Simulation and Optimization of Emitter Thickness for Indium Arsenide-Based Thermophotovoltaic Cell

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Abstract— **Thermophotovoltaic (TPV) devices are known for capturing infrared radiation from a high temperature heat source and converting them into electricity. While InAs TPV cells have the ability to harvest radiation heat from temperature source below 1000 K, the best-reported homojunction InAs efficiency is only 0.6 % under 1000 K. This is due to the lack of an optimize structure for TPV application. This research work investigates on optimizing the emitter thickness for Indium Arsenide (InAs) based TPV cells. The electrical characteristics of the InAs TPV cell were simulated using the SILVACO TCAD software. The thickness of p-type emitter ranging from 0.1 to 2.3 µm were investigated. As the emitter thickness increases, the open circuit voltage (V_{oc}) increases, while the short-circuit current density (J_{sc}) decreases. With the increase rate of V_{oc} which is faster than the decreasing rate of J_{sc}, the maximum power efficiency was achieved at an optimum thickness of 1.5 µm. At 800 °C blackbody temperature, the highest power efficiency was acquired as 0.61 % at the optimum emitter thickness.**

Keywords— InAs, III-IV semiconductor, TPV cell, SILVACO, Efficiency, Thickness

I. INTRODUCTION

Thermophotovoltaic (TPV) technology is widely employed to generate clean energy. Moreover, TPV has an additional feature of utilizing heat energy and solar energy to generate electricity [1]. TPV cells function similarly as solar cells, it absorbs radiation from heat sources as waste heat and generates electricity [2]. The semiconductor industries provide opportunities to further research on TPV cells for a series range of applications such as steel mills, thermal power plants and waste heat applications.

As of today, the recent research work on TPV cells focused more on gallium antimonide (GaSb), indium gallium arsenide (InGaAs), and gallium indium arsenide antimonide (GaInAsSb) alloys lattice matched on GaSb, which are is commonly used to generate electricity for temperatures above 1000 °C and produces high power conversion efficiency up to 16 % [3]. However, there is less investigation and studies on InAs TPV cells for lower temperature heat sources (<1000 °C) compared with the aforementioned TPV cells in previous literature [3]–[5]. At present, InAs TPV cell is regarded as one of the most suitable materials to be used in low temperature heat source application under 1000 °C [3]. This is caused by the low bandgap energy (~0.35 eV) of InAs that allows InAs TPV cell to harvest photons at a longer wavelength (infrared radiation up to 3.55 µm). Krier et al [4][5] reported one of the first low bandgap TPV system based on InAs/InAs0.61Sb0.13P0.26 photodiodes, the cell able to operate with heat source temperature of 345 °C. In 2017 Qi Lu et al [3] demonstrated the use of InAs TPV cells to harvest thermal radiation from heat source with temperature below 1000 °C. A 10 % conversion efficiency is achieved when the cell operate at 100 K cell temperature. To date, less research has been done on InAs based TPV cell at an operating cell temperature (T_{cell}) below 1000 °C, as well as to improve the cell performance by optimizing numerous parameters for example the layer thicknesses, doping concentrations and different blackbody temperatures. This paper discussed on the effect of various thickness of p-type emitter layer for the InAs based TPV cell.

We report the electrical characteristics of the InAs TPV cell operating at room temperature, T_{cell} of 27 °C (~300 K) when illuminated by low temperature thermal sources between 550 °C to 800 °C. We obtained V_{oc} of 0.027 V and 0.61 % of power conversion efficiency when the InAs TPV cell operates under a 800 °C heat source illumination spectrum.

II. METHOD OF SIMULATION

SILVACO TCAD simulation tool was incorporated in this work to determine the electrical characteristics of the TPV cell. This software consists of ATLAS, BLAZE and DevEdit modules which determine the electrical properties parameters based on the semiconductor device. DevEdit interface is use to model the InAs TPV cell structure and ATLAS module is used to further analysis on its electrical characteristics with different thicknesses of p-type emitter layers.

A. Cell Structure – InAs Based PiN TPV Cell

The InAs TPV cell structure was modelled using DevEdit software based on previous work [2]. Fig.1 shows the cross

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sectional area of the simulated structure with the dimension of 1333.33 µm x 1 µm.

The structure was integrated based on PiN regions, and each region is made up of InAs material. This InAs PiN structure has a 2 µm n-type base layer (1 $\times 10^{18}$ cm^{-3}), a 10 µm intrinsic layer (unintentionally doped with 6 $\times 10^{14}$ cm^{-3}) and a 2 µm p-type emitter layer (1 $\times 10^{18}$ cm^{-3}). The top and bottom ohmic contacts was formed by deposition of titanium/gold (Ti/Au) metal with thickness of 20/200 nm, this covers 20 % of the front surface area.

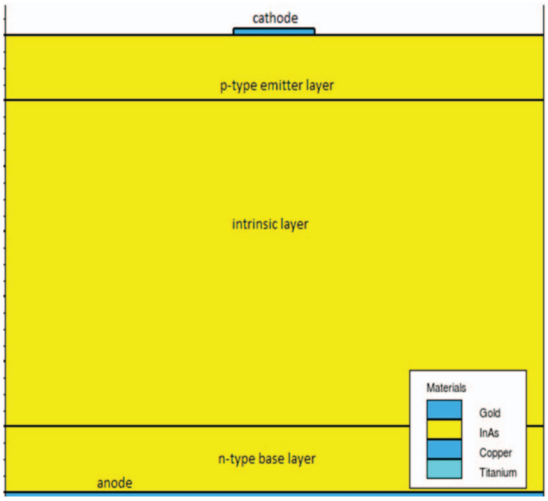

Fig.1. PiN InAs cell structure.

B. Material Parameters of InAs for Simulation

Research output in [6] and [7] successfully demonstrated the optimized material parameters suitable for TPV application. After modelling the InAs TPV cell structure, the electrical parameters were simulated by ATLAS framework. The advanced physical properties of the InAs structure and model are defined in SILVACO TCAD software to calculate and to generate the electrical parameters behaviour in InAs PiN TPV cell. Table I lists the material physical parameters of the InAs cell integrated with 300 K of cell operating temperature.

Based on Table I, the optimized physical parameters for InAs are used in this simulation. One of the challenging issues for InAs material is that there is lack of reference in experimental measurements to support the study and not all material properties can be readily found in the literature [7].

C. Model Validation

To improve the accuracy of simulation results, physical models which includes Fermi-direct, Shockley Red Hall recombination, Auger recombination and radiation recombination were all taken into consideration to ensure a high accuracy in the simulation result. Physical models in [10] was referred in this simulation work. The performance analysis of the InAs cell was conducted under a blackbody spectrum at low temperature range (<1000 °C). The experimental work done in [3] as shown in Table II is used to validate the output simulation result for benchmarking purposes. The simulation was measured at low incident power density to match the incident power intensity to the experimental work done in [3], since no concentration lenses were used in the experimental testing.

TABLE I. LIST OF INAS PHYSICAL PARAMETERS USED IN THIS WORK AND THEIR VALUES REPORTED IN OTHER LITERATURES

Parameters	**InAs Material Parameters**		**InAs Optimized Material Parameters**
	Value	**Ref**	**Value**
Bandgap (eV)	0.35 0.354 0.36	[8]–[10]	0.36
Dielectric Constant	14.6 14.985 15.15 15.34	[9]–[13]	15.15
Electron Affinity (eV)	4.13 4.29 4.73 4.9	[9], [10], [13], [14]	4.9
Effective Density of States in Conduction Bands (N_c=300 K) (cm^3)	9.33 $x10^{16}$ 8.70 $x10^{16}$	[9], [10]	8.7 $x10^{16}$
Effective Density of States in Valence Bands (N_v=300 K) (cm^3)	8.12 $x10^{18}$ 6.60 $x10^{18}$	[9], [10]	6.6 $x10^{18}$
Intrinsic Carrier Concentration (N_i)	7.70 x 10^{14} 9.99 x 10^{14} 1.00 $x10^{15}$	[6]. [7], [12]	1 $x10^{15}$
Auger Coefficients	AUGN= 2.2 $x10^{-27}$ AUGP= 2.2 $x10^{-27}$	[9]	AUGN= 2.2 $x10^{-27}$ AUGP= 2.2 $x10^{-27}$
Carrier Lifetimes (s)	taup= 3 $x10^{-6}$ taun= 3 $x10^{-9}$	[9]	taup= 3 $x10^{-6}$ taun= 3 $x10^{-9}$
Mobility Parameters (cm^2/Vs)	mun = 33,000 mun =40,000 mup = 460 mup =500	[9], [10]	mun=40,000 mup=500

TABLE II. COMPARISON OF PERFORMANCE PARAMETERS

Parameters	**Experimental Work** [3]	**This Work**
V_{oc} (V)	0.017	0.027
J_{sc} (A/cm^2)	0.23	0.262
FF (%)	25.0	26.6
Efficiency (%)	0.38	0.607

D. Optimization of p-type Emitter Thickness of InAs Based TPV Cell

Simulation results agreed with the experimental work used for validation. Further optimization was investigated by varying the thickness of p-type emitter from 1 µm to 3.5 µm. The doping concentrations for all regions as well as the physical parameters were remained as claimed in previous literature [3], [7]. Eventually, the electrical characteristics and output performance of this structure were analysed.

III. Results and Discussion

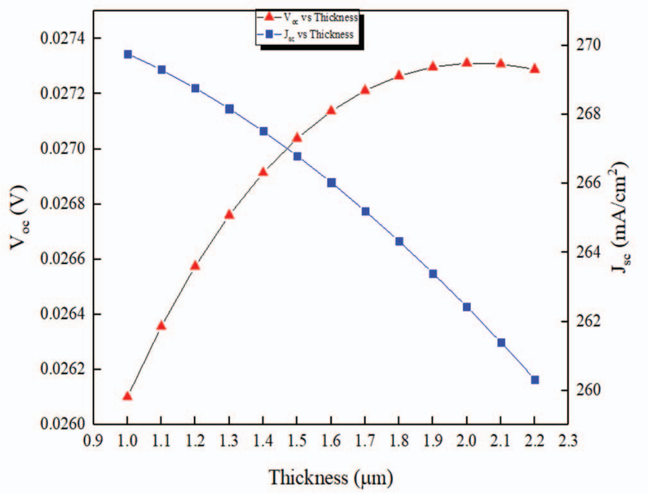

Fig. 2. Effect of varying emitter thickness on V_{oc} and J_{sc} under 800 ºC heat source.

Fig. 2 shows the trend of J_{sc} and V_{oc} as a function of emitter thickness. When the p-type emitter thickness increases from 1 µm to 2.3 µm, the J_{sc} decreases whilst the V_{oc} increases. Based on the measurement, the V_{oc} increases and reaches a plateau of 0.0273 V at the emitter thickness of about 2.1 µm. Beyond this emitter thickness, the V_{oc} gradually declines. The V_{oc} is affected by two factors: dark current due to back and front surface recombination and recombination due to the traps in space charge region (SCR) [16]. The optimum V_{oc} in this work augurs well with the emitter thickness of 2.1 µm in [16]. On the other hand, the J_{sc} declines constantly with respect to the p-type emitter thickness due to lower possibility of collecting the photogenerated electrons in thicker emitter layer. The interface between the V_{oc} and J_{sc} curve represents a critical thickness value to achieve the maximum efficiency.

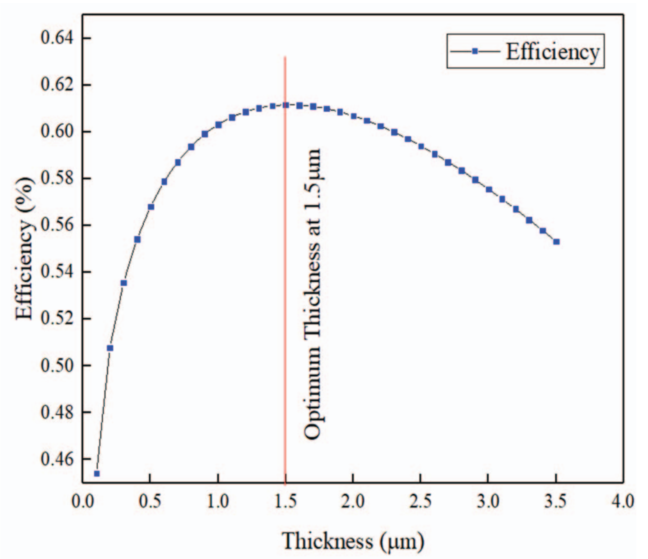

Fig. 3. Efficiency versus emitter thickness of InAs under 800 ºC heat source.

Fig. 3 illustrates the effect of varying emitter thickness on the cell efficiency. The result shows an enhancement in power efficiency from 0.45 to 0.61 % by tailoring the emitter thickness to an optimum thickness of 1.5 µm. An optimum emitter thickness improves the charge carrier collection in the emitter layer, leading to a higher V_{oc} and J_{sc} of the InAs based TPV cell. However, the efficiency shows a decreasing trend beyond the optimum emitter thickness in conjunction with the reduction in V_{oc}.

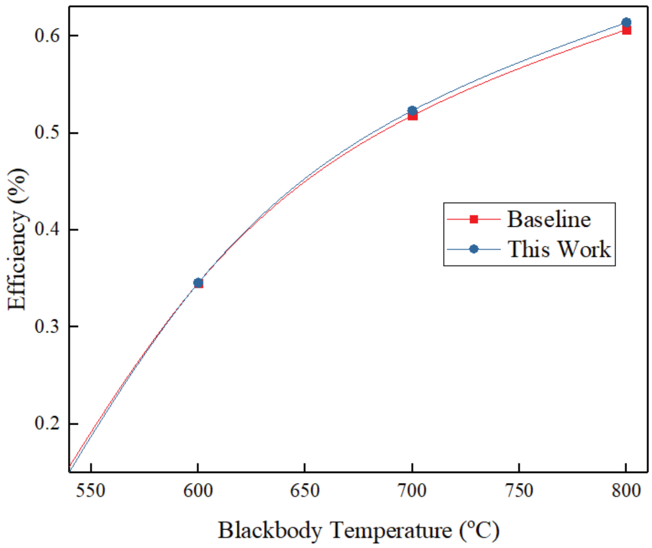

Fig. 4. Comparison in efficiency versus blackbody temperatures between this work and the baseline.

Further simulation on blackbody temperature ranging from 550 to 800 ºC was conducted using the optimized structure. The result was compared with the baseline model [2] (emitter thickness = 2 µm) as presented in Fig. 4. At 800 ºC, the InAs based TPV cell was operating at its peak performance with the highest efficiency of 0.61 % using an optimum emitter thickness of 1.5 µm. In contrary, the lowest efficiency was recorded as almost null at 550 ºC, which is attributed to less photons with higher energy than the bandgap are absorbed and converted to electricity in the emitter layer.

The increasing of the efficiency with blackbody temperature is related to the peak emissivity of the heat source. For 800 ºC, the peak emissivity is about 2.7 µm which is close to the cut-off wavelength of InAs, whereas it is 3.75 µm at 550 ºC.

For all temperatures, the efficiency is slightly higher than the baseline model. This explains that the higher energy photons are being absorbed in the intrinsic and base layer to conduct electricity, thus improving the efficiency.

However, more researches can be studied on the effect of intrinsic and base layer thicknesses on the InAs TPV cell performance. The findings of this work will contribute to more upcoming developments for InAs based TPV in waste heat recovery applications.

IV. Conclusion

In this work, we have demonstrated a comprehensive model in assessing the electrical properties of the InAs based TPV cell that is illuminated with radiation from blackbody temperatures from 550 to 800 ºC. The maximum V_{oc} and J_{sc} were resolved using SILVACO simulation software. he optimized material parameters for InAs were obtained which contributes to the electrical properties for the 1333.33 µm x 1 µm surface area of the InAs based TPV cell. The constructed TPV cell was then investigated by tailoring the p-type emitter thickness from 0.1 to 2.3 μm. The highest efficiency was acquired with an optimum emitter thickness of 1.5 μm. In conclusion, this research output will contribute to design an optimum emitter layer thickness for an InAs TPV cell, as well as provide a better insight in understanding the effect of changing the emitter thickness on the overall TPV efficiency.

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