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The Effect of SiGe/PTAA Thin Film Thickness as An Active Layer for Solar Cell Application

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This paper presents the results of electrical simulations at different active thickness layers of hybrid photovoltaic devices using GPVDM software. A combination of inorganic n-type semiconductor SiGe and organic p-type semiconductor PTAA has been chosen to be simulated in this research work. The thickness of SiGe and PTAA varies from 100 nm – 500 nm and 1000 rpm – 5000 rpm. The results show that the thickness of both semiconductor affects the electrical properties. Higher current density, $J_{sc,}$ can be obtained as the thickness of SiGe increases. PTAA as an active layer had affected the value of open-circuit voltage, $V_{oc.}$ The SiGe combination with lower rpm depicted a higher value of V_{oc} than the other combinations. The FF and efficiency rate of the solar panel is also presented in this work. This research focuses on the thickness combination of both semiconductors layer on the performance of its electrical characteristics.

Keywords: GPVDM; SiGe; PTAA; current density; open circuit voltage

I. INTRODUCTION

Silicon germanium (SiGe) thin films are one of the most well-known and widely used semiconductors in the microelectronics field. These thin films are widely applied in microelectronics and photonic devices. SiGe thin films have attracted researchers due to their ability and unique characteristics such as highly dopant solubility rate, high mobility carriers, and adjustable bandgaps, making them famously used (Ezzahri *et. al.*, 2008; Lian & Lin, 2016; Pham & Fang, 2020). Unfortunately, to get a good crystallisation form of SiGe, numerous factors, such as deposition techniques, annealing temperature, and mismatch lattice among the atom of Silicon and Germanium (Shahahmadi *et. al.*, 2016; Pham & Fang, 2020). The use of organic semiconductors on SiGe affects the crystallography structures of both materials and alters the physical properties of the combined materials (Sadki *et al.*, 2020). It also increases the light trapping capabilities due to the large interface area that boosts the materials' absorption behaviour (Srairi, Djeffal & Ferhati, 2017). Therefore, by performing a simulation, selected parameters can be controlled to examine the effects of certain variables.

In this research work, simulation was conducted using General Purpose Photovoltaic Device Model (GPVDM) software. SiGe was combined with an organic polymerPoly[bis(4-phenyl)(2,4,6 trimethylphenyl) amine] (PTAA). PTAA has also shown great performance as an active layer of electronics devices (Rani *et. al.*, 2019, 2020; Yusop *et al.*, 2020).

As shown in Rani *et al.* the value of the band edge of PTAA significantly increases with increasing spin rate value which is 2.97 eV to 3.10 eV from 1000 RPM to 5000 RPM. The smaller band edge value shows a higher conductivity level, thus affecting its ability to transfer photons energy in the materials (Rani *et al.*, 2019). Yusup *et al.* mention that PTAA helps facilitate the photons' recombination rate. As the thickness of PTAA increases, the photon is absorbed in a higher rate, causing the excitons at phase to increase (Yusop *et al.*, 2020).

PTAA possesses a wide band gap and stability in ambient conditions (Miandal, Mohamad & Alias, 2016; Ghosh *et al.*,

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2020). PTAA is selected as the active layer for the simulation with a configuration of Aluminium Electrode (Al)/ SiGe-PTAA (Hetero layer)/ ITO substrate. It is anticipated that the combination of SiGe and PTAA will improve the performance of solar cells in terms of open circuit voltage (V_{oc}), current density (J_{sc}), fill factor (FF), and also the efficiency rate of the solar cells.

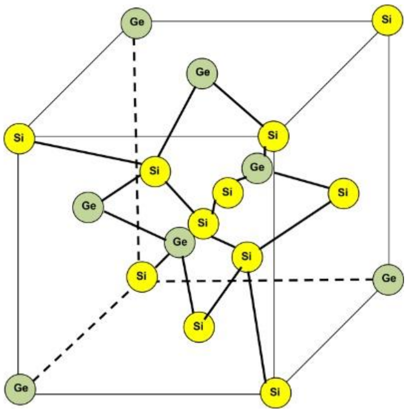

Figure 1. Chemical structure of Silicon-germanium (SiGe) (Khanna, 2017)

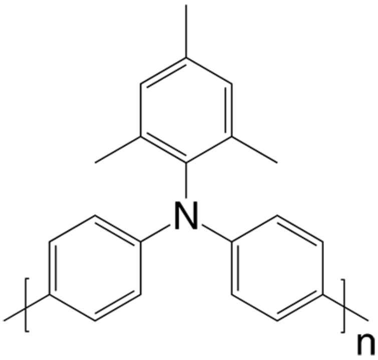

Figure 2. Chemical structure of PTAA

II. METHODOLOGY

A. Device Simulation Technique

The device simulation was done using the GPVDM software with of ITO/ SiGe-PTAA/Al device structure. The software implements the drift-diffusion equations, Poisson equations, and bipolar drift equations into the finite difference method by high power computational techniques (Kumar Mishra & Shukla, 2020; Mishra & Shukla, 2021).

$$J_p = q\,\mu_h\,p\,\nabla E_v - q\,D_p\,\nabla p \qquad (1)$$

$$\nabla \cdot J_n = q\,(R_n + T_n + \partial n_{free} / \partial t) \qquad (2)$$

$$\nabla \cdot J_p = -q\,(R_p + T_p + \partial p_{free} / \partial t) \qquad (3)$$

Nomenclature:

J_p	Hole flux density
J_p	Electron current flux density
q	Charge on an electron
μ_h	Hole mobility
p	Free hole concentration
E_v	Free hole mobility edge
D_p	Hole diffusion coefficient
R_n	Net recombination rate of electrons
R_p	Net recombination rate for holes

The simulation details and parameters used are presented in Table 1 and Table 2. The simulation was carried out by manipulating the thickness of the PTAA layer as the active layer and the thickness of SiGe film. The thickness of the PTAA layers is presented in 1000 – 5000 rpm, specifically 100 nm, 80 nm, 60 nm, 40 nm, and 20 nm.

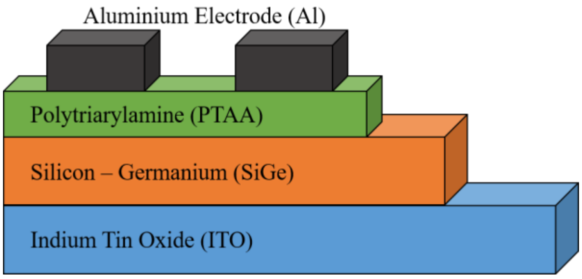

Figure 3. Solar cell device structure configuration

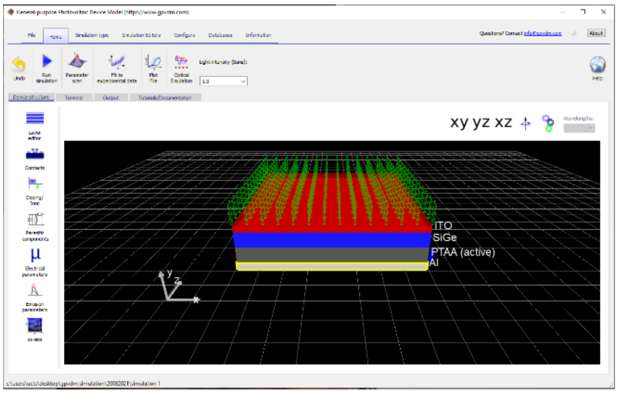

Figure 4. Graphical user interface (GUI) of GPVDM software during simulation of SiGe/PTAA solar cell

Table 1. Simulation details on the thickness of solar cells configurations

Layer name	Thickness	Layer type
Al	50 nm	Contact
SiGe	100 nm – 500 nm	n-type
PTAA	20 nm – 100 nm (5000 rpm – 1000 rpm)	p-type (Active Layer)
ITO	50 nm	Contact

Table 2. Simulation parameter for GPVDM software (MacKenzie, 2019)

Parameter	Value
Electron trap density	$3.8000e^{26}$ m^{-3} eV^{-1}
Hole trap density	1.4500 e^{25} m^{-3} eV^{-1}
Electron tail slope	0.04 eV
Hole tail slope	0.06 eV
Electron mobility	$2.48e^{-7}$ m^2 V^{-1} s^{-1}
Hole mobility	$2.48e^{-7}$ m^2 V^{-1} s^{-1}
Relative permittivity	3.8 au
Number of traps	20 bands
Free electron to trapped electron	$2.5000e^{-20}$
Trapped electron to the free hole	$1.3200e^{-22}$
Trapped hole to trapped hole	$4.6700e^{-26}$
Free hole to trapped hole	$4.8600e^{-22}$
Type of light intensity	Sun

III. RESULTS

The software was simulated for different thickness layers of SiGe and PTAA ranging from 100 – 500 nm to 1000 – 5000 rpm. As for PTAA, a higher spin speed indicates the decrease in thickness layer. The effect of active layer thickness is significant in the electrical properties of the simulated solar cell.

Figure 6 shows that the value of V_{oc} for 500 nm:5000 rpm of heterojunction SiGe/PTAA is the lowest due to the low light absorption at the thinner layer of PTAA. As the active layer decreases, it loses the ability to absorb more light and cannot transport the electron toward its hole (Chakraborty *et al.*, 2019). The combination of 100 nm:2000 rpm of SiGe/PTAA depicted the highest value of V_{oc}, which is approximately 0.5875 V. In this result, it is shown that 100 nm:1000 rpm of SiGe/PTAA is the most ideal among other simulated devices as it can maintain the value of V_{oc} without much decrement or losses of energy(voltage). The lowest V_{oc} value is 0.5251 V which is the combination of 500 nm of SiGe and 5000 rpm of PTAA.

As shown in Figure 7, the current value of density J_{sc}, decreases significantly in the device with SiGe thickness of 300 nm. This might be due to the irregular thickness ratio between the n-type and active layers. A device with 400 nm and 500 nm of SiGe thickness show an increasing value of J_{sc} due to the saturated number of Ge atom in the SiGe layer. Higher thickness generates more electron-hole pairs as the bandgap between Si and Ge gets smaller (Kadri *et al.*, 2017) and increases the recombination rate between SiGe and PTAA layer.

The simulation showed decreasing trends for FF and efficiency of the simulated solar panels. The highest FF value is 0.7716 au, which is the same combination as the highest V_{oc}. The lowest value of FF is 0.6637 au. As for the efficiency rate, the highest obtained value is 1.49% at the 1:1 ratio of SiGe and PTAA. Numerous factors affect the efficiency rate of the solar panels, and these factors affect the structure of the solar panels differently. All data are presented and tabulated in Figures 6, 7, 8, 9, and Table 3.

Figure 10 depicts the schematic band diagram of the simulated device. In this device, the ITO layer acts as the anode while Al is the cathode film. Therefore, the SiGe layer transported the holes from the anode to the PTAA layer, while the PTAA layer transported the electrons to SiGe. In a solar cell device, electrons and holes combined in the emissive layer depend on the thickness and the mobility rate charges (Zubair *et al.*, 2015). The Highest Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) levels was performed by the PTAA layer with -5.2 eV and -1.7eV, respectively, provide the direct bandgap energy of 3.5eV. The deeper HOMO level of the active layer ensures that no hole could escape to the cathode (AI layer) (Yang *et al.*, 2019). The HOMO-LUMO levels, as shown in Figure 10, were derived from the literature (Zubair *et. al.*, 2015; Khadka *et. al.*, 2017; Nehate *et. al.*, 2018; Yang *et. al.*, 2019; Fadaly *et al.*, 2020).

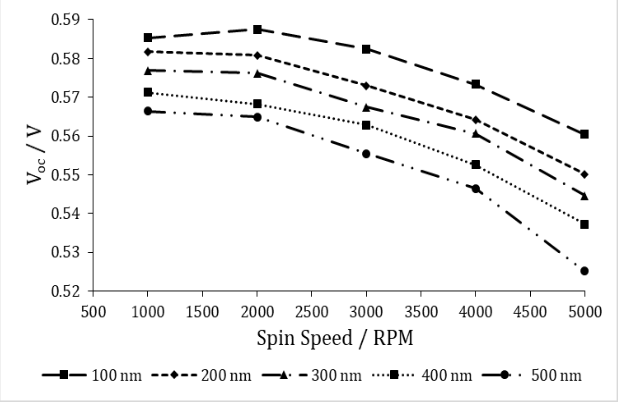

Figure 6. V_{oc} characteristic of SiGe/PTAA solar panel configuration

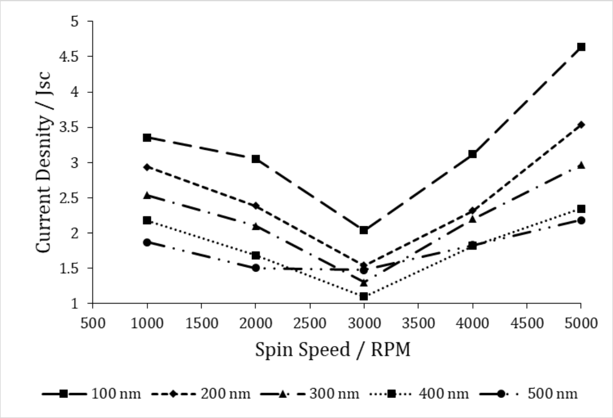

Figure 7. J_{sc} characteristic of SiGe/PTAA solar panel configuration

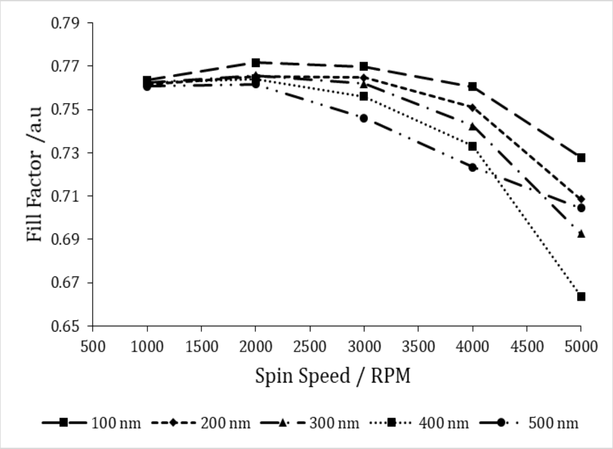

Figure 8. FF characteristic of SiGe/PTAA solar panel configuration

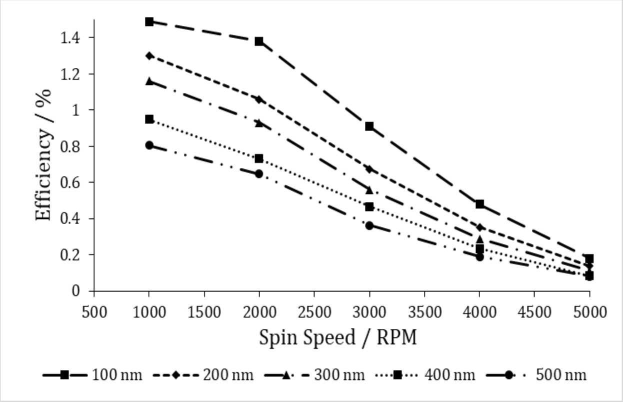

Figure 9. Efficiency rate characteristic of SiGe/PTAA solar panel configuration.

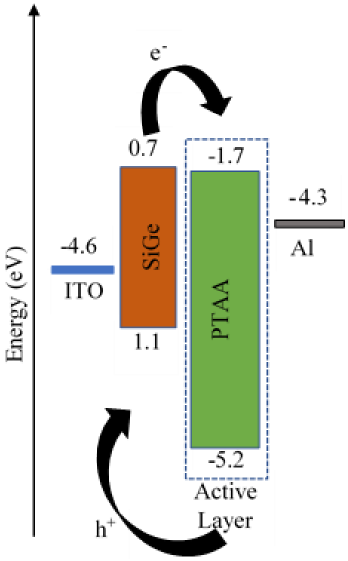

Figure 10. Energy band diagram of SiGe/PTAA

Table 3. The electrical properties of SiGe/PTAA at different SiGe and PTAA thickness

SiGe Thickness / nm	PTAA Thickness / rpm	V_{oc} / V	J_{sc} / Am^{-2}	FF / au	Eff / %
100	1000	0.5853	3.3545	0.7635	1.490
	2000	0.5875	3.0513	0.7716	1.380
	3000	0.5824	2.0372	0.7698	0.910
	4000	0.5733	3.1176	0.7604	0.480
	5000	0.5604	4.6339	0.7279	0.180
200	1000	0.5817	2.9351	0.7617	1.300
	2000	0.5808	2.385	0.7653	1.060
	3000	0.573	1.5393	0.7648	0.674
	4000	0.5642	2.3136	0.751	0.352
	5000	0.5501	3.5338	0.7086	0.137
300	1000	0.5769	2.535	0.7624	1.160
	2000	0.5762	2.1031	0.7657	0.930
	3000	0.5675	1.3004	0.762	0.560
	4000	0.5606	2.1986	0.7425	0.290
	5000	0.5446	2.9662	0.6927	0.110
400	1000	0.5712	2.1769	0.7626	0.948
	2000	0.5683	1.6825	0.7642	0.730
	3000	0.5628	1.0981	0.7561	0.467
	4000	0.5526	1.8145	0.733	0.235
	5000	0.5372	2.3463	0.6637	0.083
500	1000	0.5664	1.871	0.7606	0.806
	2000	0.5649	1.5024	0.7618	0.646
	3000	0.5554	1.4742	0.7461	0.362
	4000	0.5465	1.8271	0.7234	0.190
	5000	0.5251	2.1807	0.7044	0.081

IV. CONCLUSION

The simulation of ITO/ SiGe-PTAA/Al solar showed that the ideal ratio for the combination of SiGe/PTAA thickness is 1:1. Besides that, it was found that the current density varies depending on the thickness of SiGe film, whereby greater SiGe thickness provides more electron-hole pair. Besides that, the maximum value of FF and efficiency rate obtain is 0.7716 au and 1.49%. It is also concluded that all electrical parameters strongly depend on the thickness of the semiconductor layer. Further enhancement can be done in the future by aiding the buffer layer to decrease the work function between the electrode and the semiconductor layer.

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