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Optimization of Zinc-doped Emitter Layer Thickness and Doping Concentration for Gallium Antimonide Based Thermophotovoltaic Cells

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Gallium antimonide based thermophotovoltaic cell is a well-known photovoltaic diode that can directly convert thermal radiation into electricity. Recent investigations on the improvement of gallium antimonide thermophotovoltaic cell performance have led to a number of optimization studies, particularly on the cell design structures. However, low conversion efficiency of gallium antimonide thermophotovoltaic cell remains a major challenge in this area. An optimization study was previously demonstrated with increased efficiency up to 6.63 % incorporating an optimum emitter thickness of 0.85 μm. This work extended the optimization possibilities, aiming to achieve higher power conversion efficiency of gallium antimonide thermophotovoltaic cell. Different doping concentrations of the emitter layer ranging from 1×10^{18} to 5×10^{20} cm^{-3} were studied using Silvaco TCAD simulation software. Within the investigated doping concentrations, the optimum power efficiency of 7.51 % was achieved at 1×10^{20} cm^{-3} under AM1.5 illumination condition. Additionally, higher cell performance was achieved with a power efficiency of 7.88 % by employing an emitter layer thickness of 0.15 μm and a doping concentration of 1.7×10^{20} cm^{-3}. The success of this work will contribute to a perceptive reference for the future development in practical device fabrication of high-performance gallium antimonide thermophotovoltaic cell.

Keywords: Doping; Gallium antimonide; Optimization; Thermal radiation; Thermophotovoltaic

I. INTRODUCTION

Energy-intensive industries such as glass manufacturing, metallic-alloy fabrication as well as thermal power plants generate a huge amount of heat during the manufacturing or power generation processes, leaving almost half of the heat generated goes to waste (Thekdi & Nimbalkar 2015). Recovery and utilization of this waste heat are the key strategy for most industries to save energy, increase profit margins and minimize the global environmental impact. Whilst the waste heat recovery technology for the main exhaust streams is highly recognized and widely used, there is still ample amount of unavoidable waste heat being released in the form of radiation from the hot equipment surfaces and heat generated by the turbine. In this regard, thermophotovoltaic (TPV) system appears to be a promising candidate that can harvest and convert the waste heat into useful electricity.

The hot temperature surface of any equipment and products in industrial processing are known as a photon radiation source, commonly dubbed as a blackbody source. In principle, TPV cells operate at its peak performance when the energy bandgap of the TPV semiconductor is spectrally matched to the blackbody spectrum generated by the heat source (Bauer, 2011). TPV system has a similar working principle to the solar photovoltaic (PV) system, in which the radiation of photons is directly transitioned into electricity without involving any moving parts. This circumstance provides distinct advantages in terms of quieter operation and requires less maintenance. Nevertheless, the radiation power density of a TPV cell is about 50 to 100 times larger than that of a solar cell

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(Ferrari *et al.*, 2014). This is attributed to the close distance between the TPV cell and the incoming radiation sources, typically in the range of cm (Martín *et al.*, 2007).

Nowadays, the advances in semiconductor materials eventually broaden up the opportunity to explore the integration of TPV cells in extensive real-world applications. Figure 1 presents the basic elements of a TPV system (Nicholas & Tuley, 2012). A typical TPV system consists of a heat source, thermal emitter, spectral filter, and TPV cell. In particular, the thermal emitter is heated up by a heat source which can be solar radiation, combustion of hydrocarbon fuels or industrial waste heat (Woolf *et al.*, 2018). The heated thermal emitter transforms the heat energy into emission of the optical spectrum with photons at different energy levels which will be further channeled to a selective wavelength windows by a spectral filter. The spectral filter only allows convertible photons to be absorbed by the TPV cell to avoid thermalization and spectral losses. Finally, the TPV cell captures the photons and converts them into electrical energy via the photovoltaic effect. The efficiency of the TPV cell is determined by the types of employed semiconductor material.

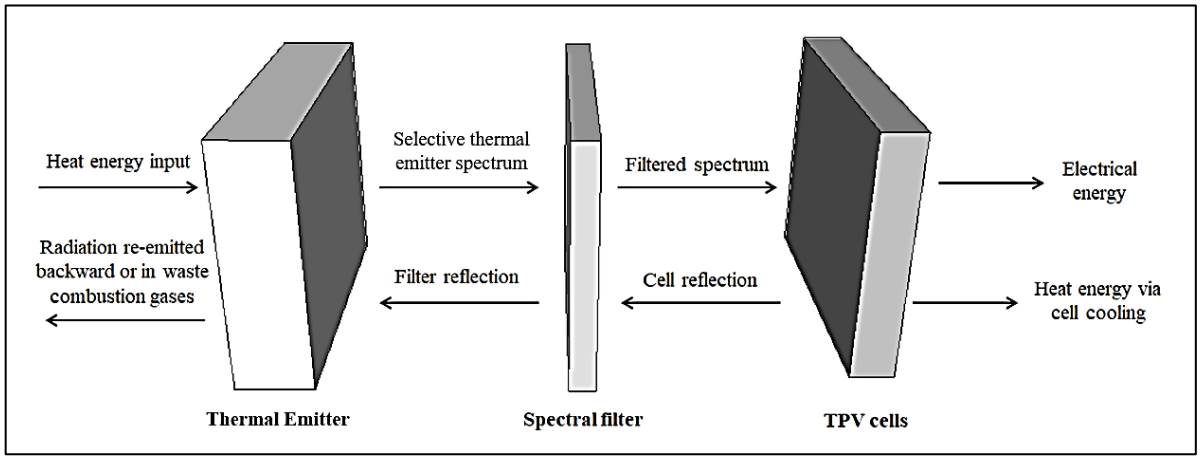


Figure 1: Main components of a TPV system (Nicholas & Tuley, 2012).

At present, gallium antimonide (GaSb) material is often regarded as one of the most ideal choices to fabricate an infrared device. GaSb-based TPV cell has received great attention since the invention and was patented by McLeod *et al.* (1988) and Fraas *et al.* (1992). Due to the properties of having a low bandgap energy (~0.72 eV), the GaSb cell has been known to be spectrally matched with the medium-temperature blackbody sources and has demonstrated good performance especially at mid-infrared wavelength up to 1800 nm (Ni *et al.*, 2016).

The GaSb TPV cells are technology matured and commercially available. However, the reported cell efficiency remains low due to the heat and electrical losses such as thermalization and recombination in the bulk and surface of the TPV cell (Basu *et al.*, 2007; Daneshvar *et al.*, 2015; Utlu & Parali 2013; Yugami *et al.*, 2003). Hence, research efforts were spurred towards maximizing the conversion efficiency of the TPV cells. Tang *et al.* (2014) reported an experimental work demonstrating a new zinc (Zn) diffusion method of fabricating GaSb TPV cell and reported a 3.3 % conversion efficiency. Licht et al. (2017) conducted a simulation study of an inverted n-on-p GaSb TPV cell configuration with a front-surface metallic photonic crystal (MPhC) and recorded an overall efficiency of 6 %. On the other hand, Meharrar *et al.* (2018) studied the effect of front contact barrier, doping concentration and thickness of the absorber layer on GaSb TPV cell performance. Meharrar reported that the highest conversion efficiency of 3 % can be achieved with a front contact barrier of 0.24 eV, a doping concentration of 1×10^{15} cm^{-3} and thickness layer of 3 μm. In particular, optimization works on the cell structure design parameters such as the layer thickness and doping concentration are the major topic exploited by various researchers.

The GaSb TPV cell performance parameters exhibit a strong dependence on the layer thickness and doping concentration. For example, the short circuit current density (J_{sc}) and open-circuit voltage (V_{oc}) are strongly influenced by the thickness and doping concentration of the emitter layer. Bett et al. (1996) conducted a comprehensive study on the optimization of the emitter thickness and found a strong dependence on the quantum efficiency (QE) when the emitter thickness is optimized. Additionally, trade-off relation between the emitter thickness and the performance parameters, such as V_{oc} and

J_{sc} values was analytically presented in the authors' previous publication (Rashid *et al.*, 2018). An increment of power efficiency from 5.91 to 6.63 % was achieved under AM1.5 illumination condition when the p-type emitter thickness was increased from 0.15 µm to 0.85 µm. Therefore, the necessity to develop a detailed optimization with precise control of the emitter thickness is very crucial. Subsequently, the doping concentration of the emitter layer is another important aspect which greatly influences the cell performance. Sulima *et al.* (2001) and Wang *et al.* (2012) studied the doping optimization of emitter layer and concluded that the optimization of the emitter doping concentration leads to an enhancement of the cell performance. Recently, Tang *et al.* (2017) performed a doping and depth optimization on Zn-diffused GaSb cell for both emitter and base regions through numerical simulation. The doping concentration of both regions was optimized to increase the QE in the long-wave ranging from 1000 to 1800 nm.

Nevertheless, previous work was limited to a direct optimization approach by manipulating one design parameter at a time. This approach allows researchers to study the tradeoff relationship of each parameter to the cell performance. However, the claiming of optimal TPV design is difficult with this approach because both thickness and doping concentration has a direct impact on the cell performance. To date, the study and optimization possibilities which consider both design parameters simultaneously have not been fully elucidated. Based on the authors' previous work, the optimized emitter layer thickness increased the power conversion efficiency up to 6.63 %.

This work extends the optimization possibilities where the effect of the doping concentration on the cell performance will be investigated, after a simultaneous optimization of both emitter thickness and doping concentration. The main goal of this study is to investigate the optimal condition of the thickness and doping concentration for the emitter layer of GaSb TPV cell that could achieve the highest performance through experimental simulation using Silvaco TCAD software.

II. MATERIALS AND METHOD

The simulation of GaSb TPV cell was carried out under AM1.5 illumination condition using Silvaco TCAD software. The software includes ATLAS, BLAZE and DEV EDIT modules that allow the user to specify the design structure and characterize the electrical behavior of semiconductor devices. The simulator is incorporated with powerful numerical methods that solve the main semiconductor equations such as Poisson's equation and carrier transport equations. The Caughey-Thomas mobility model was used as the drift-diffusion model for electrons and holes as presented by equation (1)

$$\mu_e(N_D)_{T=300K} = \mu_{min,e} + \frac{\mu_{max,e}-\mu_{min,e}}{1+\left(\frac{N_D}{N_{ref,e}}\right)^{\alpha_e}} \quad (1)$$

Where N_D denotes the doping concentration of or donor, $\mu_{min,e}$ and $\mu_{max,e}$ represents the value of electron mobility at very low and high doping level respectively, $N_{ref,e}$ denotes the doping concentration at which the mobility decreased to half the value it reaches low doping levels and α_e is a fitting parameter that can be obtained from previous literature. Besides, the physical models such as Shockley-Red-Hall (SRH) recombination, Auger (AUGER) recombination as well as optical recombination (OPTR) models were also considered in the simulation.

The performance parameter in this study will be the J_{sc}, V_{oc}, fill factor (FF) and power efficiency (η). The cell performance of the GaSb TPV cell is computed using equation (2) where the power density (P_{in}) is in the unit of W/cm².

$$\text{Efficiency}(\eta) = \frac{FF \times J_{sc} \times V_{oc}}{P_{in}} \quad (2)$$

A. GaSb TPV cell baseline model

In previous work (Rashid et al. 2018), the GaSb TPV cell structure was modeled using DEV EDIT module and the structure is almost similar to that of the experimental work done by Tang et al. (2014) and JX Crystal Inc (JXC) commercialized GaSb TPV cell. Figure 2 illustrates the schematic diagram of the modeled p on n GaSb TPV cell. A set of reliable GaSb material parameters was determined and the values were within the reported range by several pieces of literature. Table 1 summarizes the material parameters of GaSb TPV cell in the simulation.

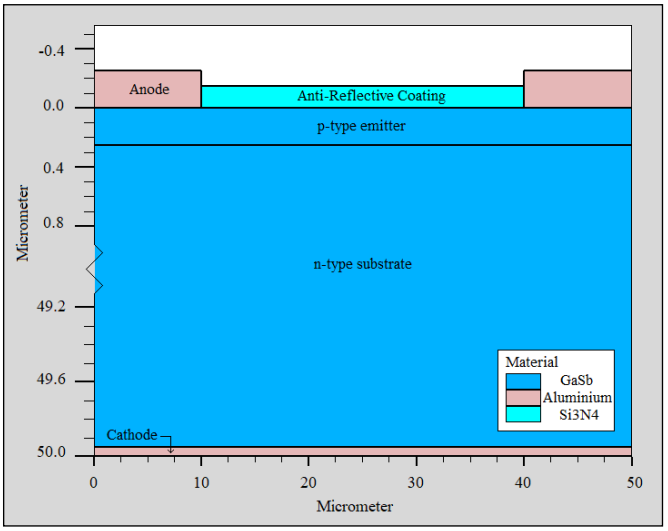


Figure 2: Schematic diagram of GaSb TPV cell.

Table 1: Summary of the integrated GaSb material parameters in the simulation (Rashid et al. 2018).

Material Parameter	Numerical value
Intrinsic carrier concentration	$1.4x10^{12}$ cm^{-3}
Electron density of states	$2.1x10^{17}$ cm^{-3}
Holes density of states	$1.8x10^{19}$ cm^{-3}
Shockley-Red-Hall lifetime electrons	$1x10^{-8}$ s
Shockley-Red-Hall lifetime holes	$6x10^{-7}$ s
Electron mobility	6600 cm^2/Vs
Holes mobility	1250 cm^2/Vs
Auger coefficient	$5x10^{-30}$ cm^6/s
Permittivity	14.4
Affinity	4.06 eV

The modeled structure was validated by having comparable performance to the experimental work and JXC commercialized GaSb TPV cell (Tang et al. 2014). Table 2 summarizes the performance comparison between experimental work done by Tang, JXC commercialized GaSb TPV cell and the present work. It can be seen that the J_{sc} and V_{oc} of the modeled GaSb TPV cell are comparable to those fabricated devices. However, the power efficiency of the simulated cell is slightly higher compared to others. This is because the series resistance is neglected in the simulation environment and the metal contact is assumed to be a perfect ohmic contact. The power efficiency of the GaSb TPV cell fabricated by Tang and associates recorded the lowest efficiency as the fabricated cell suffers from high contact resistance, leading to a lower fill factor (FF). This is due to the unoptimized structure of the fabricated cell where a silver metal was substituted from a gold metal to reduce the cost of fabrication. On the other hand, a higher efficiency was recorded by JXC commercialized TPV structure with a gold metallization deposited on the cell surface, reducing the series resistance of metal contact. From author's previous simulation result, an efficiency of 6.19 % was obtained with J_{sc} of 26.76 mA/cm² and V_{oc} of 0.316 V. This is the baseline model that will be referred in this work, incorporated with the emitter thickness of 0.25 µm and doping concentration of 1×10^{19} cm^{-3}as the baseline design structure.

Table 2: Comparison of GaSb TPV cell performance parameter

Performance parameter	Experimental By Tang et al. (2014)	JXC Commercialized GaSb TPV cell (Tang et al. 2014)	Present work
J_{sc}	29.0	32.3	26.76
V_{oc}	0.281	0.326	0.316
η	3.90	5.50	6.19

B. Optimization of the emitter layer of GaSb TPV cell

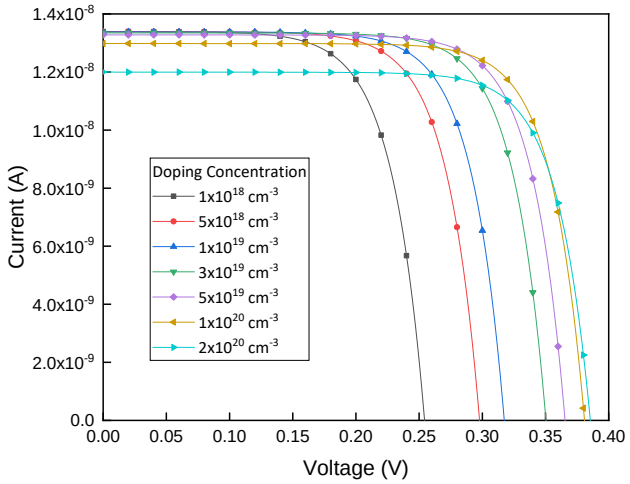
The direct optimization on the doping concentration using Zn dopants was carried out to study the trade-off relationship with the cell performance. High doping concentration is desirable for the emitter layer to obtain a better collection charge carrier in the emitter region. Therefore, a doping concentration between 1×10^{18} and 5×10^{20} cm^{-3} with 23 data points was integrated into the simulation. The baseline p-type emitter thickness, n-type substrate doping (3×10^{17} cm^{-3}), and the physical parameters were kept constant throughout the optimization. Next, further optimization with both emitter layer and doping concentration was simultaneously performed. A range from 1×10^{19} to 2×10^{20} cm^{-3} doping concentrations was chosen because the highest cell performance is predictably obtained within this range. On the other hand, the emitter thicknesses ranging from 0.15 to 1.20 µm was employed in the simulation. A total of 460 simulations were conducted, which corresponds to all possible combinations between these two design parameters. Subsequently, the cell performance on each combination was analyzed to determine the optimum

power conversion efficiency.

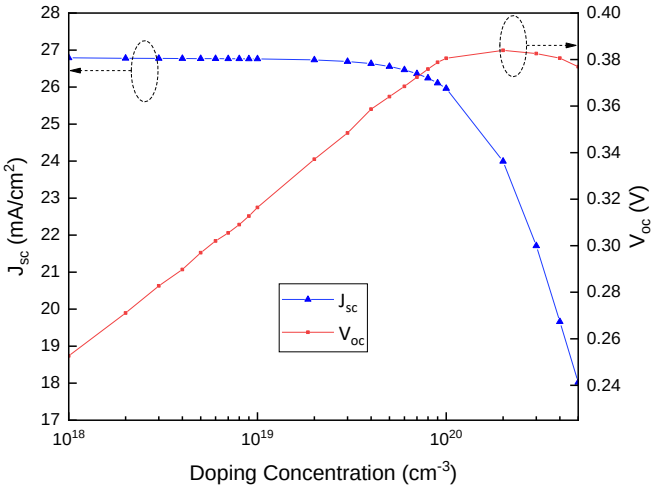
III. RESULTS AND DISCUSSION

A. The effect of emitter doping concentration on cell performance

In this subsection, the simulation results from a direct optimization on emitter doping concentration is presented. The emitter thickness of 0.25 µm and other baseline parameters are kept constant. Figure 3 shows the effect of different doping concentrations on the electrical characteristic of GaSb TPV cell.



(a)



(b)

Figure 3: (a) Current-Voltage characteristic for GaSb TPV cell with different emitter doping concentrations and (b) Effect of doping concentration on the J_{sc} and V_{oc}.

As shown in Figure 3(a), increasing the doping concentration of the emitter layer from 1×10^{18} to 1×10^{20} cm^{-3} increases the V_{oc} from 0.25 to 0.38 V, but reduces the J_{sc} from 26.79 to 25.96 mA/cm² of the GaSb TPV cell. Theoretically, higher doping concentration reduces the carrier (electron and hole) mobility and lifetime, leading to the deterioration of charge carrier diffusion length (Wang et al. 2012). Despite the fact of reduction in diffusion length, only a minor decrement was observed for the J_{sc} at higher doping concentration up until 1×10^{20} cm^{-3}. This may imply that the diffusion length remains longer than the active part of the emitter thickness within these concentration windows.

On the other hand, the reverse saturation current (J_o) will also be affected by the doping concentration. The J_o is reduced with respect to higher doping concentration, resulting in a significant increase in the V_{oc}. However, the V_{oc} reaches the plateau at the doping concentration of 2×10^{20} cm^{-3}. Beyond this doping concentration, the V_{oc} and J_{sc} decrease as depicted in Figure 3(b). When the emitter layer is doped at high concentration (greater than 1×10^{20} cm^{-3}), the mobility and minority carrier lifetime will eventually be reduced, resulting in a sudden drop on J_{sc}. Consequently, the power efficiency would also be decreased.

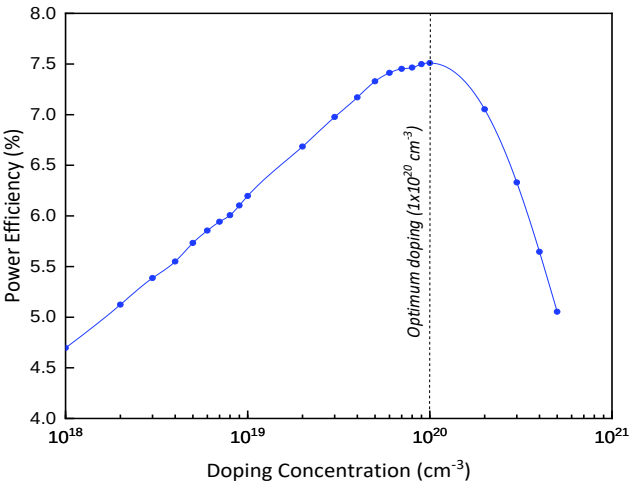


Figure 4: Effect of p-type emitter doping concentration on the power efficiency

Figure 4 illustrates the optimum doping concentration based on the simulation results. Under AM1.5 illumination condition, a remarkable increment from 4.70 to 7.51 % was achieved when the doping concentration was increased from 1×10^{18} to 1×10^{20} cm^{-3}. The optimum point is a trade-off between high doping levels and efficient transport of charge carriers. Beyond the doping concentration of 1×10^{20} cm^{-3}, the diffusion length of charge carriers will

reduce to a certain length, shorter than that of the emitter thickness, which in this case is 0.25 μm. This phenomenon greatly contributes to the loss of carrier generation hence reducing the power conversion efficiency of the GaSb TPV cell.

A. The effect of both emitter thickness and doping concentration on the cell performance

Previously, the demonstration of a direct correlation between the doping concentration and emitter thickness proved the importance of optimizing both parameters simultaneously. The doping concentration window of interest in this study lies within the range between 1×10^{19} to 2×10^{20} cm^{-3}. Figure 5 depicts the dependence of power efficiency of GaSb TPV cell on the emitter thickness and doping concentration. In the author's previous work, a direct optimization on emitter thickness ranging from 0.15 μm to 1.20 μm was investigated at an emitter doping concentration of 2×10^{19} cm^{-3}. Based on the author's previous findings, the optimum emitter thickness was found to be at 0.85 μm, where a maximum power efficiency of 6.63 % was obtained. It was highlighted that the trade-off relation between the emitter thickness, J_{sc}, and V_{oc} determine the optimum emitter thickness of the GaSb TPV cell. However, this study demonstrated that the power efficiency increases with thinner emitters. This is due to the incorporation of higher doping concentrations in the emitter region.

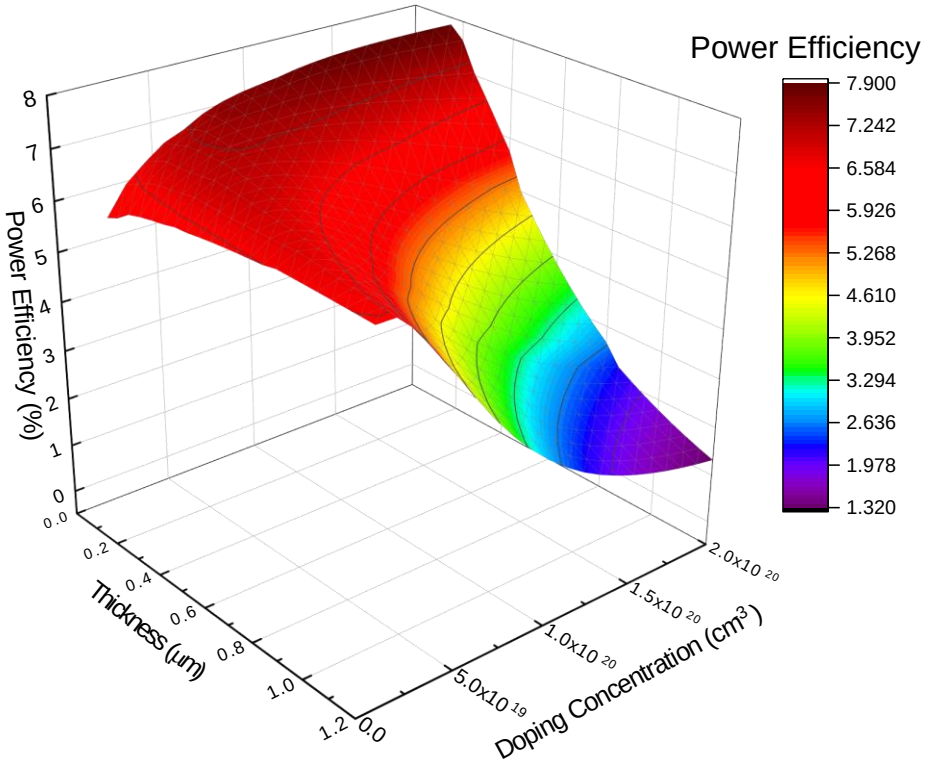


Figure 5: The effect of emitter thickness and doping concentration of GaSb TPV cell on power efficiency.

Furthermore, the optimal condition was determined to be within a high doping concentration range. As aforementioned, the optimum point of power efficiency is attained by the trade-off between high doping levels and the mobility charge carriers. In solid states physics, high carrier mobility is required to ensure efficient transport of the charge carrier through the semiconductor. At high doping levels, the primary scattering mechanism for the electrons and holes will collide with a substantial amount of impurity dopants, thus the collision time and mobility become inversely proportional to the doping (Chubb, 2007). This resulted in the reduction of the diffusion length of charge carriers, leading to a tendency of the charge carriers to recombine faster.

In particular, the diffusion length must be longer than the emitter thickness to generate maximum electron-hole pairs in the active region. When the diffusion length is shorter than the emitter thickness, increasing the doping concentrations in the emitter region would reduce the

overall efficiency due to the recombination of charge carriers prior to reaching the p-n junction. This suggests that the thickness of the emitter layer could be reduced simultaneously with an increase in doping concentrations to achieve higher power efficiency. Moreover, reducing the emitter layer would maximize the collection of generated carriers, particularly under the illumination condition of AM 1.5. Since the majority of photons in the AM1.5 spectrum are at short wavelengths of 300-600 nm, these high energy photons will be absorbed near the surface of the active layer. Therefore, decreasing the emitter layer will reduce the distance traveled of the generated carriers from the cell surface to the p-n junction. In this work, optimum power efficiency of 7.88 % was achieved with the best combination of design parameters with 0.15 µm and 1.7×10^{20} cm^{-3}. Significantly, this result demonstrates a better cell performance as compared to the authors' previous finding on direct optimization of emitter thickness and doping concentration separately. Eventually, a comparison between the optimum design of GaSb TPV cell in this work and the baseline model was illustrated in Figure 6.

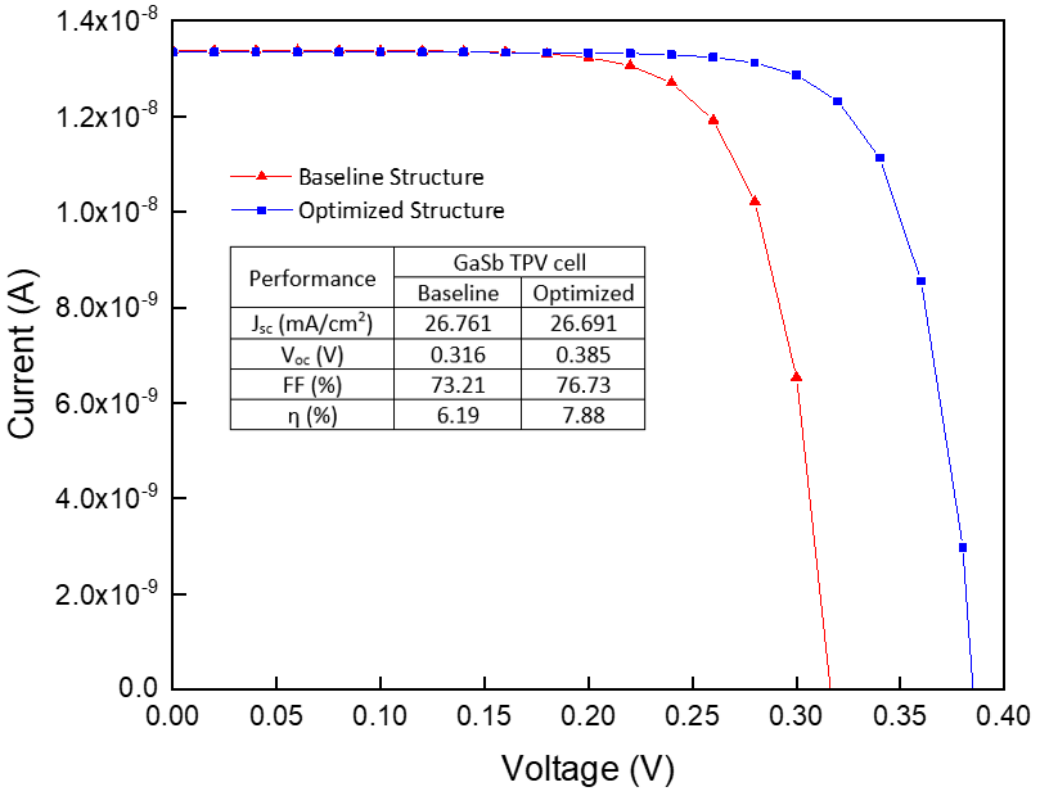


Figure 6: The current-voltage characteristic of both baseline and optimized structure.

A significant improvement on V_{oc} can be achieved through optimization of the cell structure according to Figure 6. Even though a slight decrease of J_{sc} was observed for the optimized structure, the fill factor (FF) of the cell is still high as compared to the baseline structure. For this reason, the optimized structure could generate more power, leading to an enhancement in power efficiency (η) from 6.20 to 7.88 %.

IV. CONCLUSION

The effect of both emitter thickness and doping concentration on the power efficiency under AM1.5 illumination condition was investigated and presented. The outcome of this study indicates that the emitter thickness and doping concentration plays an important role in fabricating a high-performance GaSb TPV cell. The right combination of both parameter selection is necessary to produce high output power density that contributes to high conversion efficiency. The results show an increment in power efficiency from 4.70 to 7.51 % when the doping concentration was increased from $1 \times 10^{18}$to 1×10^{20} cm^{-3}. Moreover, it was found that higher power efficiencies were recorded at thinner emitter layer with high doping concentration levels. Through simultaneous optimization, the optimum design parameter

of emitter thickness and doping concentration was found to be at 0.15 μm and 1.7×10^{20} cm^{-3} respectively, and found to increase the power efficiency up to 7.88 %. Further studies on other design parameters such as base layer thickness and doping will need to be performed to extend the optimization possibilities and enhance cell performance.

V. ACKNOWLEDGMENT

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