SYNTHETIZATION AND NUMERICAL SIMULATION OF MODIFIED TiO_2 FOR EMERGING FLEXIBLE SOLAR CELL

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in fulfillment of the requirements for the degree of
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DECLARATION

I declare that this thesis entitled "Synthetization And Numerical Simulation Of Modified Tio_2 For Emerging Flexible Solar Cell" 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 : Nur Syamimi Binti Noorasid

Date : 12/04/2023

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 Master of Science in Electronic Engineering.

Signature : _____

Supervisor Name : Ts. Dr Faiz Bin Arith

Date : 12/04/2023

DEDICATION

This thesis is wholeheartedly dedicated to,

my beloved parents,

(Noorasid bin Noordin and Nur Azlinda binti Mahat),

who have been my source of inspiration and gave me strength when I thought of giving up,

who continually provide theirmoral, spiritual, emotional, and financial support.

all of my siblings,

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who shared their words of advice and encouragement to finish this study.

and all my relatives, mentor, lectuers, friends, and classmates,

Thank you for supporting me during ups and downs in finishing my master study.

ABSTRACT

Dye-Sensitized solar cells (DSSCs) have attracted massive attention due to simple and low-cost fabrication process. In addition, it also suitable to be used for indoor application. Compared to commercially available silicon-based solar cells, which require complicated equipment, higher cost and heavy, flexible DSSCs are lighter in weight, thinner, and lower fabrication cost. In conventional DSSCs structure, anatase (TiO_2) has been used as a photoanode layer. However, the TiO_2 paste required a high-temperature treatment (> 450 °C) in order to obtain crystalline structure. The high-temperature process cannot be applicable to flexible DSSCs due to the flexible polymer substrates such as polyethylene terephthalate (PET) that are vulnerable to temperature, specifically below 150 °C. This study has conducted two analyses based on experiment and simulation. Titanium dioxide (TiO_2) layer was synthesized and deposited with varying concentrations of titanium tetrapropoxide (TTIP) within the range of 0.3–0.7 M using the sol gel and spin coat method during deposition onto flexible substrates (ITO/PET). The impact of TTIP concentration on the electrical, structural, and optical properties has been studied. Ultraviolet visible (UV-Vis) spectrum demonstrates that the visible transmittance of the TiO_2 layer lies between 10% to 23% and direct band gap energy within the range from 3.08 eV to 3.49 eV. X-ray diffraction (XRD) spectrum revealed that the average size of TiO_2 crystallites ranged from 4.35 to 5.23 nm. According to the IV curve, the current density obtained within the range of 0.0011 µA to 0.0064 mA. Scanning electron microscopy (SEM) images for the concentration of 0.5 M achieved the most porosity structure than others. Thus, the layer of TiO_2 with a concentration of 0.5 M TTIP demonstrates the ideal concentration of TTIP due to it high achievement of electrical, structural and optical properties. Next, the simulation carried out in this study used solar capacitance simulator (SCAPs) software and this simulation is based on the best band gap (3.2 eV) obtained from the experiment. Simulation part consists of 3 stages where all these stages use TiO_2 as the main semiconductor material. The first stage is a simulation based on the DSSC structure. The simulation achieved efficiency of up to 8.14% by applying a 50 nm ultra-thin layer of TiO_2 with a doping concentration of 1×10^{18} cm^{-3} and the results show that the four factors (thickness, temperature, doping concentration and defect density) analyzed are highly influential in improving the efficiency of DSSC. The next stage is a simulation based on the SSDSSC structure. This simulation examined the performance of SSDSSC with a variety of ETLs, including TiO_2, ZnO, and SnO_2. The simulation result indicates that the best ETL is TiO_2, with maximum efficiency of 5.6%. The last stage is a simulation based on the structure of the PSC. In this simulation, it is found that each layer affects the performance of the PSC and proves that the optimization of each layer effectively improves the performance of the PSC. Remarkable results of the optimized structure have achieved impressive PSC efficiency 28.30% by the parametric analysis. This study will lead the path and can be a guidance to increase and enhancing the performance of generation photovoltaic cells.

SINTESIS DAN SIMULASI BERANGKA TiO_2 TERUBAH SUAI UNTUK SEL SURIA FLEKSIBEL MEMUNCUL

ABSTRAK

Sel suria Peka Pewarna (DSSC) telah menarik perhatian besar-besaran kerana proses fabrikasi yang mudah dan kos rendah. Selain itu, ia juga sesuai digunakan untuk aplikasi dalaman. Berbanding dengan sel suria berasaskan silikon yang tersedia secara komersil, yang memerlukan peralatan yang rumit, kos yang lebih tinggi dan berat, DSSC yang boleh lentur adalah lebih ringan, nipis dan kos fabrikasi yang lebih rendah. Dalam struktur DSSC konvensional, anatase TiO_2 telah digunakan sebagai lapisan fotoanod, di mana ia boleh memberikan struktur mesoporous yang sangat baik untuk penyerapan pewarna. Walau bagaimanapun, pes TiO_2 memerlukan rawatan suhu tinggi (> 450 °C) untuk mendapatkan struktur kristal. Proses suhu tinggi tidak boleh digunakan untuk DSSC boleh lentur kerana substrat polimer boleh lentur seperti polietilena tereftalat (PET) yang terdedah kepada suhu, khususnya di bawah 150 °C. Kajian ini telah menjalankan dua analisis berdasarkan simulasi dan eksperimen. Lapisan titanium dioksida (TiO_2) telah disintesis dan didepositkan dengan kepekatan titanium tetrapropoksida (TTIP) yang berbeza-beza dalam julat 0.3-0.7 M menggunakan kaedah sol gel dan spin coat semasa pemendapan ke substrat boleh lentur (ITO/PET). Kesan kepekatan TTIP terhadap sifat elektrik, struktur dan optik telah dikaji. Spektrum ultraviolet visible (UV-Visible) menunjukkan bahawa penghantaran kelihatan lapisan TiO_2 terletak antara 10% sehingga 23% dan tenaga jurang jalur terus dalam julat dari 3.08 eV kepada 3.49 eV . Spektrum pembelauan sinar-x (XRD) mendedahkan bahawa anggaran saiz purata kristal TiO_2 adalah antara 4.35 hingga 5.23 nm. Mengikut keluk IV, ketumpatan arus yang diperoleh dalam julat 0.0011 µA to 0.0064 mA. Imej SEM untuk kepekatan 0.5 M mencapai struktur keliangan yang paling banyak daripada yang lain. Oleh itu, lapisan TiO_2 dengan kepekatan 0.5 M TTIP menunjukkan penghantaran dan ketumpatan arus terbaik. Seterusnya, simulasi yang dijalankan dalam kajian ini menggunakan perisian solar capacitance simulator (SCAPs) dan simulasi ini adalah berdasarkan jurang jalur terbaik (3.2 eV) yang diperolehi daripada eksperimen. Simulasi ini terdiri daripada 3 peringkat di mana kesemua peringkat ini menggunakan TiO_2 sebagai bahan semikonduktor utama. Peringkat pertama adalah simulasi berdasarkan struktur DSSC. Simulasi mencapai kecekapan sehingga 8.14% dengan menggunakan lapisan ultra-nipis 50 nm TiO_2 dengan kepekatan doping 1×10^{18} cm^{-3} dan keputusan menunjukkan bahawa empat faktor (ketebalan, suhu, kepekatan doping dan ketumpatan kecacatan) yang dianalisis sangat berpengaruh dalam meningkatkan kecekapan DSSC. Peringkat seterusnya ialah simulasi berdasarkan struktur SSDSSC. Dalam simulasi ini, prestasi SSDSSC dengan pelbagai ETL seperti TiO_2, ZnO, dan SnO_2 telah dikaji. Simulasi ini membuktikan TiO_2 sebagai ETL memperoleh kecekapan terbaik sehingga 5.6%. Peringkat terakhir ialah simulasi berdasarkan struktur PSC. Dalam simulasi ini, didapati setiap lapisan mempengaruhi prestasi PSC dan membuktikan pengoptimuman setiap lapisan berkesan meningkatkan prestasi PSC. Keputusan luar biasa bagi struktur yang dioptimumkan telah mencapai kecekapan PSC yang mengagumkan sebanyak 28.30% dengan analisis parametrik. Kajian ini akan menerajui laluan dan boleh menjadi panduan untuk meningkatkan dan meningkatkan prestasi penjanaan sel fotovoltaik.

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AZO	-	Aluminium Zinc Oxide
AG-MP-NA	-	Acetic Acid Gelation-Mechanical Press-Ammonia Activation
Ag-NW	-	Silver Nanowire
Au	-	Gold
C_2H_3OH	-	Ethanol
$C_2H_6O_2$	-	Ethylene Glycol
CB	-	Conduction Band
CdTe	-	Cadmium telluride
CH_3COOH	-	Acetic Acid
$CH_3NH_3PbI_3$	-	Methylammonium Lead Halide
$CH_3NH_3SnI_3$	-	Methylammonium Tin Iodide
CIGS	-	Copper Indium Gallium Selenide Solar Sells
CIP	-	Cold Isostatic Compression
Cr	-	Chromium
CSCNT	-	Cup-Stacked Carbon Nanotubes
Cu	-	Copper
CuI	-	Copper (I) Iodide
CuSCN	-	Copper Thiocynate
CVD	-	Chemical Vapor Deposition
D	-	Crystallite Size
DFT	-	Density Functional Theory
DGT	-	Double-Graphene-Tubes
DSSC	-	Dye-Sensitized Solar Cell
Ec	-	Conduction Band
Eg	-	Bandgap

Ev	-	Valence Band
EPD	-	Electrophoretic Deposition
ETL	-	Electron Transport Layer
eV	-	Electron Volt
FDSSC	-	Flexible Dye-Sensitized Solar Cell
FESEM	-	Field Emission Scanning Electron Microscope
FF	-	Fill Factor
FPSC	-	Flexible Perovskite Solar Cell
FTO	-	Fluorine doped Tin Oxide
GQD	-	Graphene Quantum Dot
Gr	-	Graphene
HOMO	-	Highest Occupied Molecular Orbit
HTL	-	Hole Transport Layer
HTM	-	Hole Transport Material
Im	-	Maximum Current
IPCE	-	Incident Photon-to-Electron Conversion Efficiency
I_{SC}	-	Short Circuit Current
ITO	-	Indium Tin Oxide
IV	-	Current - Voltage
J_O	-	Saturation Current
J_{SC}	-	Current Density
K	-	Scherrer Constant
KI	-	Potassium Iodide
LSL	-	Light Scattering Layer
LUMO	-	Lowest Unoccupied Molecular Orbit
$MAPbI_3$	-	Methylammonium Lead Iodide
MD	-	Molecular Dynamic
Mo	-	Molybdenum
MoO_3	-	Molybdenum Trioxide
MPa	-	Megapascal
MWCNT	-	Multi-Wire Carbon Nanotube
N_3	-	Nitride
N719	-	Ruthenizer

N_A	-	Acceptor Density
N_C	-	Density of Charge at Conduction Band
N_{CB}	-	Effective State Density
N_D	-	Donor Density
Nt	-	Defect Density
NH_3	-	Ammonia
Ni	-	Nickel
NP	-	Nanoparticle
NR	-	Nanorod
NRP	-	Nanorods Particle
N_V	-	Density of Charge at Valence Band
NW	-	Nanowire
PCBM	-	Phenyl-C61-Butyric acid Methyl ester
PCE	-	Power Conversion Efficiency
PEDOT:PSS	-	poly(3,4-ethylenedioxythiophene) polystyrene sulphonate
PEN	-	Polyethylene naphthalate
PES	-	Polyethersulfone
PET	-	Polyethylene terephthalate
PLD	-	Pulse Laser Deposition
PSC	-	Perovskite Solar Cell
Pt	-	Platinum
PTAA	-	poly[bis(4 phenyl)(2,4,6-trimethylphenyl)amine]
PV	-	Photovoltaics
PVD	-	Physical Vapour Deposition
R_{SH}	-	Shunt Resistance
SCAPs	-	Solar cell Capacitance Simulator Software
SEM	-	Scanning Electron Microscope
SLGQD	-	Single-Layer Graphene Quantum Dots
$SnIn_2O_3$	-	Indium Tin Oxide/Polyethylene terephthalate
SnO_2	-	Tin Oxide
SRH	-	Shockley–Read–Hall
SSDSSC	-	Solid State Dye-Sensitized Solar Cell
Spiro Ometad	-	2,2’,7,7tetrakis(N,N-pdimethoxyphenylamino)-9,9’-

		pirobifluorene;
TCO	-	Transparent Conducting Oxide
TEM	-	Transmission Electron Microscopy
TG	-	Titanium Dioxide-Graphene Quantum Dot
TIO_2	-	Titanium Dioxide
TTIP	-	Titanium Isopropoxide
UV	-	Ultraviolet
UV-O_3	-	Ultraviolet–ozone
UV-Vis	-	Ultraviolet–Visible Spectroscopy
V_2O_5	-	Vanadium Pentoxide
V_B	-	Valence Band
Vm	-	Voltage Maximum
V_{OC}	-	Open Circuit Voltage
WTP	-	Water-Assisted Transfer Printing
XPS	-	X-ray photoelectron spectroscopy
XRD	-	X-ray Diffraction
$YBa_2Cu_3O_7$	-	Yttrium barium copper oxide
$Zn(NO_3)_2$	-	Zinc Nitrate
ZnO	-	Zinc Oxide
α	-	Alpha (absorption coefficient)
εr	-	Relative Permittivity
χ	-	Electron Affinity
µm	-	Micrometre
µn	-	Electron Mobility
µp	-	Hole Mobility
a,c	-	Lattice Constant
hkl	-	Miller Indices
d	-	Interplanar Spacing
$\mathcal{E}$	-	Lattice Strain
θ	-	Angle
λ	-	Radiation Wavelength

LIST OF PUBLICATIONS

1. **N. S. Noorasid**, F. Arith, A.N. Mustafa, P. Chelvanathan, MI Hossain and N. Amin, Improved performance of lead-free Perovskite solar cell incorporated with TiO_2 ETL and CuI HTL using SCAPs. *Applied Physics A: Materials Science and Processing* 129(2), 2023, pp. 1–16.(WoS Q2 IF:2.983 and Scopus Indexed)

2. **N. S. Noorasid**, F. Arith, A. Y. Firhat, A. N. Mustafa, and A. S. M.Shah, SCAPS Numerical Analysis of Solid-State Dye-Sensitized Solar Cell Utilizing Copper (I) Iodide as Hole Transport Layer, *Engineering Journal*, vol. 26, no. 2, pp. 1-10, Feb. 2022 (WoS ESCI and Scopus Indexed).

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CHAPTER 1

INTRODUCTION

1.1 Research Background

As the world is becoming more advanced in economy and technology, more energy is being consumed to keep up with the development and demand on energy boomed over past decades. Presently, the energy demands are still highly dependent on fossil fuels, natural gases and coal with percentages of 31.2%, 24.7% and 27.2% respectively (bp, 2022). However, the world will shortly come to an end of fossil fuels due to its non-renewable. Meanwhile, the wasteful use of fossil fuels actually causes irreversible environmental damage, geopolitical tensions, and tragically climate changes (Kabeyi and Olanrewaju, 2022). Our world definitely must move toward a more sustainable energy economy. Of all the available technologies to produce renewable energy, solar energy has become a hot topic in current research for replacing fossil fuels. One simple reason is that the earth receives 1.2 × 1017 W insolation or 3 × 1024 Joule energy per year from the sun and this means covering only 0.13% of the Earth's surface with solar cells with an efficiency of 10% would satisfy humanities' energy needs (Edward et al., 2019). Apart from the abundance of potentially exploitable solar energy, photovoltaic cells also have other competitive advantages such as little need for maintenance, off-grid operation and silence, which are ideal for usage in remote sites or mobile applications (Kabeyi and Olanrewaju, 2022). Currently, mankind has made use of three main ways of converting sunlight to a useable source of energy.