INVESTIGATION OF LEAD-FREE MATERIAL FOR PEROVSKITE SOLAR CELLS

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This report is submitted in partial fulfilment of the requirements for the degree of Bachelor of Electronic Engineering with Honours

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DECLARATION

I declare that this report entitled "Investigation of Lead-free Material for Perovskite Solar Cells" is the result of my own work except for quotes as cited in the references.

Signature : ………………………………………

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Date : 23 JANUARY 2023

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 Bachelor of Electronic Engineering with Honours.

Signature : ……………………………………

Supervisor Name : TS. DR. MUHAMMAD IDZDIHAR BIN IDRIS

Date : 23 JANUARY 2023

DEDICATION

This thesis is dedicated to the people who have supported me throughout my education. Thanks for making me see this adventure through the end.

ABSTRACT

Due to the development of photovoltaic technology, it is now possible to convert sunlight into electrical energy. With high power conversion efficiency and low cost, perovskite solar cells have advanced for the generation of power in the fields of photovoltaic research. The main issues with lead-based perovskite solar cells are their poor stability and high toxicity. Investigation of environmentally safe lead-free perovskite solar cells have been studied from variety of non-toxic materials, some of which have good optoelectronic properties and can improved device performance. Simulation of tin-based perovskite solar cell is where the lead (Pb) material is substitute with tin (Sn) material, where the tin-based perovskite layer was optimized to achieve the highest efficiency. To analyse the parameters of solar cells configurations such as Power Conversion Efficiency (PCE), Fill Factor (FF), short circuit current density (Jsc) and an open circuit voltage (Voc). Finally, it is expected for the lead-free perovskite solar cells to achieve the PCE of more than 20%.

ABSTRAK

Disebabkan oleh perkembangan teknologi fotovoltaik, kini boleh menukar cahaya matahari kepada tenaga elektrik. Dengan kecekapan penukaran kuasa tinggi dan kos rendah, sel solar perovskite telah maju untuk penjanaan kuasa dalam bidang penyelidikan fotovoltaik. Isu utama dengan sel solar perovskite berasaskan plumbum adalah kestabilan yang lemah dan ketoksikan yang tinggi. Penyiasatan sel suria perovskite bebas plumbum yang selamat dari segi alam sekitar telah dikaji daripada pelbagai bahan bukan toksik, sesetengah daripadanya mempunyai sifat optoelektronik yang baik dan boleh meningkatkan prestasi peranti. Simulasi sel suria perovskit berasaskan timah adalah di mana bahan plumbum (Pb) digantikan dengan bahan timah (Sn), di mana lapisan perovskite berasaskan timah telah dioptimumkan untuk mencapai kecekapan tertinggi. Untuk menganalisis parameter konfigurasi sel suria seperti Kecekapan Penukaran Kuasa (PCE), Faktor Isi (FF), ketumpatan arus litar pintas (Jsc) dan voltan litar terbuka (Voc). Akhirnya, sel suria perovskite bebas plumbum dijangka mencapai PCE lebih daripada 20%.

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LIST OF SYMBOLS AND ABBREVIATIONS

ANOVA	:	Analysis of Variance
ETL	:	Electron Transport Layer
FF	:	Field Factor
HTL	:	Hole Transport Layer
ITO	:	Indium Tin Oxide
Jsc	:	Short Circuit Current
$MASnBr_3$	:	Methylammonium Tin Bromide
$MASnBr_3$	:	Methylammonium Tin Iodide
NiO	:	Nickel Oxide
OA	:	Orthogonal Array
PCE	:	Power Conversion Efficiency
PSCs	:	Perovskite Solar Cells
SCAPS 1D	:	Solar Cell Capacitance Simulator
SEM	:	Scanning Electron Microscope
SNR	:	Signal Noise Ratio
UV- Vis	:	Ultraviolet Visible Spectroscopy
Voc	:	Open Circuit Voltage

XRD	:	X-ray Diffraction
ZnO	::	Zinc Oxide

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CHAPTER 1

INTRODUCTION

1.1 Project Introduction

Solar cell also known as photovoltaic cell is a type of device that can converts light energy into electrical energy through photovoltaic effect. Most commonly use type of solar cells are fabricated from silicon material with the efficiency of 21%-22%. Perovskite solar cells (PSCs) is new technology that can provides simple manufacturing, highly efficient photovoltaics, and low-cost solar cell application. A new class of lead-free perovskites material is developed to solved problems regarding the issue of toxicity lead based halide perovskite. An alternative to produce a lead-free perovskite solar cell devices from variety choices of nontoxic perovskite materials for development of environmentally friendly solar cells with excellent performance and properties. The substitution metals for lead (Pb) use in perovskite solar cells with the use of tin (Sn) material to achieve the targets of this project, others material that can be used to replace the use of lead that have similar semiconducting characteristics is germanium (Ge), bismuth (Bi), and antimony (Sb). Sn- based perovskites have high optical absorption coefficients and low optical band gaps that are similar to Pb- based perovskites [1]. Metal halide perovskite general from formula ABX_3, where A is organic cation usually organic methylammonium, B is a metal cation and X is a halogen anion. Sn-based perovskites able to exhibit higher charge carrier, the highest efficiency reported for Sn-based perovskite solar cells reached up to 27.43% [2].

The simulation process was done by using device simulator, OghmaNano software where in the simulation process the experimental and theoretical data were used for simulating thin film devices. The fundamentals of photovoltaic devices will be discussed and examined. There are several important parameters that can manipulate the performance of a device such as thickness of material, bandgap energy, electron affinity etc. Therefore, an analysis needs to be done before identifying the parameters that would impact most on device characteristics. One of the most significant methods that are being used widely nowadays are known as Taguchi Method. Simulation can help in terms of more understanding on factors that can be controlled and identify appropriate process before actual implementation.

Fabricating devices can be done after investigation process by simulation, spin coating is one of the low-cost preparation methods of perovskite thin film by using depositing techniques. After fabricating, the sample need to be characterized, X-ray diffraction pattern (XRD) of the material confirms the formation of perovskite structure whereas, UV–vis absorption spectroscopy shows the absorption range of these material. Crystal formation of the perovskite is confirmed from the scanning electron microscope (SEM). Comparison of perovskite material is discussed in depth in terms of structural, optical, and electrical properties.

1.2 Problem Statement

Lead perovskites are considered for next generation photovoltaic technology, but perovskites are generally to be assume as toxic because of the lead (Pb), the exposure to perovskite can cause serious hazard on health and toxic to the environment [3]. Therefore, alternative to do a simulation of lead-free solar cells that focus on compound that have similarity in the perovskite structure and improves the performances that suitable for optoelectronic applications such as solar cell. Besides, the traditional solar cell such as silicon required higher cost for manufacturing compared to perovskite material. Other than that, the efficiency of the tin-based solar cells still needs an improvement due to instability.

1.3 Objectives

The objectives of this project are:

i. To simulate a methylammonium tin bromide and methylammonium tin iodide, lead-free material for perovskite layer using OghmaNano software simulator.

ii. To analyze the output parameters such as power conversion efficiency (PCE), fill factor (FF), short circuit current (Isc), open circuit voltage (Voc) in perovskite layer.

iii. To optimize the input parameters, thickness of material used and temperature in lead-free perovskite solar cells using Taguchi Method.

1.4 Project Scope

This project aims to construct a lead-free perovskite solar cells model by simulation and optimization process.

1.4.1 Simulation using OghmaNano Software

To design and simulate a lead-free perovskite solar cell models that can achieve the maximum efficiency using OghmaNano simulator, a computer-based software tool for simulating and to analyzing the photovoltaic (PV) devices. This software can be used to design several types of devices using different input parameters. This simulation study will provide useful information to make perovskite solar cells and appropriately choose parameters and attain the high efficiency. The design of lead-free perovskite solar cell model configuration contains of metal oxide material: zinc oxide (ZnO) as the Electron Transport Layer (ETL) and nickel oxide (NiO) as the Hole Transport Layer (HTL).

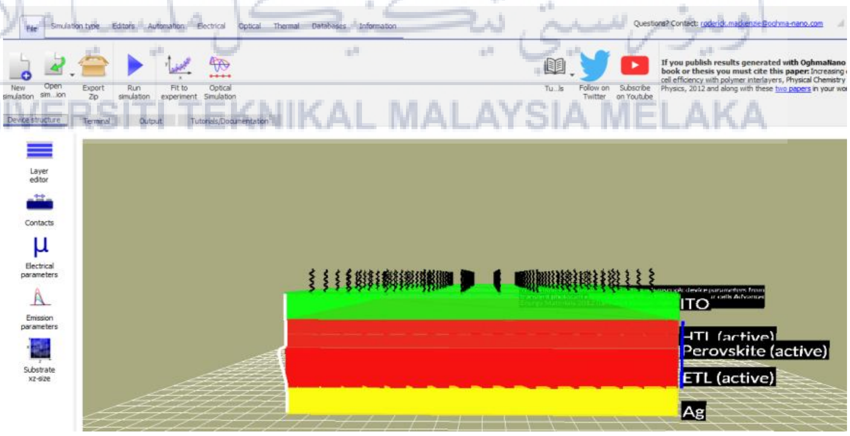

Figure 1.1: Simulation of solar cell using OghmaNano

1.4.2 Analyze and Comparison of Lead-free Perovskite Solar Cells

From collected data, optimization of various input parameters such as the thickness of layer, temperature and electrical parameters of material will be implemented by using appropriate analysis techniques. To make comparison in between two types of tin halides material used at perovskite layer and observe the devices performance after optimization and analyze the output parameters.

1.5 Significant and Importance

The importance of this project is to improve the performance of solar devices, to develop a low cost and easy to fabricate solar cell devices that meet the market's demand for greater functionality and performance. Furthermore, to manufactured perovskite with thinner layer compared to the traditional solar cell. Therefore, this project can help to achieved Sustainable Development Goals 7 which is to ensure access to affordable, reliable, sustainable, and modern energy for all.

It is also essential to conduct a statistical analysis such as Taguchi Method that can identify the parameters affecting the most on devices performances. Taguchi method is being used to ensure the devices produced are in the acceptable quality range [4].

1.6 Summary of Work

In the first chapter, explanation about the problem statement, objectives, and scope of work that will be done to complete the project. For the next part in the project, it will focus on the gathering information to understand the concept and process of the project. Most of the information is obtained from articles and journals. The research was continued with running several experiments of simulation with different parameters after the initial design of device structure was done by using

OghmaNano software. Finally, the results were analyzed and optimized by using appropriate statistical method.

1.7 Thesis Outline

This thesis consists of five chapters. The first chapter provide an introduction about the project tittle for readers. This includes the problem statement, objectives, scope of work and summary. For second chapter, it consists of literature review, theory and information about lead-free perovskite solar cells, simulation, statistical analysis, and another relevant research.

The method studied from passed research will be conducted in this project and later will be discussed in detail. The project flow will be explained from the beginning of data collection until acceptable results is obtained. Two types of lead-free material for simulation, which is methylammonium tin bromide ($MASnBr_3$) and methylammonium tin iodide ($MASnI_3$). Next, the explanation for optimization of lead-free perovskite solar cells efficiency.

In Chapter 4, the summary of results obtained from the simulation of the solar cell devices using OghmaNano software. The data and result will be analyzed and optimized by using suitable method. Analysis for power conversion efficiency (PCE), fill factor (FF), short circuit current (Jsc) and open circuit voltage (Voc) will be discussed.

Lastly, in Chapter 5 is the conclusion and suggestions for the project improvement. The results from analysis with objectives of the project will be compared to determine the achievements of this project.

CHAPTER 2

LITERATURE REVIEW

This chapter contains the research results from a previous study that is relevant to this project. These studies also serve as the primary source of information, with the theoretical, methodology, and interpretation of the studies assisting in the support of the project's material.

2.1 Renewable Energy

Renewable energy is energy from source that will not depleted when used, this limitless energy is derived from earth’s natural resources such as wind and sunlight. To reduce the use of traditional energy that mostly relies on sources that comes from fossil fuels, the use of renewable energy is an alternative to reduce the dependence on imported fuels and reduce the greenhouse gas emissions into atmosphere for healthier environment.

Implementation of renewable energy is the key to combating climate changes, this is due to renewable energy do not emit carbon dioxide or any other greenhouse gases that causing rise in temperature and contribute to global warming. Wind and solar are the fastest growing renewable sources in the United States [5].

2.2 Solar Cell

Solar cell is a photovoltaic cell that can produce electricity by photovoltaic effect and in a form of p-n junction diode. Solar cell is a photoelectric cell which a device that can change it electrical characteristics such as current, voltage and resistance when being exposed to light. The first modern solar cell made of silicon wafers was invented by Russel Ohl [6]. When light reaches the p-n junction of semiconductor material, light energy or photons with sufficient energy will create electron -hole pairs and generate electrical power. The most used material for photovoltaic solar cells is in the form of silicon that can be categorized into different classes. First generation solar cell that are produced on silicon wafers is the oldest and popular technology due to the high-power efficiencies, but this type of solar cell suffered from high fabrication and installation costs. For second generation solar cells is thin film solar cells that required less material usage as compared to the first-generation solar cell that resulting in low production cost and can cause the devices to have low-power efficiency. Third generation solar cell is a new technology approaches to achieve high-efficiency of photovoltaics (PVs) while maintaining low production cost and enhance the electrical performance in solar cells [7], the technologies involves such as dye- sensitized solar cell (DSSC), perovskite solar cells (PSC) and hybrid organic solar cell.

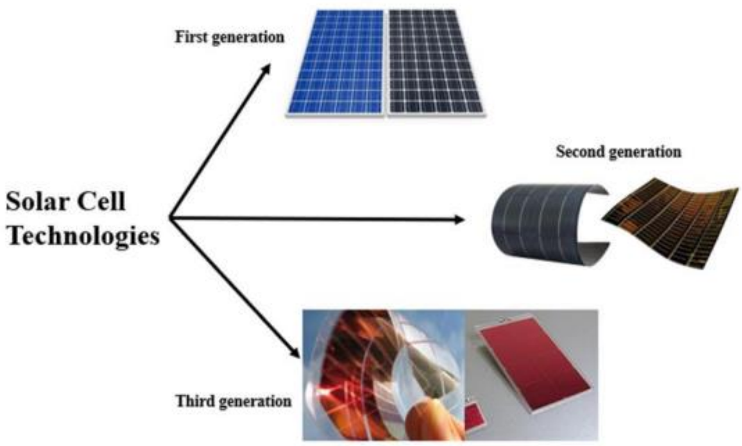

Figure 2.1: Photovoltaic cell generation

2.3 Lead-free Perovskite

Silicon-based cells have been used for industrial uses for many years due to their high solar-to-power conversion efficiency. Research shows that silicon solar cells reliability is only 12% to 17.5% for every power conversion efficiency [8]. In comparison, perovskites solar cells are much cheaper to manufactured than silicon based solar cell, this led to new research technology and design for photovoltaic hybrid (organic inorganic) materials as the primary material for perovskite solar cell production.

The efficiency of perovskites solar cells has been increased through years from 3.8 % in 2009 to 22.7% in 2017 [8]. Perovskite solar cells made of lead have the efficiency up to 20% but this lead-based material has low lifetime period due too low stability and the issues of high toxicity material that can affect the environment. According to researchers at Brown University and the University of Nebraska-Lincoln (UNL), the use of lead- free perovskite solar cells can improve the stability while removing the need for hazardous elements such as lead [9]. Other types of material that can replace the used of lead-based material is with the substitution of materials such as tin, titanium, and bismuth. Important components to construct a standard perovskite based structure are the gold electrode, hole transport layer, organic-inorganic hybrid perovskite as absorption layer, electron transport layer and glass transport electrode [9].

2.3.1 Tin (Sn) Based Perovskite

Methylammonium tin halide, CH3NH3SnX3 (X = I, Br, Cl) perovskite is one contender that has emerged from the group of lead-free perovskites [10]. This substance has a straight band gap and a high absorption coefficient comparable to lead perovskites. Methylammonium tin halides ($MASnX_3$) have more optimal band gap which is 1.2 to 1.4 eV compared to Methylammonium lead halides ($MAPbX_3$) 1.6 to 1.8 eV [11]. The limitation of using Sn based perovskites is the oxidation from Sn^{2+} to Sn^{4+} in the presence of air. Perovskite material that are affected by environmentally factors such as temperature, light, oxygen, and moisture can lead to fast degradation of device performance due to instability [12]. The stability of Sn based perovskite can be increase by reducing the chances of oxidation.

2.4 Inverted Solar Cell

Conventional structures of perovskite solar cells (n-i-p structure) have experience fast development and has reached efficiency for over 20%. Recent developments of perovskite solar cells with inverted structure (p-i-n structure) has progress in the device performance and stability [13]. Mainly, the low performance of inverted structure of perovskite solar cells are associated with the reduced current extraction and non-radiative recombination losses that limit the device photovoltage and fill factor [14]. Development to overcome this limitation including interface and bulk passivation of traps that can led to improvement of device performance due to increase of open-circuit voltage (Voc).

2.5 Current-Voltage (I-V) Measurement

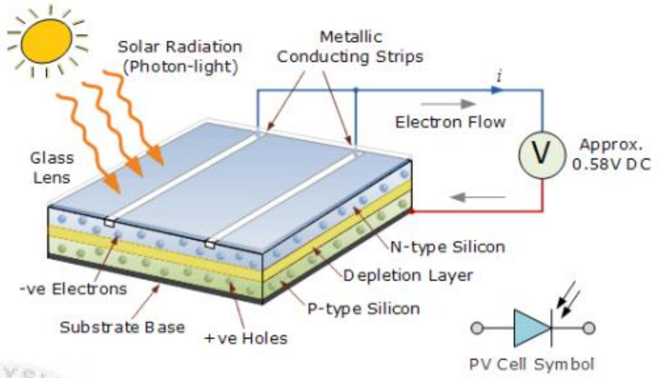

Figure 2.2: Construction of a solar Cell

Solar cell is a semiconductor p-n junction device. The formation of p-n junction by combining p-type and n-type semiconductor material. The excess electrons at n-type will diffuse to the p-type and vice versa. Movement of electron and hole resulting in an electric field and forming a depletion region. When solar cell illuminates with sunlight, photon energy that are greater than the band gap will be absorbed by the cell and generate an electron-hole pair. The common solar cell or photovoltaic device has negative and positive contact, where p-n junction of semiconductor is formed and current can flow from positive to the negative terminal. This is the basic working principle applied in solar cell, each material has its own band gap level [15]. Solar cell I-V curve is the superposition on the I-V curve of solar cell diode in absence and presence of light. Various parameters can be obtained such as short circuit current (Jsc), open circuit voltage (Voc), fill factor (FF) and efficiency, these parameters determine the performance of solar cell. Jsc is current flow in the solar cell when the solar cell is short circuit. Voc is the maximum voltage obtained by the solar cell that occurs at zero current. Fill factor is a parameter where the interval of Voc and Jsc, that can determine the maximum power produces in solar cell. The efficiency of a solar cell can be used to make comparison on the performance with others type of solar device. The efficiency defined the ratio energy output to input energy.

2.6 Simulation of Solar Cells

Device modelling of lead-free perovskite has been implemented to investigate the effects amphoteric defect and interface defects states on the photovoltaic parameters of lead-free perovskite solar cell using Solar Cell Capacitance Simulator (SCAPS-1D) [16]. The simulation is to observe the influences of few parameters in the electron transport layer. The optimization parameters of methylammonium tin bromide solar cells achieved the efficiency of 21.66%. The simulation provides for a better understanding about the behavior of optical properties in any solar cell. Simulation of lead-free tin-based perovskite as the absorber layer with two transport layers. The configuration for the device structure is FTO/TiO_2/$CH_3NH_3SnBr_3$/NiO. Observation for Voc, Jsc, FF and efficiency can be done when amphoteric defect on solar parameters were influenced. Investigation on the metal work function of different materials with different bandgap level.

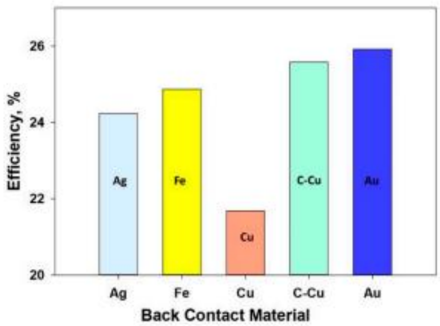

Figure 2.3: Solar cell efficiency with different back contact metal

2.7 Taguchi Method

To determine the optimal processing parameters, this journal aims to do research on the practical use of Taguchi method in the optimization of processing parameter. Optimization approaches is to enhance the efficiency of the optimization process [16]. To improve the design and performance of Dye Solar Cell (DSC), practical use of Taguchi method by simulation showed that the thickness of material and other parameters that contribute to the efficiency. There are lots of problems that can be addressed in DSC such as low efficiency. Optimization of the solar cell by using Taguchi method shows that efficiency of solar cell can be increases by utilizing the optimized parameters in designing the devices [17].

2.8 Previous Work

Tables below shows the comparison of previous work based on journal and articles that have been studied about perovskite solar cells such as the deposition method, type of material use and thickness for perovskite layer.

Table 2.1: Comparison of previous work

Author	**Tittle**	**Finding**
A. Hima, A. Khechekhouch, I. Kemerchou , N. Lakhdar , B. Benhaoua , F. Rogti , I. Telli , A. Saadoun5	GPVDM simulation of layer thickness effect on power conversion efficiency of CH3NH3PbI3 based planar heterojunction solar cell [18].	• Use GPVDM software. • To study the effect of parameters on the PCE. • Thickness of layer can improve the efficiency, from 9.96% to 12.9%
Amrit Kumar Mishra, R.K. Shukla	Electrical and optical simulation of typical perovskite solar cell by GPVDM software [19].	• Use GPVDM software for simulation of different types of lead perovskite. • Enhancement in PCE by changing the thickness of layer. • Active layer is varied in range of 100nm to 900nm. • The maximum efficiency of 5.6% obtained at 200nm thickness.
Faisal Baig, Yousaf Hameed Khattak, Bernabe´ Mari´,	Efficiency Enhancement of CH3NH3SnI3 Solar	• Simulations using SCAPS-1D software • To analyze the PCE, FF, Voc and Jsc. PCE of 18.71% when absorber layer

Saira Beg, Abrar Ahmed, And Khurram Khan	Cells by Device Modeling [12]	thickness of 500nm with doping concentration of $1x10^{16}$ cm^{-3} • Increase in defect density will limit the thickness of absorber layer.
Saquib Ahmed, Jon Shaffer, Jalen Harris, Michael Pham, Abishai Daniel, Shaestagir Chowdhury, Aboubakr Ali, Sankha Banerjee	Simulation Studies of Non-toxic Tin-based Perovskites: Critical Insights into Solar Performance Kinetics through Comparison with Standard Lead-based Devices [20].	• Simulations using GPVDM software • Comparison between tin-based and lead-based perovskite • Tin-based perovskite efficiency is at 21.3%, for lead- based perovskite is 23.4%
Kassahun Lewetegn Damena	Investigation of Organic Solar Cell at different Active Layer Thickness and Suns using GPVDM [21]	• Simulation of device model at different active layer width and different light intensity. • J-V characteristics are affected by active layer thickness and different light intensity • Optimization for each layer
Abdelkader HIMA, Nacereddine Lakhdar, Boubaker Benhaoua, Achour Saadoune, Imad Kemerchou, Fatiha Rogti	An optimized perovskite solar cell designs for high conversion efficiency [22]	• Thickness layer of different material are modified. • The maximum PCE of 18.16% for lead material, and 9.56% for lead-free material. Lead perovskite has better electrical performances

Yasodharan R, Senthilkumar A P, Mohankumar P, Ajayan J	Effects of layer thickness on Power Conversion Efficiency in Perovskite solar cell: A numerical simulation approach [23]	• The efficiency of simulation increases to 14.5%. • The resistance is varied at different series level. • The layer configuration assumed in this simulation is Glass/ FTO/ Tio2/Perovskite/Spiro/Silver
Mahmoud N Zidan, Tawfik Ismail, and Irene S Fahim	Effect of thickness and temperature on flexible organic P3HT:PCBM solar cell performance [24]	• Simulation using GPVDM software. • Range of operating temperature are from 10 °C to 40 °C • Highest PCE of .3.4%
Manish Kumar a , Abhishek Raj , Arvind Kumar, Avneesh Anshul	An optimized lead-free formamidinium Sn-based perovskite solar cell design for high power conversion efficiency by SCAPS simulation [25].	• Simulation using SCAPS 1D software. • Absorber layer of formamidinium tin iodide. • Optimization of absorber layer, ETL, HTL, defect density, doping concentration, carriers capture cross section and interfacial defects. • Power conversion efficiency improved to 19.08%

CHAPTER 3

METHODOLOGY

This chapter will explain the project methodology and flow of the project. The explanation for simulation process and steps to construct a lead-free perovskite solar cell using OghmaNano software. Next, the methodology on statistical approach by Taguchi Method will be discussed.

3.1 Methodology

The process of simulation for the lead-free perovskite solar cells has been carried out for this project using OghmaNano software. This process consists of studying about the parameters that were required for the simulation based on different type of material and to obtain the highest efficiency of material being used. The data obtained will later be compared to the actual data and theoretical data. The process of simulation is shown in Figure 3.1. Few research based on different journals has been studied to know on how to do a statistical analysis technique for optimization. As shown in Figure 3.4 and Figure 3.5 are the process flow using analysis of variance (ANOVA) and the process flow of optimization by using Taguchi method.

3.2 Simulation Process

The simulations conducted is to study the effects of different temperature and thickness of each layer on solar devices. The thickness and temperature are varied in range to observe the PCE, Jsc, Voc and fill factor using two different types of lead-free perovskite material.

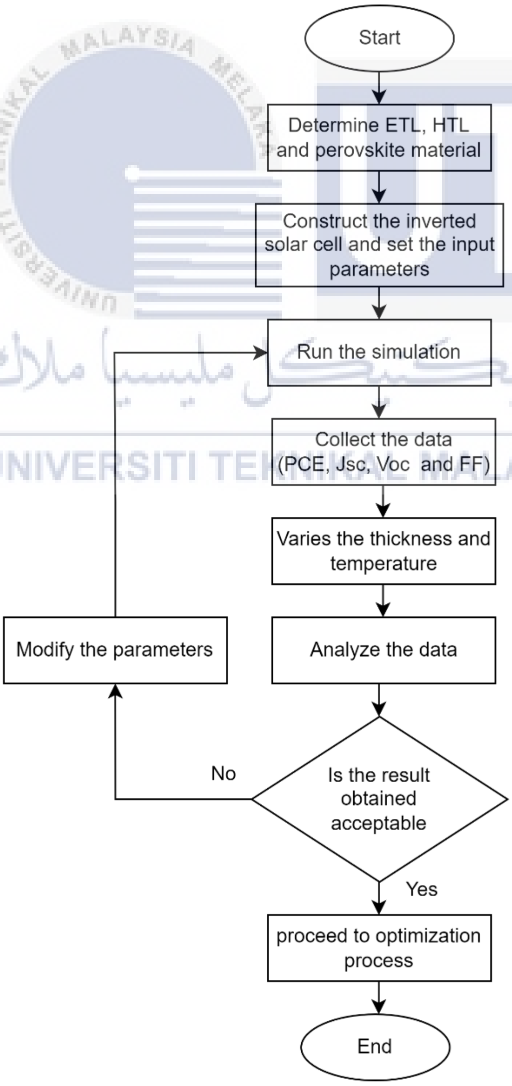

Figure 3.1: Lead-free perovskite solar cell simulation process

3.2.1 Device Structure

Before starting the simulation process for solar cells using OghmaNano software, first need to find the electrical parameters and default thickness for each type of material used. In Figure 3.2 and Figure 3.3 shown the structure of solar cell devices with two different type of lead-free perovskite layer which are $MASnBr_3$ and $MASnI_3$. The layer configuration for both simulations is ITO/ HTL/ lead-free perovskite/ ETL/ silver, where the material used for HTL is NiO and material used for ETL is ZnO. The device structure constructed in inverted layer.

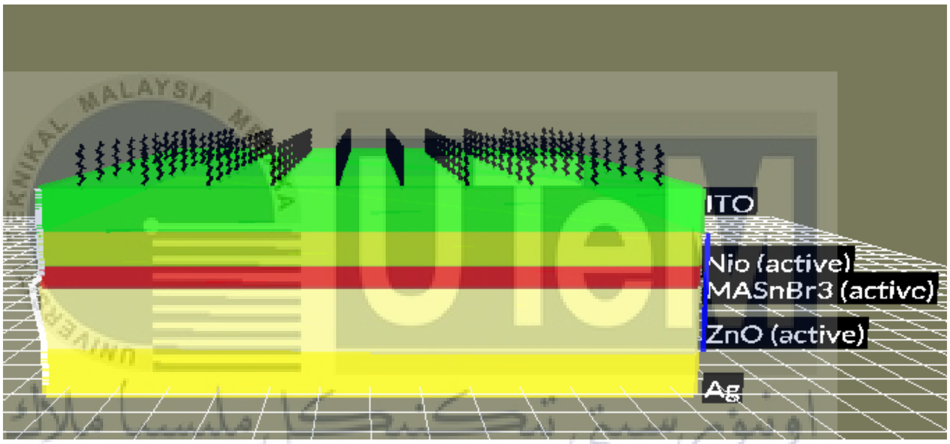

Figure 3.2: Planar heterojunction architecture of $MASnBr_3$

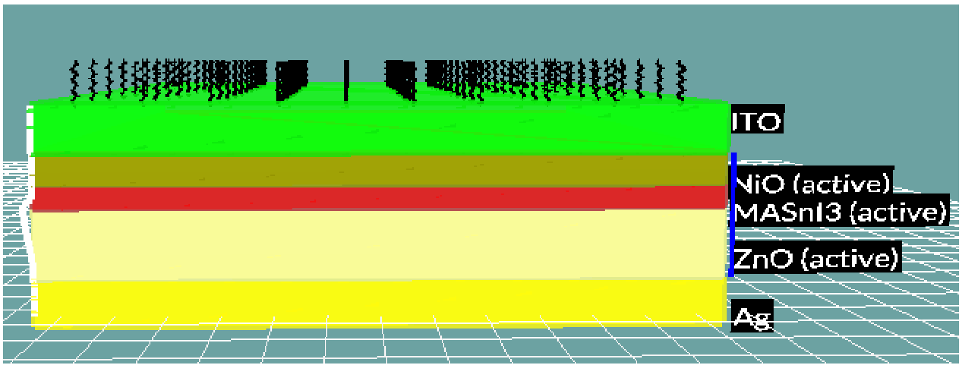

Figure 3.3: Planar heterojunction architecture of $MASnI_3$

3.2.2 Device Simulation Parameters

The initial parameters shown in Table 3.1 were chosen from theoretical and practical source [2][16]. The electrical parameters at ITO glass, HTL, ETL, lead-free perovskite layer and metal layer were fixed for each simulation.

Table 3.1: Parameters for device modelling

Material Properties	NiO	ZnO	$MASnBr_3$	$MASnI_3$
Thickness, d (nm)	50	1.6	50	50
Bandgap, Eg (eV)	3.6	3.37	1.3	1.3
Electron affinity, x (eV)	1.8	4	4.17	4.2
Dielectric Permittivity, ε (relative)	11.7	9	10	10
CB effective density of states, NC (cm^{-3})	2.5×10^{20}	2×10^{18}	2.2×10^{18}	1×10^{18}
VB effective density of states, NV (cm^{-3})	2.5×10^{20}	1.8×10^{19}	1.8×10^{18}	1×10^{18}
Electron thermal velocity, Vc (cm/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
Hole thermal velocity, Vh (cm/s)	1×10^{7}	1×10^{7}	1×10^{7}	1×10^{7}
Electron mobility, µe (cm2 /Vs)	2.8	25	1.6	1.6
Hole mobility, µp (cm2 /Vs)	2.8	25	1.6	1.6
Density of donor, ND (cm^{-3})	NA	1.5×10^{17}	NA	NA
Density of acceptor, NA (cm^{-3})	1×10^{19}	NA	1×10^{13}	3.2×10^{15}

3.2.3 Thickness of Layer and Temperature of Solar Devices

The thickness of each material layer from the solar cell is varied in the range of 50nm to 200nm for simulation and analysis. Next, the temperature range is set between 300 Kelvin to 500 Kelvin. The electrical parameters of each material layer were fixed for every simulation to obtained accurate data.

In all simulation, the default temperature was set at 300 Kelvin. The default thickness for each layer is determined to obtain the initial output data and later to observed and analyzed the output data. The output data are collected in table and a graph is constructed based on the output data for each solar cells to make analysis and comparison.

Table 3.2: Default thickness of each layer

Material Layer	Default Thickness (nm)
ITO	100
NiO (HTL)	50
$MASnBr_3$	70
$MASnI_3$	70
ZnO (ETL)	130
Ag	100

3.3 Optimization Process

Optimization method used in the simulation is to fix the parameters used and to modify one by one until a parameter that gives maximal PCE value is obtained [18].

3.3.1 Analysis Process of Default Parameters

Make an analysis to identify the thickness that can gives maximal value of PCE for each layer of perovskite solar cell using default thickness in Table 3.3.

To find the thickness that can give the maximal PCE for perovskite layer, first the thickness value of nickel oxide layer (HTL) was fixed at 50nm and 130 nm for zinc oxide layer (ETL). Next, the thickness value for perovskite layer is varied from 50nm until 200nm and the output data of perovskite layer thickness on PCE is recorded.

The procedure is repeated to find the thickness that can give the maximal PCE value for nickel oxide layer (ETL) zinc oxide layer (ETL). All the data from the effect of layer thickness on PCE is recorded for observation.

For the temperature, the simulation process is conducted in the range of 300 Kelvin to 500 Kelvin on solar cell with default value of thickness. From the simulation, the maximal PCE value can be identified.

From default thickness and temperature, an analysis can be made to find the maximal PCE value for optimization process using Taguchi method.

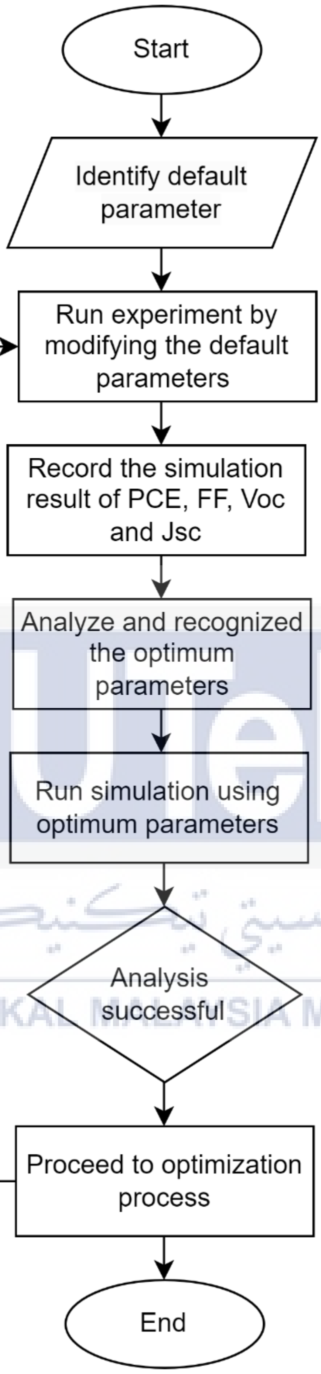

Figure 3.4: Flowchart of analysis process

3.3.2 Taguchi Method

To design a lead-free perovskite solar cell, it requires an optimization approach to obtain the optimum efficiency for third generation solar technology. Taguchi method emphasizes on designing and performing experiment that allow investigation the variance of control factors towards output responses. This method uses special orthogonal arrays to study all possible factors in designing process with minimum number of experiments. Figure 3.5 shows the sequence flow in implementing Taguchi method for the control factors.

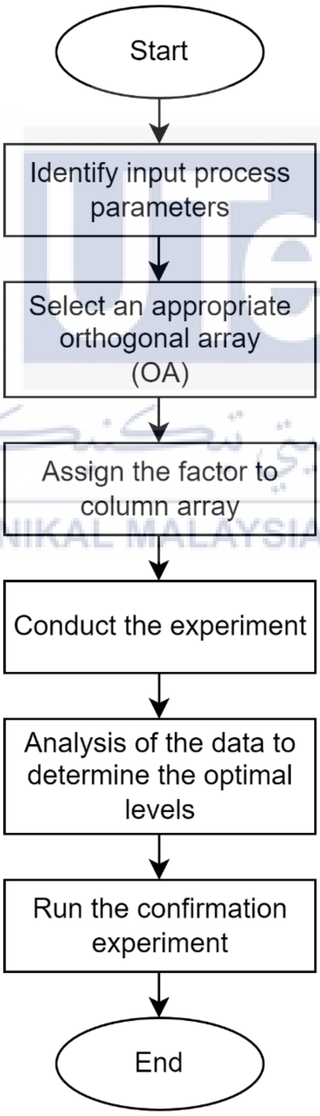

Figure 3.5: Flowchart of Taguchi method

3.3.3 Control Factors

The main control factors that were choose for optimization in designing solar cells are thickness layer of perovskite, nickel oxide, zinc oxide, and temperature of solar cell. To identify whether these parameters give the most impact on the solar cell performances, Taguchi method will be implemented. Table 3.3 shows the control factors that has been choose for optimization and represented by symbol A, B, C and D.

Table 3.3: Control factors for optimization

Symbol	Control Factors	Units
A	Thickness $MASnBr_3$ / $MASnI_3$	nm
B	Thickness of Nickel Oxide	nm
C	Thickness of Zinc Oxide	nm
D	Temperature of perovskite	Kelvin

3.3.4 Selection of Orthogonal Array

The selection of an orthogonal array (OA) depends on the total degrees of freedom of the parameters. In this project, an L_9 orthogonal array were used. The experimental layout for the control factors using L_9 are shown in Table 3.4.

Table 3.4: Experimental layout using L_9 orthogonal array

Exp. No	**Control Factors**				**S/N ratio**
	A	B	C	D	**η (dB)**
1	1	1	1	1	η_1
2	1	2	2	2	η_2
3	1	3	3	3	η_3
4	2	1	2	3	η_4
5	2	2	3	1	η_5
6	2	3	1	2	η_6
7	3	1	3	2	η_7
8	3	2	1	3	η_8
9	3	3	2	1	η_9

For the two types of lead-free perovskite solar cells, the L_9 orthogonal array is implemented to study the effect of four control factors which were varied into three levels. The experiment was conducted to obtained data that will be observed with the signal noise ratio calculated.

CHAPTER 4

RESULTS AND DISCUSSION

This chapter includes all results related to this project and project implementation. The optimization of four input parameters with three levels using L_9 orthogonal array Taguchi modelling will be discussed. The experiment is carried out using OghmaNano simulator. From simulation, four important output parameters which are power conversion efficiency, fill factor, open circuit voltage and short circuit current will be observed.

4.1 Result

From the default input parameters, an analysis has been implemented to obtain the input parameters value that can be used for optimization. The parameters that have been analyzed and optimized in this project are thickness layer of material and temperature of solar cells. Comparison between two types of lead-free perovskite solar cells in terms of efficiency after optimized.

4.2 Analysis of Parameters

Table 4.1 until 4.7 shows the output parameters for each type of solar cells after analysis using default input parameters. The thickness of nickel oxide (HTL), zinc oxide (ETL), and perovskite material was varied in range of 50nm to 200nm, the temperature was varied in range of 300 Kelvin to 500 Kelvin.

4.2.1 Methylammonium Tin Bromide

The input parameters obtained from the analysis for every layer of methylammonium tin bromide solar cells are 50nm for NiO, 50nm for $MASnBr_3$, 160nm for ZnO while the temperature is 350K.

The power conversion efficiency obtained by simulation using optimum parameters from analysis is 22.88%. Table 4.1 until Table 4.4 shows the output parameters after analyzed.

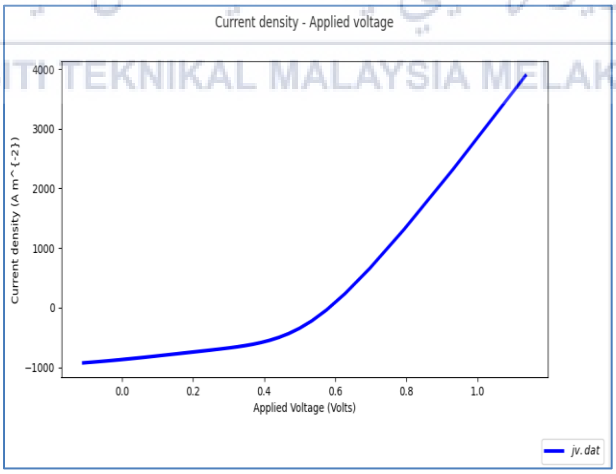

Figure 4.1: J-V characteristics for $MASnBr_3$

Table 4.1: Thickness of the $MASnBr_3$

Thickness $MASnBr_3$ (nm)	PCE (%)	Isc (mA/cm2)	FF (a.u)	Voc (V)
50	12.52	4.01	0.56	0.56
60	11.62	3.69	0.54	0.56
70	9.95	3.4	0.53	0.55
80	4.83	1.51	0.61	0.52
90	5.1	1.3	0.73	0.54
100	4.79	1.23	0.73	0.54
110	4.48	1.16	0.73	0.53
120	4.84	1.27	0.72	0.53
130	4	1.07	0.72	0.52
140	3.75	1.01	0.72	0.52
150	3.5	9.55	0.71	0.51
160	3.3	9.15	0.71	0.51
170	3.07	8.61	0.7	0.51
180	3.13	8.9	0.7	0.5
190	2.65	7.66	0.7	0.5
200	2.73	8.03	0.68	0.5

Table 4.2: Thickness of nickel oxide

Thickness NiO (nm)	PCE (%)	Isc (mA/cm2)	FF (a.u)	Voc (V)
50	9.95	3.4	0.53	0.55
60	5.48	1.38	0.73	0.54
70	5.1	1.3	0.72	0.54
80	4.81	1.2	0.72	0.54
90	4.48	1.16	0.72	0.53
100	4.21	1.1	0.72	0.53
110	4.02	1.07	0.72	0.52
120	3.74	1.01	0.72	0.52
130	3.52	9.6	0.71	0.51
140	3.51	9.6	0.71	0.51
150	3.08	8.67	0.7	0.51
160	3.13	8.9	0.7	0.5

170	2.67	7.72	0.69	0.5
180	2.73	8.03	0.68	0.49
190	2.51	7.51	0.68	0.49
200	2.21	7.13	0.64	0.48

Table 4.3: Thickness of zinc oxide

Thickness ZnO (nm)	**PCE (%)**	**Isc (mA/cm2)**	**FF (a.u)**	**Voc (V)**
50	0.33	7.52	0.77	0.52
60	0.89	2.25	0.76	0.52
70	1.36	3.4	0.76	0.53
80	1.64	4.14	0.76	0.53
90	1.85	4.66	0.76	0.53
100	2.43	6.12	0.75	0.53
110	3.04	7.63	0.75	0.53
120	7.25	2.3	0.58	0.54
130	9.45	3.4	0.53	0.55
140	10.04	3.58	0.51	0.55
150	16.09	6.09	0.47	0.57
160	16.99	6.54	0.56	0.57
170	12.55	4.95	0.46	0.55
180	13.98	5.45	0.46	0.56
190	14.43	5.61	0.46	0.56
200	14.38	5.52	0.46	0.56

Table 4.4: Temperature of $MASnBr_3$ solar cell

Temperature (K)	PCE (%)	Isc (mA/cm2)	FF (a.u)	Voc (V)
300	9.95	3.4	0.53	0.55
350	10.34	3.41	0.62	0.49
400	9.13	3.41	0.62	0.44
450	7.68	3.43	0.58	0.38
500	5.94	3.44	0.53	0.32

4.2.2 Methylammonium Tin Iodide

The input parameters obtained from the analysis for every layer of methylammonium tin iodide solar cells are 50nm for NiO, 50nm for $MASnI_3$, 180nm for ZnO while the temperature is 300K.

The power conversion efficiency obtained by simulation using the optimum parameters from analysis is 24.7%. Table 4.5 until Table 4.8 shows the output parameters after analyzed.

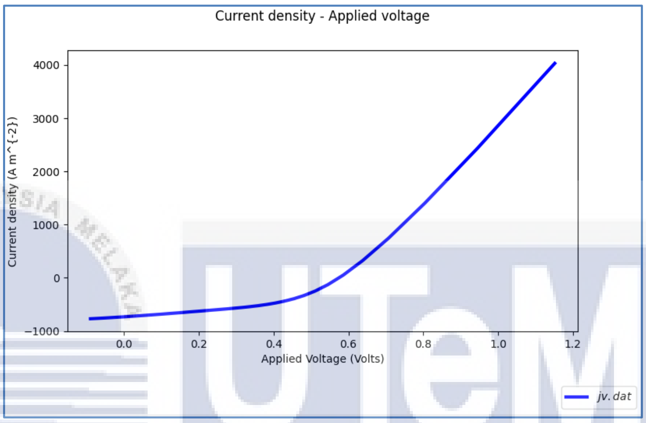

Figure 4.2: J-V characteristics for $MASnI_3$

Table 4.5: Thickness of MASnI3

Thickness MASnI3 (nm)	PCE (%)	Isc (mA/cm2)	FF (a.u)	Voc (V)
50	14.13	3.59	0.66	0.59
60	12.92	3.34	0.66	0.59
70	11.82	3.1	0.65	0.58
80	5.38	1.4	0.69	0.55
90	5.14	1.19	0.76	0.57
100	4.85	1.13	0.76	0.57
110	4.57	1.08	0.75	0.56
120	4.92	1.16	0.75	0.56
130	4.14	9.92	0.75	0.56
140	3.91	9.43	0.75	0.55
150	3.68	8.96	0.75	0.55

160	3.5	8.62	0.75	0.55
170	3.28	8.15	0.74	0.54
180	3.36	8.39	0.74	0.54
190	2.9	7.31	0.74	0.53
200	3.01	7.62	0.74	0.53

Table 4.6: Thickness of nickel oxide

Thickness NiO (nm)	PCE (%)	Isc (mA/cm2)	FF (a.u)	Voc (V)
50	11.82	3.1	0.65	0.58
60	5.48	1.26	0.75	0.58
70	5.14	1.19	0.76	0.57
80	4.87	1.14	0.76	0.57
90	4.51	1.08	0.75	0.56
100	4.34	1.03	0.75	0.56
110	4.16	9.96	0.74	0.56
120	3.93	9.48	0.75	0.55
130	3.7	9.01	0.75	0.55
140	3.73	9.13	0.75	0.55
150	3.31	8.2	0.74	0.54
160	3.36	8.37	0.74	0.54
170	2.88	7.26	0.74	0.53
180	3	7.59	0.74	0.53
190	3.03	7.7	0.74	0.53
200	2.6	6.73	0.74	0.53

Table 4.7: Thickness of zinc oxide

Thickness ZnO (nm)	PCE (%)	Isc (mA/cm2)	FF (a.u)	Voc (V)
50	0.77	3.13	0.77	0.54
60	1.26	3.03	0.77	0.54
70	1.57	3.8	0.77	0.55
80	1.77	4.03	0.77	0.55
90	2.39	5.54	0.77	0.56
100	2.55	5.92	0.77	0.56
110	5.86	1.31	0.76	0.58
120	8.83	2.26	0.67	0.58
130	11.82	3.1	0.65	0.58
140	12.49	3.35	0.64	0.58
150	20.06	5.74	0.58	0.6
160	21.57	6.37	0.56	0.6
170	16.51	4.86	0.58	0.59
180	22.67	7.15	0.53	0.6
190	21.67	6.66	0.54	o.6
200	21.94	6.96	0.53	0.6

Table 4.8: Temperature of $MASnI_3$ solar cell

Temperature (K)0.58	PCE (%)	Isc (mA/cm2)	FF (a.u)	Voc (V)
300	11.82	3.1	0.65	0.58
350	11.03	3.09	0.66	0.53
400	9.62	3.1	0.65	0.47
450	7.91	3.11	0.61	0.41
500	6.04	3.11	0.56	0.35

4.3 Performance Based on Simulation

From simulation, the observation for the lead-free material for perovskite layer shows that $MASnI_3$. has better power conversion efficiency compared to $MASnBr_3$. the highest value for PCE.

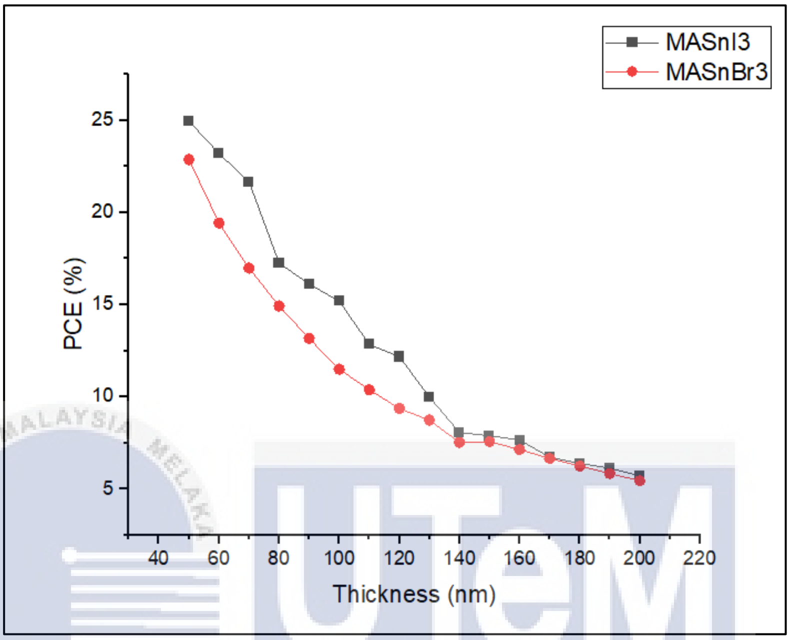

Figure 4.3: Thickness vs PCE for lead-free material

The input parameter that has been analyzed, will be optimized using Taguchi method to obtain the optimum thickness and temperature value for designing the solar cells. The optimized value will be compared with the analyzed value in terms of efficiency of the solar devices.

Table 4.9: PCE value before optimization

Lead-free Material	PCE (%)
$MASnI_3$.	24.7
$MASnBr_3$.	22.88

4.4 Optimization Using Taguchi L_9 (3^4)

Table 4.10 and Table 4.11 shows the control factors of input parameters and their appropriate levels for the experiment for both lead-free solar cells. For L_9 (3^4) Orthogonal Array it will have a total number of nine experiments. From analyzed input parameter, three variables value from each control factors were chosen for the experiment.

Table 4.10: Control factors and their levels of $MASnBr_3$ solar cell

Symbol	Control Factors	Units	Level 1	Level 2	Level 3
A	Thickness of $MASnBr_3$	nm	50	60	70
B	Thickness of Nickel Oxide	nm	50	60	70
C	Thickness of Zinc Oxide	nm	150	160	170
D	Temperature of Perovskite	K	300	350	400

Table 4.11: Control factors and their levels of $MASnI_3$ solar cell

Symbol	Control Factors	Units	Level 1	Level 2	Level 3
A	Thickness of $MASnI_3$	nm	50	60	70
B	Thickness of Nickel Oxide	nm	50	60	70
C	Thickness of Zinc Oxide	nm	170	180	190
D	Temperature of Perovskite	K	300	350	400

4.4.1 L_9 (3^4) Orthogonal Array

From nine experiment, each experiment was run using OghmaNano software for four times with different bandgap level as noise factors. The noise factor chosen is bandgap level at HTL that give minimal differences at the output data. Different in bandgap level will varies the PCE output value after simulation at each experiment. The noise factors are varied for two levels to obtain four readings for every row of experiment. The values of noise factors at different levels are shown in Table 4.14.

Table 4.12: Experimental table for $MASnBr_3$

Expt. No.	Thickness of MASnBr3, A	Thickness of Nickel Oxide, B	Thickness of Zinc Oxide, C	Temperature of Perovskite, D
1	50	50	150	300
2	50	60	160	350
3	50	70	170	400
4	60	50	160	400
5	60	60	170	300
6	60	70	150	350
7	70	50	170	350
8	70	60	150	400
9	70	70	180	300

Table 4.13: Experimental table for $MASnI_3$

Expt. No.	Thickness of MASnI3, A	Thickness of Nickel Oxide, B	Thickness of Zinc Oxide, C	Temperature of Perovskite, D
1	50	50	170	300
2	50	60	180	350
3	50	70	190	400
4	60	50	180	400
5	60	60	190	300
6	60	70	170	350
7	70	50	190	350
8	70	60	170	400
9	70	70	180	300

Table 4.14: Bandgap as noise factors

Noise Factor	Units	Level 1	Level 2
Bandgap Nickel Oxide	eV	1.1	1.2
Bandgap Nickel Oxide	eV	1.3	1.4

4.4.2 Taguchi Method Analysis

Nine different experiments for lead free solar cells are performed using the design parameter in the specified orthogonal array table. Several experiments are run to determine which control factor or variable that contributes the most significant effect on the output response, power conversion efficiency. Furthermore, it can also give the most recommendable value or optimum value for certain factor. There are four control factors of the solar cells that is altered for observation on the power conversion efficiency. The PCE value for each individual experiment is obtained by

OghmaNano simulator, the control factor level is varied according L9 (3^4) orthogonal array layout and the result from experiments are recorded in Table 4.14 and Table 4.15 for two types of lead-free material.

Table 4.15: PCE values for $MASnBr_3$ solar cell

Experiment number	Bandgap (eV)			
	1.1	**1.2**	**1.3**	**1.4**
1	21.78	21.81	21.8	21.79
2	23.54	23.56	23.56	23.55
3	15.01	15.03	15.03	15.02
4	21.73	21.76	21.76	21.75
5	12.69	12.69	12.69	12.69
6	17.6	17.62	17.61	17.61
7	16.09	16.1	16.1	16.09
8	16.23	16.25	16.25	16.25
9	13.16	13.17	13.17	13.16

Table 4.16: PCE values for $MASnIr_3$ solar cell

Experiment number	Bandgap (eV)			
	1.1	**1.2**	**1.3**	**1.4**
1	21.78	21.81	21.8	21.79
2	23.54	23.56	23.56	23.55
3	15.01	15.03	15.03	15.02
4	21.73	21.76	21.76	21.75
5	12.69	12.69	12.69	12.69
6	17.6	17.62	17.61	17.61

7	16.09	16.1	16.1	16.09
8	16.23	16.25	16.25	16.25
9	13.16	13.17	13.17	13.16

4.4.3 Signal to Noise Analysis

After nine experiments of L9 array have been completed, the next step is to determine which control factors would give the most significant impact on the output data, PCE. Signal-to-Noise (S/N) ratio is utilized to figure out the optimal input parameters and analyze the experimental data. In this project the best efficiency to be obtained for the solar cells is above 20%. The S/N ratio is implemented to obtain thickness and temperature that can obtain the target value.

The S/N ratio obtained from Taguchi method implemented for $MASBr_3$ is 28.62 and for $MASnIr_3$ is 29.35. The effect of each input parameter on the S/N ratio at each level will be separated out because the experimental design is orthogonal. The S/N ratio for each of the control factor is shown.

The overall mean SNR for nine set of experiment is computed. From Table 4.18 the highest levels for each control factors are selected, the new level for $MASnBr_3$ is Level 1 for control factor A, B, and C, Level 2 for control factor D. From Table 4.19 the new level for $MASnI_3$ is Level 1 for control factor A, B and D, Level 3 for control factor C. From the S/N result it can be concluded that the optimization for $MASnBr_3$ is in the predicted range, meanwhile for $MASnIr_3$ the S/N result is approximately closed to the predicted range and the optimization is acceptable, refers to Table 4.17.

Table 4.17: S/N ratio obtained from the Taguchi

Solar Cells	S/N ratio	Range of S/N ratio
$MASBr_3$	28.62	28.83 - 28.67
$MASnIr_3$	29.35	30.97 - 30.80

Table 4.18: S/N response to the control factor for $MASnBr_3$

Control Factors	Levels		
	1	2	3
Thickness of $MASnBr_3$	26.53	24.58	23.58
Thickness of Nickel Oxide	26.50	24.57	23.61
Thickness of Zinc Oxide	25.92	25.53	23.25
Temperature of Perovskite	24.36	25.50	24.83

Table 4.19:S /N response to the control factor for $MASnI_3$

Control Factors	Levels		
	1	2	3
Thickness of $MASnI_3$	27.91	25.74	24.78
Thickness of Nickel Oxide	27.88	25.72	24.82
Thickness of Zinc Oxide	25.10	26.09	27.23
Temperature of Perovskite	26.88	26.29	25.26

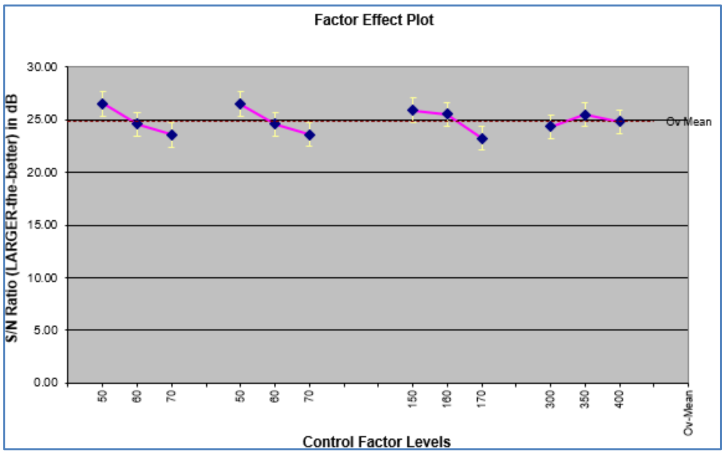

Figure 4.4: Control factor effect plot $MASnBr_3$

From Figure 4.4 above shows a graph that display the control factors parameters. At control factor A, B, and C level 1 was chosen but for control factor D, level 2 was chosen because it has the highest S/N ratio.

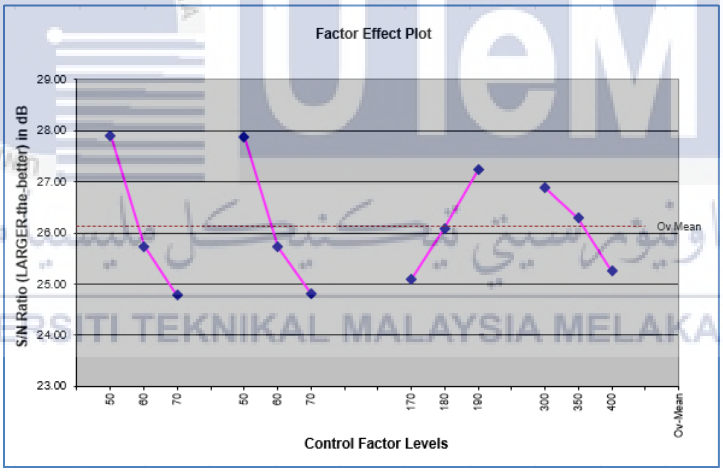

Figure 4.5: Control factor effect plot $MASnI_3$

From Figure 4.5 above shows a graph that display the control factors parameters. At control factor A, B, and D level 1 was chosen but for control factor C, level 3 was chosen because it has the highest S/N ratio.

4.5 Comparison Before and After Optimization.

From optimization of two types of perovskite solar cells which are $MASnBr_3$ and $MASnI_3$, the efficiency obtained has been improved. The efficiency from the simulation with different noise factor of the two levels will be calculated to obtain the average value. From the optimized result, $MASnI_3$ have higher efficiency which is 29.33% compared to $MASnBr_3$ at 26.98%.

Table 4.20: Optimized result of $MASnI_3$ and $MASnBr_3$,

Perovskite Solar Cells	Before Optimization	After Optimization
$MASnI_3$	24.7%	29.33%
$MASnBr_3$	22.88%	26.98%

CHAPTER 5

CONCLUSION AND FUTURE WORKS

This chapter analyzed the project, and it was finished with recommendations for future enhancements. From the result obtained, it has been determined the achievement of this project.

5.1 Conclusion

In conclusion, this project presents the expansion of low-cost perovskite solar cells and the use of non-toxic materials. Through research, investigation to design a lead-free perovskite solar cell that substitute the use of lead material with tin material. Methylammonium tin bromide and methylammonium tin iodide are two types of material use as absorber layer in the solar cells for further investigation of the device performance. To find the parameters that would give the optimum impact on the device performance, an optimization method was implemented. Through this research project, Taguchi Method was implemented to do the statistical analysis from the various parameters that can affect the solar cells performance. Furthermore, the observation was conducted using a computer simulation tools, known as OghmaNano. From analysis, the efficiency of solar cells performances has been improved after optimization. Based on optimization, the highest efficiency of 29.33% has been achieved for NiO/$MASnI_3$/ZnO solar cell and 26.98% has been achieved for NiO/ $MASnBr_3$/ZnO solar cell. This project demonstrates a low-cost and non-toxic material, tin-based perovskite solar cell is a good candidate to be implement in the photovoltaic technology. To sum up, the objectives of this project have been achieved which is to do simulation of methylammonium tin-based perovskite layer, to analyze the parameters of solar cells such as the power conversion efficiency and to optimize the thickness and temperature of material used in lead-free perovskite solar cells by using Taguchi method.

5.2 Future Works

For future work, some of the improvements that can be made for lead-free perovskite solar are by optimizing others input parameters for further study and investigation. Moreover, the performance of lead-free perovskite solar cell can be compared by using different type of material of tin-halides material for the absorber layers, and varies the material used at ETL and HTL. Finally, the investigation can be implemented by using other type of simulation software for thin film photovoltaic device known as SCAPS-1D.

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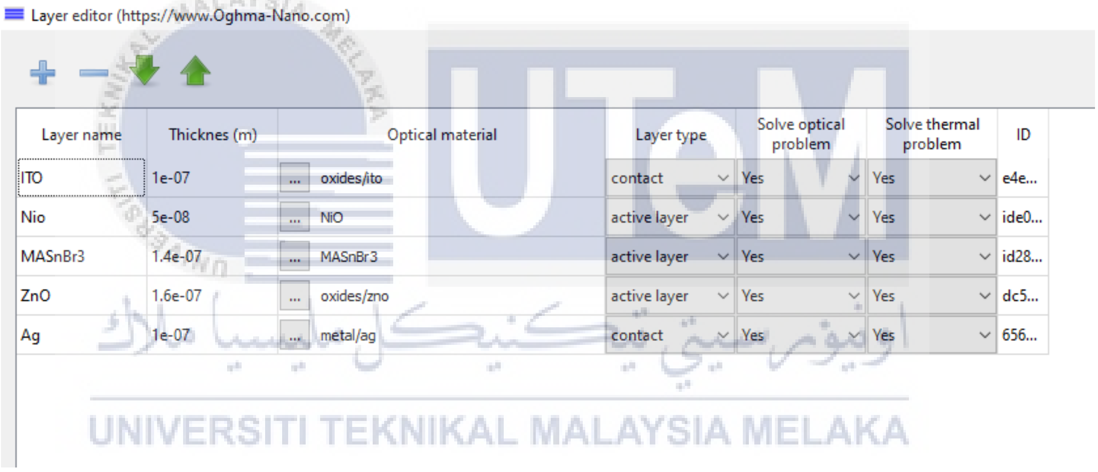
APPENDICES

Appendix A

Layer Editor in OghmaNano Simulator



Layer name	Thicknes (m)	Optical material	Layer type	Solve optical problem	Solve thermal problem	ID
ITO	1e-07	oxides/ito	contact	Yes	Yes	e4e...
Nio	5e-08	NiO	active layer	Yes	Yes	ide0...
MASnBr3	1.4e-07	MASnBr3	active layer	Yes	Yes	id28...
ZnO	1.6e-07	oxides/zno	active layer	Yes	Yes	dc5...
Ag	1e-07	metal/ag	contact	Yes	Yes	656...

Appendix B

L_9 (3^4) Orthogonal Array Taguchi Method $MASnBr_3$

Type 'NEW' levels as 1,2 or 3

L9 ASSIGNMENT	Control Factor Names	Level 1	Level 2	Level 3	SELECT	LevelName	Opt Level	% Factor Effects	Contribution of SELECTed Level to S/N Ratio (in dB)	DOMINANT or Significant or neutral/negligible	"F" after Pooling
Column 1	ickness of MASnBr3, A	50	60	70	1	50	50	33	1.64	D O M I N A N T	6.91
Column 2	kness of Nickel Oxide,	50	60	70	1	50	50	32	1.60	D O M I N A N T	7
Column 3	ckness of Zinc Oxide,	150	160	170	2	160	150	30	0.63	D O M I N A N T	6
Column 4	perature of Perovskite	300	350	400	2	-	-	5	0.00	neutral/negligible-	-
								Ov-Mean	24.90		
					28.8			S/N Ratio	28.77		
				31.03		26.50		"+-" error in dB	2.27		
	See the 'RESULTS' here			3.56E+01	to	2.11E+01		Material Removal Rate Range Center Value	2.74E+01		

Appendix C

L_9 (3^4) Orthogonal Array Taguchi Method $MASnI_3$

Type 'NEW' levels as 1,2 or 3

L9 ASSIGNMENT	Control Factor Names	Level 1	Level 2	Level 3	SELECT	LevelName	Opt Level	% Factor Effects	Contribution of SELECTed Level to S/N Ratio (in dB)	DOMINANT or Significant or neutral/negligible	"F" after Pooling
Column 1	hickness of MASnI3, A	50	60	70	1	50	50	37	1.76	D O M I N A N T	7692.31
Column 2	kness of Nickel Oxide,	50	60	70	1	50	50	36	1.74	D O M I N A N T	7421
Column 3	ckness of Zinc Oxide,	170	180	190	3	190	190	17	1.09	D O M I N A N T	3401
Column 4	perature of Perovskite	300	350	400	2	350	300	10	0.15	SIGNIFICANT	2017
								Ov-Mean	26.14		
					30.9			S/N Ratio	30.88		
				30.97		30.80		"+-" error in dB	0.08		
	See the 'RESULTS' here			3.53E+01	to	3.47E+01		Material Removal Rate Range Center Value	3.50E+01		