SIMULATION, CHARACTERIZATION AND ANALYSIS OF SILICON GERMANIUM AND POLY (TRIARYLAMINE) HETEROJUNCTION FOR PROSPECTIVE PHOTO-DEVICES

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FACULTY OF ENGINEERING
UNIVERSITI MALAYSIA SABAH
2023

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DECLARATION

I hereby declare that the material in this thesis is my own except for equations, summaries, and references, which have been duly acknowledged.

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ABSTRACT

Silicon (Si) is a common electrical and optoelectronic materials technology in the semiconductor industry. Furthermore, transparent device applications with visible to near-infrared band absorption edge shifting are sought. Germanium (Ge) is a promising material that enhances absorption and greater carrier mobility of electronic devices. Poly (triarylamine) (PTAA) in room temperature deposition scope, and as an excellent p-type conductive polymer, it has good visible band transparency. This study initially investigated the PTAA/SiGe and PTAA/Si prospective photo device performance using Solar Cell Capacitance Simulator (SCAPS) software simulation. PTAA thin films are developed using the spin coating process, and SiGe thin films are deposited by the radio frequency sputtering method. The active SiGe morphology is varied by varying the % of Ge composition in SiGe materials and deposition time. In contrast, PTAA morphology is set with a fixed number of drops and spin coating device rotational speed. The structural, compositional, and surface characterisations are performed by x-ray diffraction, scanning electron microscopy with energy dispersive x-ray spectroscopy, and atomic force microscopy, respectively. The ultraviolet-visible spectroscopy for optical and source measurement unit (SMU-2400) instruments for current density - voltage characterizations are also investigated in this study. The SCAPS simulation of 0.3 μm SiGe revealed very high current density (48.1 mA/cm^2) and the highest 8.55% photo-electrical energy conversion efficiency in contrast to similar thickness Si photovoltaic technology is revealed. $Si_{0.8}Ge_{0.2}$ has the highest 36.78 nm grain size and 52.49 μm^{-2} grain density and at 800 °C annealing temperature is achieved. Transparency analysis has shown that the $Si_{0.8}Ge_{0.2}$ deposited after 30 minutes is highly transparent for visible light in the wavelength range of 600-700 nm. The highest transparency of $Si_{0.8}Ge_{0.2}$ at 600 °C is realized at 87.87%. $Si_{0.8}Ge_{0.2}$ deposited is shown 5.19 rectifying ratio, while $Si_{0.9}Ge_{0.1}$ is 7.67. However, both $Si_{0.8}Ge_{0.2}$ and $Si_{0.9}Ge_{0.1}$ deposited on quartz substrate is revealed at 14.76 and 7.91 rectifying ratio respectively. From simulation result, PTAA/SiGe microstructure is shown preferable than PTAA/Si microstructure and experimental work $Si_{0.8}Ge_{0.2}$ is revealed more promising than $Si_{0.9}Ge_{0.1}$.

ABSTRAK

SIMULASI, PENCIRIAN, DAN ANALISIS SILIKON GERMANIUM DAN POLI (TRIARILAMIN) HETERO-SIMPANG UNTUK PERANTI FOTO PROSPEKTIF

Silikon (Si) ialah teknologi bahan elektrik dan optoelektronik dalam industri semikonduktor. Tambahan pula, pencarian peralihan sudut penyerapan jalur inframerah boleh dilihat menggunakan aplikasi peranti lutsinar. Germanium (Ge) dapat meningkatkan penyerapan dan mobiliti pembawa dalam sesebuah peranti elektronik. Poli (triarilamin) (PTAA) bersuhu rendah, dapat menghasilkan polimer yang baik, serta mempunyai kadar ketelusan cahaya yang tinggi, di mana bahan tersebut mempunyai kadar ketelusan yang baik. Kajian ini menyiasat tentang prestasi PTAA/SiGe dan PTAA/Si menggunakan simulasi perisian SCAPS. PTAA menggunakan proses salutan putaran dan SiGe menggunakan kaedah percikan frekuensi radio. Berbeza dengan morfologi, PTAA diset dengan bilangan titisan yang ditetapkan dan kelajuan salutan putaran. Pencirian struktur, optik, dan elektrik menggunakan pembelauan sinar-x, pengimbasan mikroskopi elektron dengan spektroskopi sinar-x penyebaran tenaga, dan mikroskop daya atom. Spektroskopi ternampakkan ultraviolet digunakan untuk pencirian optik manakala instrument unit ukuran sumber (SMU-2400) untuk ketumpatan arus- voltan telah dikaji dalam kajian ini. Simulasi SCAPS pada 0.3 μm SiGe menunjukkan ketumpatan arus tinggi (48.1 mA/cm^2) dan kecekapan peranti pada 8.55% menunjukkan nilai tinggi berbanding teknologi Si pada ketebalan sama. Struktur $Si_{0.8}Ge_{0.2}$ dicapai pada saiz butiran yang besar dan juga ketumpatan butiran tinggi, masing-masing 36.78 nm dan 52.49 μm^{-2} pada 800 °C. Analisis ketelusan cahaya menunjukkan $Si_{0.8}Ge_{0.2}$ yang dipercikkan selepas 30 minit sangat telus cahaya pada julat gelombang 600-700 nm. Nilai ketelusan cahaya bagi $Si_{0.8}Ge_{0.2}$ pada 600 °C adalah 87.87%. $Si_{0.8}Ge_{0.2}$ yang dimendapkan mempunyai jumlah nisbah kelurusan tinggi iaitu 5.19, manakala $Si_{0.9}Ge_{0.1}$ telah dimendapkan hanya 7.67. Namun begitu, kedua-dua $Si_{0.8}Ge_{0.2}$ and $Si_{0.9}Ge_{0.1}$ yang dimendapkan pada substrat kuarza yang mempunyai nisbah kelurusan yang tinggi, masing-masing pada 14.76 dan 7.91. Simulasi mikro-struktur PTAA/SiGe diutamakan daripada mikro-struktur PTAA/Si dan kerja uji kaji $Si_{0.8}Ge_{0.2}$ adalah lebih baik berbanding $Si_{0.9}Ge_{0.1}$.

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LIST OF SYMBOLS

α	-	Alpha
A	-	Ampere
Å	-	Angstrom
β	-	Beta
cm	-	Centimetre
A/W	-	Current per watt
°	-	Degree
°C	-	Degree Celsius
ŋ	-	Ens
ε	-	epsilon
fA	-	Farthingales
fA/cm^2	-	Farthingales per square centimetre
K	-	Kelvin
λ	-	Lambda
μm	-	Micrometre
mA/cm	-	Milliampere per centimetre
mW	-	Milliwatt
mW/cm^2	-	Milliwatt per square centimetre
nm	-	Nanometre
ln	-	Natural logarithm
Ω	-	Ohm
%	-	Percentage
Rad	-	Radian
s	-	Second
Scm^{-1}	-	Siemens per centimetre
σ	-	Sigma
Cm^2	-	Centimetre squares
$Cm^2 V^{-1}s^{-1}$	-	Centimetre squares per volt second
θ	-	Theta
2θ	-	Two thetas

Torr	-	Torricelli
V	-	Volt
W	-	Watt
Wt.%	-	Weight percent
Ωm	-	Ohm metres

LIST OF ABBREVIATIONS

AFM	-	Atomic Force Microscopy
Ag	-	Silver
Al	-	Aluminium
Ar	-	Argon
ASCII	-	American Standard Code for Information Interchange
CB	-	Conductive Band
CdTe	-	Cadmium Telluride
CdZnS	-	Cadmium Zinc Sulphide
CPC-PV	-	Compound Parabolic Concentrators- Photovoltaic
CPCs	-	Compound Parabolic Concentrators Solar
DC	-	Direct Current
EBIC	-	Electron Beam Induced Current
E_g	-	Optical Bandgap
EQE	-	External Quantum Efficiency
eV	-	Electron Volt
FDTD	-	Finite-Difference-Time-Domain
FF	-	Fill Factor
Ge	-	Germanium
GO	-	Graphene Oxide
GPVDM	-	General Purpose Solar Cell Simulator
HTL	-	Hole Transfer Layer
HTM	-	Hole Transfer Material
Hz	-	Hertz
IR	-	Infrared

IT	-	Information Technology
ITO	-	Indium Tin Oxide
Jsc	-	Short-Circuit Current
J-V	-	Current Density - Voltage
LBIC	-	Light Beam Induced Current
LiF	-	Lithium Floride
mcSi	-	Multi-Crystalline Silicon
MoS_2-QD	-	Molybdenum Disulfide – Quantum Dots
NA	-	Acceptor Density
ND	-	Donor Density
NIR	-	Near-Infrared
Pb	-	Plumbum
PC1D	-	Personal Computer One Dimension
PCE	-	Power Conversion Efficiency
PEDOT: PSS	-	Poly (3,4-ethylenedioxythiophene) polystyrene sulfonate
PTAA	-	Poly (Triarylamine)
QE	-	Quantum Efficiency
RF	-	Radio Frequency
RMS	-	Root Mean Square
rpm	-	Revolution per Minute
R_s	-	Series Resistance
R_{sh}	-	Shunt-Recombination Resistance
SCAPS	-	Solar Cell Capacitor Simulator
sccm	-	Standard Cubic Centimetre per Minute
SC	-	Solar cell

SEM EDX	-	Scanning Electron Microscopy with Energy Dispersive X-Ray Spectroscopy
Si	-	Silicon
SiGe	-	Silicon Germanium
SILVACO -TCAD	-	Silvaco Technology Computer Aided Design
Sn	-	Tin
TCAD	-	Technology Computer Aided Design
UV	-	Ultra-Violet
UV-Vis	-	Ultra-Violet Visible
UV-Vis-NIR	-	Ultra Violet-Visible-Near Infrared
VB	-	Valence Band
Vmp	-	Maximum Peak Voltage
Voc	-	Open- Circuit Voltage
wt.	-	Weight
XRD	-	X-Ray Diffraction
Zn	-	Zinc

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CHAPTER 1

INTRODUCTION

1.1 Research Background

The physical properties of hybrid inorganic-organic materials have been recognised for their impressive physical properties and ability to be used as a layer in photo devices. Photo device is one of the most well-known renewable energy sources, even though it is also one of the most expensive and inefficient due to the high manufacturing cost and technologies to make solar cells as photo device. A hybrid semiconductor device offers excellent barrier and rectifying properties (Gullu, Kilicoglu, & Turut, 2010; Concilio et al., 2014; El-Shabaan & Gaml, 2022). Photo devices should not be as expensive if specific low-cost materials are utilised, as this will strengthen the photodiode business and make it more accessible to the public. It has been over a decade since photo devices were used in the country. Photo devices will reduce electric bills, and it is beneficial for the environment. Hybrid semiconductor devices reduce energy consumption, which results in lower electricity bills. By using low-cost materials, the cost of photo devices can be reduced, making them more accessible. Hybrid semiconductor devices are more efficient and can use less energy, resulting in lower electricity bills. It helps to reduce environmental impact. Additionally, this technology can be used to produce clean energy, which reduces carbon emissions and is more sustainable.

The first photo device was invented in the mid-19th century in 1856 (Popoola, 2015; Groeneveld et al., 2022). They developed the first silicon (Si) photo device with low percentage efficiency, which has resulted in a wide range of photo device bulk materials. In time, photo devices have developed, and many researchers have attempted to increase the performance of photo devices. Si cells have become a hot