NUMERICAL ANALYSIS OF ONE-DIMENSIONAL PEROVSKITE SOLAR CELL USING DRIFT DIFFUSION EQUATIONS

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MASTER OF SCIENCE IN ELECTRICAL ENGINEERING

2024

Faculty of Electrical Technology and Engineering

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

Faculty of Electrical Technology and Engineering

UNIVERSITI TEKNIKAL MALAYSIA MELAKA

2024

DEDICATION

To my beloved son and my parents,

Thank you for giving all your love and support even though there are a lot of things we have been through with a lot of roller-coaster emotions along this master journey. Their prayer of them is a strength for me.

To my respective supervisors,

Thank you for the support, teaching, and knowledge that is being shared, only God can repay your kindness of yours.

ABSTRACT

Solar energy, one of the renewable energies with infinite sources all over the world apart from wind, biomass, water, and geothermal, is gaining much attention from researchers since the invention of wafer-based technology (using silicon), thin film technologies using Cadmium Telluride (CdTe) and Copper Indium Gallium Selenide (CIGS), and emerging film technologies, including perovskites solar cells. The perovskites solar cell (PSC) has been proven to possess a high-efficiency achievement. However, the instability issue in its moisture, light and temperature leads to current-voltage hysteresis, which always becomes a major concern for the perovskite solar cell under operational conditions. The situation is caused by the diffusion of mechanisms of charge transport and charge release at the interface between layers by the migration mechanism, which dominates the global electrical field. Another challenge in modelling the solar cell is to account for the dynamic physics behaviour, which requires a comprehensive model to relate all the dynamic mechanisms that can give information and insight into the perovskite solar cell. Hence, this study is carried out to identify the one-dimensional drift-diffusion equation of the n-i-p perovskite solar cell that accounts for the dynamic process of the solar cell mechanism, to solve the equation of the perovskite solar cell numerically and develop the current density against voltage (J-V) curve using the folding method, as well as to analyse the performance of perovskite solar cells. The numerical scheme used the Method of Line (MOL) procedure and Chebfun. An analysis of the efficiency of perovskite solar cell's factors based on the effect of varying thickness, doping density, diffusion coefficient, temperature, photo-generated current density, recombination current density and resistivity in steady-state conditions was studied. Findings revealed that the optimisation of thickness, diffusion coefficient, doping density level, resistivity, and recombination current density of the perovskite solar cell increased the efficiency of perovskite solar cells from 10.69% to 28.53%. The main contribution of this work is providing a reliable and flexible numerical scheme to the dynamic perovskite solar cell model that requires high and complex numerical literacy skills. The MOL is an efficient numerical technique for the conversion of partial differential equations (PDE) into ordinary differential equations (ODE) in drift-diffusion equations of the perovskite solar cell in unsteady-state conditions. The folding method can reduce the complexity of the numerical scheme by transforming the drift-diffusions equations in three types of transport layers into a set of transformed equations in one transport layer for steady-state conditions. The results of the analysis of parameter variation provide information on the idea of improving perovskite solar cell efficiency in the future.

ANALISIS BERANGKA SATU-DIMENSI SEL SURIA PEROVSKIT MENGGUNAKAN PERSAMAAN RESAPAN HANYUT

ABSTRAK

Tenaga suria ialah sejenis tenaga boleh baharu yang mudah diperoleh secara global selain daripada tenaga angin, tenaga biojisim, tenaga air, dan tenaga geoterma serta mendapat perhatian daripada para penyelidik sejak penciptaan teknologi berasakan wafer (menggunakan silicon), teknologi filem nipis yang mengunakan Kadmium Telluride (CdTE) dan Kupurum Indium Gallenium Seleneid (CIGS), tekonologi pencantuman filem nipis termasuklah sel suria perovskit. Sel suria perovskit telah terbukti mampu menyumnbang ke arah kecekapan tinggi. Walau bagaimanapun, isu ketidakstabilannya dari aspek kelembapan, pencahayaan dan suhu semasa sel suria perovskit beroperasi telah menyebabkan masalah histerisis arus-voltan yang menjadi perkara yang perlu dititikberatkan. Situasi berpunca daripada mekanisme penyerapan iaitu hasil daripada proses pengangkutan dan pembebasan cas pada permukaan lapisan semasa mekanisme migrasi berlaku, dan mendominasi gelombang eletrik global. Selain itu, masalah fizikal sel suria perovskit yang dinamik memerlukan model yang komprehensif yang boleh mengaitkan mekanisme dinamik untuk menyampaikan maklumat secara jelas mengenai sel suria perovskit. Sehubungan itu, objektif projek ini adalah untuk mengenal pasti persamaan resapan-hanyut untuk sel suria perovskit jenis n-i-p satu dimensi yang merangkumi proses yang dinamik berdasarkan mekanisme sel suria, untuk menyelesaikan persamaan model sel suria perovskit mengggunakan kaedah berangka dan menghasilkan graf ketumpatan arus dan voltan dengan menggunakan kaedah lipatan dan juga menganalisis prestasi sel suria perovskit. Skema berangka menggunakan teknik garisan dan Chebfun. Analisis terhadap faktor yang mempengaruhi kecekapan sel suria perovskit dari segi kesan perubahan ketebalan lapisan pengangkutan sel solar, ketumpatan doping, pekali resapan, suhu, ketumpatan arus yang dijana oleh cahaya, ketumpatan arus hasil daripada cantuman hole dan elektron serta rintangan telah dilakukan dalam keadaan pegun. Kajian ini mendapati bahawa dengan pengoptimuman ketebalan lapisan pengangkutan, pekali resapan, tahap ketumpatan doping, kerintangan, dan ketumpatan arus hasil daripada cantuman hole dan elektron oleh sel suria perovskit telah meningkatkan prestasi sel suria perovskit dari 10.69% kepada 28.53%. Sumbangan utama penyelidikan ini adalah menyediakan penyelesaian yang boleh dipercayai serta fleksibel menggunakan kaedah berangka terhadap model sel suria perovskit yang dinamik yang memerlukan kemahiran kaedah berangka yang tinggi dan kompleks. Teknik garisan ialah kaedah berangaka yang cekap dalam menukar persamaan pembezaan separa kepada persamaan perbezaan biasa yang terkandung dalam persamaan resapan hanyut sel suria perovskit untuk keadaan tidak pegun. Manakala kaedah kaedah lipatan mampu mengurangkan kesukaran skema numerikal yang kompleks dengan menukar persamaan resapan hanyut pada tiga jenis lapisan pengangkutan berbeza kepada satu persamaan dalam satu lapisan pengankutan dalam keadaan pegun. Hasil analalisis terhadap parameter yang bervarisi dapat memberikan informasi tentang idea untuk menambah baik kecekapan sel suria perovskit pada masa akan datang.

ACKNOWLEDGEMENT

In the Name of Allah, the Most Gracious, the Most Merciful. First and foremost, I would like to take this opportunity to express my sincere acknowledgment to Universiti Teknikal Malaysia Melaka with the fund by the Ministry of Higher Education Malaysia under the Fundamental Research Grant Scheme (FRGS), FRGS/1/2020/STG06/UTEM/02/2.

I also want to acknowledge my supervisor Dr. Rahifa Ranom, and my co-supervisor, Professor Madya Dr. Hidayat Zainuddin for guiding and teaching me while conducting the research.

In addition, I want to give acknowledgment to Professor Madya Mohd Adib Ibrahim and Associate Professor Dr. Mohd Asri Mat Teridi from Solar Energy Research Institute, Universiti Kebangsaan Malaysia (UKM) for collaboration in sharing the outcomes and suggestions regarding the perovskite solar cell.

Furthermore, I want to acknowledge Ts. Dr. Muhammad Idzdihar Idris from the Faculty of Technology Electronics Engineering and Computer Science at Universiti Teknikal Malaysia Melaka (UTeM) for sharing the information regarding the perovskite solar cell during the workshop of fabrication of solar cells.

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LIST OF ABBREVIATIONS

UTeM	-	Universiti Teknikal Malaysia Melaka
BVP	-	Boundary Value Problem
ETL	-	Electrons Transport Layer
FDA	-	Finite Difference Approximation
HOMO	-	Highest Occupied Molecular Orbital
HTL	-	Hole Transport Layer
J-V	-	Current density-voltage
LUMO	-	Lowest Unoccupied Molecular Orbital
MOL	-	Method of Line
ODE	-	Ordinary Differential Equation
PDE	-	Partial Differential Equation

LIST OF SYMBOLS

ϕ	-	Potential Difference
q	-	Elementary Charge
k	-	Boltzmann Constant
T	-	Temperature
$\epsilon_i, \varepsilon_i$	-	Permittivity
D_i	-	Diffusion Coefficient
b	-	Recombination coefficient
η	-	Efficiency
L_i, l_i	-	Thickness
t	-	Time
V	-	Voltage
J	-	Current density
G	-	Generation
N_i	-	Doping Density
R	-	Resistivity
P	-	Power
FF	-	Fill Factor
p	-	Holes
n	-	Electrons

LIST OF APPENDICES

LIST OF PUBLICATIONS

The following is the list of publications related to the work of this thesis:

R. Ranom, R. S. Bacho, and S. N. A. S. A. Jamal, 2022 “The effect of electrolyte parameter variation upon the performance of lithium iron phosphate (LiFePO4),” *Indonesian Journal of Electrical Engineering and Computer Science (IJEECS).*, vol. 28, no. 1, pp. 58–66, 2022, (SCOPUS indexed).

B.Y. Seah, R. Ranom, S. N. A. S. A. Jamal, 2021. Numerical simulation of one-dimensional solar cell model, in *Proceedings of Malaysian Technical Universities Conference on Engineering and Technology (MUCET) 2021*, pp. 425-426.

S. N. Aisyahtun Sakinah Ahmad Jamal, Rahifa Ranom, 2024. Method of line technique to solve the drift-diffusion equation for perovskite solar cell in *AIP Conference Proceeding.* 7 March 2024; vol. 2895, no. 1, pp. 020013. https://doi.org/10.1063/5.0193418. (SCOPUS indexed).

Sakinah, S.N.A., Ranom, R., Basmin, S.H. and Yao, L.J., 2024. Numerical simulation of one-dimensional perovskite solar cell model. *Bulletin of Electrical Engineering and Informatics*, vol. 13, no. 4, pp.2221-2230. https://doi.org/10.11591/eei.v13i4.6463. (SCOPUS indexed).

CHAPTER 1

INTRODUCTION

1.1 Introduction

This chapter introduces solar cells, perovskites solar cells, the instability issue of perovskites solar cells, the importance of the studies, the objectives and hypothesis to encounter perovskites solar cell issue in terms of instability of Perovskites, mechanism of the solar cell, types of the solar cell, modelling of Perovskites and numerical procedure of PSC. God created the sun and the moon for balance in the world, which contributes to the benefits for living creatures. Solar energy is among the renewable energies highly demanded to generate electricity. Sunlight is the most preferable over other renewable energies such as wind, hydro, tidal and biomass owing to its sustainability, harmless radiation, cost-effective, pollution-free and continuous sources compared to the consumption of nuclear power, which gives rise to global warming, while fossil fuels and oil will be depleted and finish if keep being used (Kabir et al., 2018; Letcher, 2018; Overland, 2019; Rabaia et al.,2021).

1.2 Motivation

Since 1970, the issue of the oil crisis during the war has motivated scientists to use renewable energy as a source to generate electricity and transportation (Overland, 2019). The evolution of solar cells started with the first-generation, second-generation and third-generation categories to improve their efficiencies and performance (Ahmadi, 2018). The first generation of solar cells uses wafer-based technologies such as Si-solar cells, the second generation utilises thin-film technologies such as CdTe and CIGS solar cells, whereas the third generation of solar cells uses emerging photovoltaic technologies such as Perovskites solar cell, DSSC, quantum dot and tandem solar cell (Dragulinescu and Dragulinescu, 2020; Kodati and Radhika, 2020; Kodati and Rao, 2020; Lin and Peng, 2021). The types of materials used in solar cells display different levels of efficiency, which rely on the process of fabrication technologies and climate changes to achieve maximum light absorption (Alarifi, 2021). Today, the application of solar photovoltaics covers indoor applications; for instance, wireless sensor nodes in automated buildings and calculators, as well as outdoor applications to generate electricity, such as traffic lights, universities, housing areas and outer space (Lee and Ebong, 2017; McMillon-Brown et al. 2021). Figure 1.1 presents an example of solar panels installed at the faculty of electrical engineering at the Universiti Teknikal Malaysia Melaka (UTeM), Melaka.

Figure 1.1 The example of solar cell application at the university

The Malaysian government has implemented a few incentive programs to encourage citizens to harness solar energy, such as Net Energy Metering (NEM), Net Energy Metering (NEM), Large Solar Scale (LSS), Supply Agreement with Renewable Energy (SARE), Self-Consumption Scheme (SELCO) and ‘Peer-to-Peer’ (P2P) for individual or commercial usage (Zainuddin et al., 2021) NEM is a program replacing the feed-in tariff mechanism that offers the same tariff for selling and buying electricity and automatically gives smart meters for registered solar energy consumers under the NEM program (Abdullah et al., 2019). All the programs benefit both parties and contribute to the economic growth of Malaysia.

Related to the benefit given by the government, the perovskite solar cell could be one of the potential panels suggested to be used in Malaysia. The efficiency of perovskite solar cell data from 2018 to 2023, was obtained from the National Renewable Energy Laboratory, (NREL) and is summarized in Figure 1.2 (Cell Efficiency Data Table 2024, 2024).

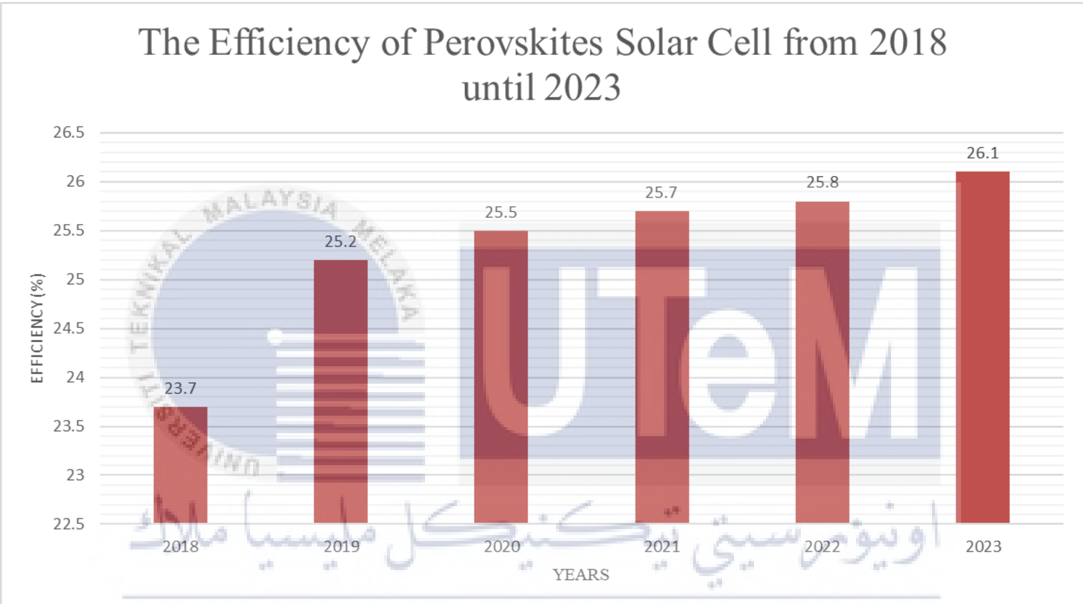

Figure 1.2 The efficiency of perovskite solar cell status from 2018 until 2023 (Cell Efficiency Data Table 2024, 2024)

Figure 1.2 shows the efficiency of perovskite solar cell status from 2018 until 2023. The efficiency of PSC is soaring from 23.7% in 2018 to 26.1% in 2023. The perovskite solar cell has advantages in cost-effectiveness, high-power conversion efficiency, high ability of light absorption, solution processability, and low cost (Ijaz et al., 2020; K. Zhang et al., 2020; Zhao and Park, 2015) besides other intrinsic properties such as tuneable bandgap, high coefficient of absorption, high ability carrier transport and mobility (Suresh Kumar and Chandra Babu Naidu, 2021). Recent progress revealed that the flexible perovskites solar cell could be used for specified applications such as smart integrated buildings, solar-powered outdoor flight, wearable PSCs as a power source to power a smartwatch, a solar-powered wearable sensor and solar-powered tents (Tang and Yan, 2021).

1.3 The Problem of Instability of Perovskite Solar Cell

Perovskite solar cells are one of the advanced technologies from dye-sensitised solar cells well known for their rapid efficiencies, low cost, and tunable bandgap. However, there is an issue related to perovskite solar cells that requires further attention. Despite the high toxicity level of the materials and short lifetime, the main problem with the perovskite solar cell is its instability issue (Q. Chen, 2020), which is affected by moisture, light, and thermal exposure in terms of intrinsic chemical and electronic properties (A. Mahapatra et al., 2020; Zhao and Park, 2015). The instability issue of the perovskite solar cell leads to hysteresis (Guo et al., 2020; A. Mahapatra et al., 2020; Miyashita et al., 2021) which is related to the structural distortion and unbalanced distribution of electrons and holes in the perovskite solar cell (W. Chen et al., 2018; Nemnes et al., 2017).

The behaviour of holes and electrons in perovskite solar cells is dynamic, resulting in the fluctuation of the current values upon the cycling of the voltage (Ravishankar et al., 2017). During the ion migration, the charge is trapped or de-trapping and accumulated at the interface of the perovskite solar cell due to diffusion mechanisms of charge transport and charge release at the interface between layers, further dominating the global electrical field depending on the carrier lifetime and concentration of mobile ions (Boldyreva et al., 2019; Chang et al., 2020; Khorramshahi and Takshi, 2019). Courtier et al. (2018) suggested tunable doping density or permittivity of each transport layer to reduce loss due to interfacial recombination for the perovskite solar cell model. This suggestion is related to the issue of describing the dynamic mechanism related to the generation, transportation and collection process in PSC.

Another related problem is identifying the best and most comprehensive model to relate all the above dynamic mechanisms that can give information and insight into the perovskite solar cell. This problem requires an expensive and complex numerical procedure to solve the evolution of charge density across three different layers: donor phase, blend phase, and acceptor phase with different properties, which requires a set of solar cell parameters that are difficult to obtain such as diffusion coefficient where radiotracer is used to extract the diffusion coefficient of mobile ions in a controlled environment (Thomas and Thankappan Aparna, 2018). The costs required to provide such a controlled and safe environment are expensive. Thus, the numerical procedure must offer high accuracy and efficiency that can simulate the whole Perovskite solar cell system. Nevertheless, the model would still face difficulty in determining numerous values of parameters for validating the model with experimental data.

1.4 Objective

The objectives of the research are:

i) To identify the drift-diffusion model of a one-dimensional perovskite solar cell.

ii) To numerically solve the equations of perovskite solar cells using the method of line technique and folding method.

iii) To analyse the performance of perovskite solar cells (J-V curve) and the effect of the thickness variations, diffusion coefficient variation, temperature variation,