

Investigation of Nickel Oxide / Perovskite Interfacial in Inverted Perovskite Solar Cell

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**INVESTIGATION OF NICKEL OXIDE / PEROVSKITE
INTERFACIAL IN INVERTED PEROVSKITE SOLAR CELL**

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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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APPROVAL

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DEDICATION

I dedicate this thesis to my beloved parents, Mr. Chee Kong Wing and Mrs. Ng Guat Wan, my supervisor, Dr. Zul Atfyi Fauzan bin Mohammed Napiah, and co-supervisor, Dr. Muhammad Idzdihar bin Idris, as well as all my friends, seniors, and colleagues for their moral support, cooperation, encouragement, and understanding throughout my educational pursuit. Thank you very much.

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ABSTRACT

Inverted perovskite solar cells (IPSC) have gotten a lot of interest in recent years because of their consistent operational stability, reduced hysteresis, and low fabrication procedure. Among the materials used in p-type semiconductor, NiOx is the most widely applied as the hole transport layer (HTL) because the organic HTL has poor stability and complicated doping process. However, NiOx has some drawbacks, which are low conductivity and unsatisfactory interface contact with perovskite. In this project, the work is divided into two sections. The first section was simulation of IPSC, and the second section was the deposition and characterization of NiOx/MAPbI3 layer. For the first section, the focus of this project was on simulating NiOx as HTL in IPSC using the GPVDM software. The simulated results were evaluated by extracting the important parameters such as power conversion efficiency (PCE), short circuit current density (Jsc), open circuit voltage (Voc) and fill factor on different variation of layers. A complete modelling device structure of ITO/NiOx/MAPbI3/C60/BCP/Ag was successfully simulated with better PCE, which is 18.227% compared to previous work, which is 17.57%. For the second section, the project was focused to characterize the NiOx/MAPbI3, which is synthesized by sol-gel method. Then, the deposited layers were characterized by UV-Vis, SEM and XRD.

It was found that the annealed NiOx/MAPbI3 has improved the performance and stability, resulting in a good stability compared with non-anneal NiOx/MAPbI3. From these findings, the ITO/NiOx/MAPbI3/C60/BCP/Ag in IPSC has a potential for the development of IPSC with higher PCE.



ABSTRAK

Sel suria perovskit tersongsang (IPSC) telah mendapat perhatian sejak beberapa tahun ini kerana kestabilan operasi yang konsisten, histeresis yang berkurangan dan prosedur pembikinan yang rendah. Antara bahan yang digunakan dalam semikonduktor jenis-p, NiOx adalah yang paling banyak digunakan sebagai lapisan pengangkutan lubang (HTL) kerana HTL organik mempunyai kestabilan yang lemah dan proses doping yang rumit. Walau bagaimanapun, NiOx mempunyai beberapa kelemahan, iaitu kekonduksian rendah dan hubungan antara muka yang tidak memuaskan dengan perovskit. Projek ini dibahagikan kepada dua bahagian. Bahagian pertama adalah simulasi IPSC, dan bahagian kedua ialah pemendapan dan pencirian lapisan NiOx/MAPbI3. Untuk bahagian pertama, tumpuan projek ini adalah untuk mensimulasikan NiOx sebagai HTL dalam IPSC menggunakan perisian GPVDM. Hasil simulasi dinilai dengan mengekstrak parameter penting seperti kecekapan penukaran kuasa (PCE), ketumpatan arus litar pintas (Jsc), voltan litar terbuka (Voc) dan faktor isian pada variasi lapisan yang berbeza. Model struktur ITO/NiOx/MAPbI3/C60/BCP/Ag yang lengkap telah berjaya disimulasikan dengan PCE yang lebih baik, iaitu 18.227% berbanding kerja sebelumnya, iaitu 17.57%. Untuk bahagian kedua, projek ini difokuskan untuk mencirikan

NiOx/MAPbI3, yang disintesis dengan kaedah sol-gel. Kemudian, lapisan yang dimendapkan dicirikan oleh UV-Vis, SEM dan XRD. Didapati bahawa penyepuhlindapan NiOx/MAPbI3 telah meningkatkan prestasi dan kestabilan yang menghasilkan jangka hayat yang lebih lama berbanding dengan NiOx/MAPbI3 tanpa penyepuhlindapan. Daripada penemuan penyiasatan ini, ITO/NiOx/MAPbI3/C60/BCP/Ag dalam IPSC mempunyai potensi untuk pembangunan IPSC dengan PCE yang lebih tinggi.



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LIST OF SYMBOLS AND ABBREVIATIONS

HTL	: Hole transport layer
NiOx	: Nickel Oxide
IPSC	: Inverted Perovskite Solar Cell
α	: Absorption coefficient
n	: Refractive index
Voc	: Open circuit voltage
Jsc	: Circuit current density
FF	: Fill factor
PCE	: Power Conversion Efficiency
PV	: Photovoltaic
ITO	: Indium Tin Oxide
FTO	: Fluorine doped Tin Oxide
ETL	: Electron transport layer
HTL	: Hole transport layer
PEDOT: PSS	: Poly (3,4-ethylenedioxythiophene) polystyrene sulfonate
PCBM	: Phenyl C-61 Butyric acid methyl ester
Rs	: High serial resistance
PSCs	: Perovskite solar cells

C_{60}	:	Fullerene
BCP	:	Bathocuproine
IPA	:	Isopropyl alcohol
KOH	:	Potassium Hydroxide
$C_4H_6NiO_4$:	Nickel (II) Acetate
MAI	:	Methylammonium iodide
PbI_2	:	Lead (II) iodide
DMSO	:	Dimethyl sulfoxide
DMF	:	Dimethylformamide



CHAPTER 1

INTRODUCTION



The project introduction is covered in this chapter. Furthermore, it emphasizes the issue of the current state of industry, which leads to the project's development. In addition, the research background, objective, problem statement and scope of work will all be covered in this chapter.

1.1 Project background

With the fast expansion of society and the economy, excessive use of fossil fuels has created significant concerns such as energy shortages, environmental harm, and global warming. Therefore, renewable energy is frequently at the top of any discussion on how the globe might mitigate the worst effects of increasing temperatures. The researchers are motivated to maximize the generation of renewable energy in order to solve climate change challenges.

According to Shahzad (2015), renewable energy is the energy which is derived from a limitless source [1]. Renewable energy is also often referred to as clean energy due to the fact that renewable energy sources like sun and wind do not create carbon dioxide or other greenhouse gases, which contribute to global warming. Figure 1.1 show the example of generic renewable energy technologies.

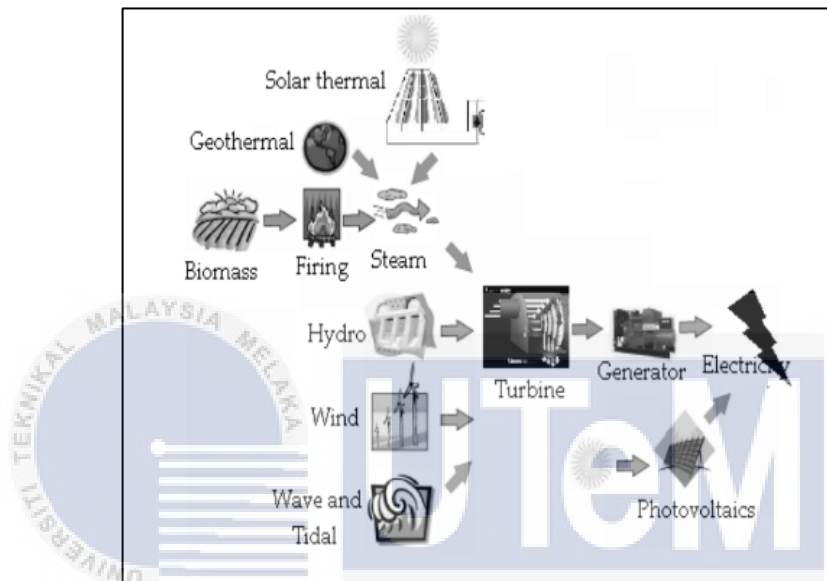


Figure 1.1: Generic renewable energy. [2]

For the planet Earth, the sun is a primary source of unlimited free energy such as solar energy. This energy may be harvested directly for use in homes, companies, schools, and hospitals using a variety of technologies. Photovoltaic cells and panels, are one of the examples of solar energy technology. PV is a type of active solar technology that was discovered in 1839 by Alexandre-Edmond Becquerel, a 19-year-old French physicist. Photovoltaic cells are semiconductor devices that convert light energy to electrical energy. There are three generations of solar PV technologies as shown in Figure 1.2.

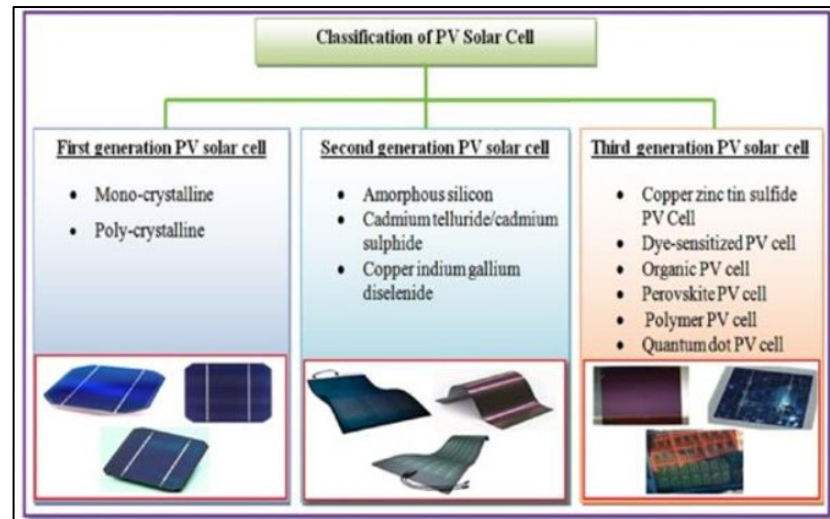


Figure 1.2: The generation of solar PV cells

The underlying technology for first-generation PV cells is silicon wafer technology. This generation includes monocrystalline and polycrystalline silicon PV cells. The solar cell of this generation is more efficient and lasts longer than other PV cells. However, the cost of production is higher, and it easily degrades at higher temperatures [1].

Thin film PV technology is used to produce second generation PV cells. In comparison to the first generation of PV cells, they are simpler and use fewer semiconductor materials. The third generation PV cells, on the other hand, are designed to manufacture high-efficiency devices using thin-film technology, as opposed to the second-generation PV cells.

Therefore, in this project focus on Inverted Perovskite Solar (IPSC), which is under the third generation of solar PV cells. IPSC is a form of solar cell that uses a perovskite-structured compound as the light-harvesting active layer, most typically a hybrid organic-inorganic lead or tin halide-based material. In inverted p-i-n perovskite

solar cells, the HTL is deposited first and the light falls first on HTL before it encounters ETL. Figure 1.3 showed the general structure of IPSC. Inverted p-i-n (substrate/HTL/perovskite/ETL/top electrode) have attracted a lot of attention due to their simple device fabrication technique, high power conversion efficiency (PCE), and low hysteresis.

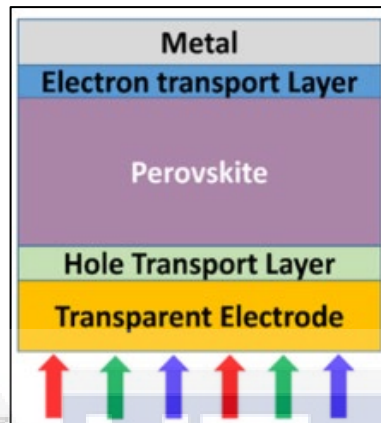


Figure 1.3: General structure of IPSC. [2]

ITO or FTO glass is commonly used as the transparent electrode. These glasses are transparent conductive substrate. The electron transport layer (ETL) is responsible for extracting electrons from the perovskite layer and preventing recombination between electrons in the ITO or FTO and holes in the perovskite layer. Perovskite is used to transport the electric charge whenever the light presents in the material. Hole transport layer (HTL) is used to covers the perovskite and collects the hole. HTL can be organic or inorganic. Lastly, metal is used as back contact.

1.2 Problem statement

Spiro-OMeTAD and PEDOT: PSS are frequently employed as HTL, but the complicated doping process and poor stability of organic HTL make them not so promising for real applications [3]. Alternatively, inorganic p-type semiconductors,

specially NiOx which is the most widely used as HTL can provide intrinsically higher stability and exhibits lower cost compared to organic polymer-based HTL.

However, NiOx has some drawbacks such as intrinsic low conductivity of NiOx [4] and unsatisfactory interface contact between NiOx and perovskite. [5]. The low conductivity of NiOx results in increased charge carrier recombination and degraded hole extraction efficiency. Moreover, the interface contact issue of the NiOx film with a perovskite layer not only influences the interfacial charge transfer but also affects perovskite crystallite growth.

Thus, in this project will simulate NiOx as HTL, then deposit the NiOx / MAPbI₃, which synthesized by sol-gel method to investigate the interface contact in NiOx on perovskite.

1.3 Project objective

The project aims to simulate nickel oxide as HTL in the inverted perovskite solar cell using GPVDM. Secondly, to evaluate the performance of simulated IPSC by extracting the important parameters such as PCE, fill factor, open-circuit voltage and short circuit photocurrent on different variation of layers in GPVDM software. Lastly, to characterize the NiOx / MAPbI₃ layer, which is synthesized by sol-gel method.

1.4 Project scope

This project scope involves the simulation of IPSC by using GPVDM software. NiOx is chosen as inorganic material as HTL. Then, the important parameters are extracted from the simulation, such as PCE is used to evaluate the efficiency of IPSC on different variation such as electrical parameters, thickness of active layers in the simulation, temperature dependency, absorption coefficient (α) and refractive index