-	Transient Photovoltage
IS	-	Impedance Spectroscopy
IMPS	-	Intensity Modulated Photocurrent Spectroscopy
TMM	-	Transfer Matrix Method

LIST OF SYMBOLS

J_{SC}	-	short circuit current
V_{OC}	-	open circuit voltage
FF	-	fill factor
η	-	power conversion efficiency
L	-	thickness
χ	-	electron affinity
E_g	-	energy bandgap
ε_r	-	relative permittivity
N_C	-	conduction band density
N_V	-	valence band density
N_D	-	donor doping density
N_A	-	acceptor doping density
μ_n	-	electron mobility
μ_p	-	hole mobility
c	-	direct recombination factor
P_{in}	-	input power
e	-	electron
h	-	hole
E	-	electric field
q	-	charge density
ε	-	dielectric permittivity
ϕ	-	electrostatic potential
p	-	hole charge density

n	-	electron charge density
N_D	-	donor ionized doping concentration
N_A	-	acceptor ionized doping concentration
p_t	-	trapped hole
n_t	-	trapped electron
J_n	-	electron total current density
$J_n(drift)$	-	electron drift current density
$J_n(diffusion)$	-	electron diffusion current density
J_p	-	hole total current density
$J_p(drift)$	-	hole drift current density
$J_p(diffusion)$	-	hole diffusion current density
F	-	electrostatic force
m	-	mass of the electron
a	-	acceleration of the electron
V_{drift}	-	drift velocity of the electron
t	-	time
μ_n	-	electron mobility
μ_p	-	hole mobility
D_n	-	electron diffusion coefficient
D_p	-	hole diffusion coefficient
k_B	-	Boltzmann's constant
T	-	temperature
G_n	-	electron generation rate
G_P	-	hole generation rate
R_n	-	electron recombination rate

R_p	-	hole recombination rate
R_{b-b}	-	band-to-band recombination rate
n_i	-	intrinsic carrier density
R_{SRH}	-	SRH recombination rate
τ_n	-	electron minority carrier lifetime
τ_p	-	hole minority carrier lifetime
E_i	-	intrinsic energy level
E_t	-	trap state energy level
R_{Auger}	-	Auger recombination rate
γ_n	-	Auger recombination constant for electron
γ_p	-	Auger recombination constant for hole
ε_o	-	vacuum permittivity
E_C	-	conduction band energy level
E_V	-	valence band energy level
V	-	applied voltage
J_{max}	-	current density at maximum power
V_{max}	-	voltage at maximum power
P_{max}	-	maximum power

LIST OF APPENDICES