



GaTlAs Quantum Well Solar Cells for Sub-band Gap Absorption

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ABSTRACT

Despite the improvements seen in efficiency of GaAs cells over the years, there remains room for improvement for it to approach the theoretical single junction limit posited by Shockley and Quieser decades ago. One of the more pursued options is the growth of quantum wells within the structure of GaAs to enhance its photon absorption below its bandgap. Multiple Quantum Wells (MQW) have been an ongoing topic of research and discussion for the scientific community with structures like InGaAs/GaAs and InGaP/GaAs quantum wells producing promising results that could potentially improve overall energy conversion. Here, we used WEIN2K, a commercial density functional theory package, to study the ternary compound $\text{Ga}_{1-x}\text{Tl}_x\text{As}$ and determine its electronic properties. Using these results combined with experimental confirmation we extend these properties to simulate its application to form a MQW GaAs/ $\text{Ga}_{1-x}\text{Tl}_x\text{As}$ solar cell. $\text{Ga}_{1-x}\text{Tl}_x\text{As}$ is a tunable ternary compound, with its bandgap being strongly dependent on the concentration of Tl present. Concentrations of Tl as low as 7% can reduce the bandgap of $\text{Ga}_{1-x}\text{Tl}_x\text{As}$ to roughly 1.30 eV from GaAs's 1.45 eV at room temperature with as little as a 1.7% increase in lattice constant. The change in bandgap, accompanied by the relatively small change in lattice constant makes $\text{Ga}_{1-x}\text{Tl}_x\text{As}$ a strong candidate for a MQW cell with little to no strain balancing required within the structure to minimize unwanted defects that impede charge collection within the device. Our GaAs photodiode with TlGaAs MQWs shows an expanded absorption band and improved conversion efficiency over the standard GaAs photovoltaic cell with dilute concentrations of Tl incorporated into the compound.

INTRODUCTION

The material properties, and relative ease of fabrication have made III-V compounds ideal for many novel solar energy harvesting structures. Chief among these prospective solutions are Multiple Quantum Well (MQWs) cells, which have shown promising results in GaAs/AlGaAs, InGaAs/GaAs and InGaN/GaN devices [1]–[5]. With relative modelled efficiencies of approximately 10% higher than the standard bulk III-V single junction cell, it becomes worthwhile to research how far the efficiency envelope can be pushed in similar setups with various material choices. MQWs allow for the absorption and conversion of sub-bandgap photons into collectable electrical energy. This is mostly due to the improved carrier transport through the device, allowing for an increased short circuit current (J_{sc}) and for some devices, the open circuit voltage (V_{oc}) as demonstrated with GaAs/AlGaAs MQW solar devices [1].

In the course of this study, we consider the ternary compound $Ga_{1-x}Tl_xAs$ which contains the exotic material Thallium (Tl). First mentioned by Van Schilfgaarde et al in the early 90s, Tl-based semiconductors were proposed as mid-far infrared detectors due to their theorized semimetal properties [6]–[8]. Through the course of this paper, we study the properties of Tl incorporation into the III-V compound GaAs, how it changes its electronic properties and its incorporation into a MQW structure for photovoltaic energy collection.

PARAMETERS

The growth and study of $Ga_{1-x}Tl_xAs$ compounds was sparked with the increased research for materials in the optical communication, and heterostructure field effect transistor applications[6], [9]–[11]. The initial studies showed that with increasing Thallium content into the ternary compound $Ga_{1-x}Tl_xAs$, the optical and electronic properties of the material changed. The bandgap in particular showed a significant decrease at every additional Tl content (x) added.

To better understand the performance of these compounds, we used the commercial package WIEN2k developed by Blaha et. al., to calculate the electronic properties of the semiconductor $Ga_{(1-x)}Tl_xAs$ while varying x -content. WIEN2k uses the Density Functional Theory (DFT) to calculate the electronic structure of materials, where the exchange-correlation potential can be approximated using Linear Density Approximation (LDA) or the Generalized Gradient Approximation (GGA). To avoid the overbinding that could result from using LDA, we employ the Wu-Cohen GGA method for the ab-initio calculations in our work [12], [13].

Our key result with regards to the change of bandgap as a function of Tl content can be seen in Figure 1. As previously theorized, we show that increasing Tl content reduces the bandgap of the material allowing for a tunability in the compound that is a function of the Tl in it. Attempts to grow these compounds however have shown that Thallium does not incorporate well at x values exceeding 8% [14]. XRD measurements presented by Asahi et. al show that at higher contents of Tl, Tl diffuses up to the surface of the compound forming micro-islands of Tl on top of grown layers of GaAs [15]. This unfavorable result has made it difficult to pursue structures with additional Tl in them despite their simulated advantages. Some key parameters of GaTlAs at different concentrations are listed in Table 1.

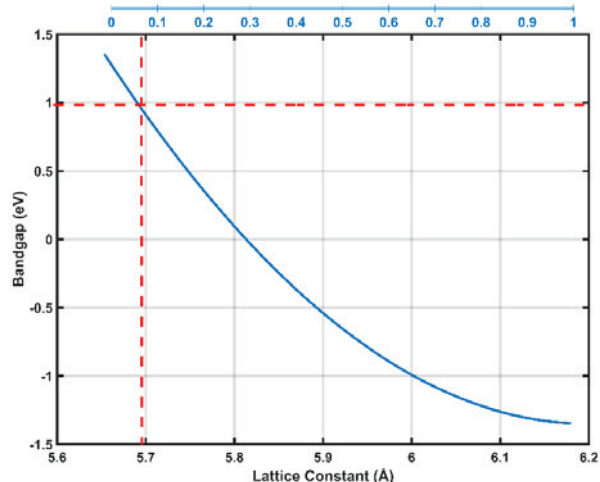


Figure 1: Optical bandgap of $\text{Ga}_{(1-x)}\text{Tl}_x\text{As}$ and lattice parameter as a function of increasing Tl content.

In lieu with this restriction, the MQW solar cell we designed considers a well $x = 0.07$ (7% Tl, highlighted in Figure 1), with a GaAs barrier repeated for N times. Table 1 shows the basic design of the structure.

Table 1: 1-D Device Structure of the MQW solar cell used in the simulations below

Layer	Material	Thickness
p-Contact	p-GaAs, $1 \times 10^{19} / \text{cm}^3$	20 nm
Emitter	p-GaAs, $1 \times 10^{18} / \text{cm}^3$	200 nm
MQW-Barrier	i-GaAs	10 nm
MQW-Well	i-GaTlAs	3 nm
Base	n-GaAs, $5 \times 10^{17} / \text{cm}^3$	1000 nm
n-Contact	n-GaAs, $3 \times 10^{18} / \text{cm}^3$	250 nm
Back Surface Field	i-GaAs	30 nm

Further design considerations like the thicknesses of the Quantum Well and Quantum Barrier regions were also derived off the experimental results obtained by Asahi et. al and were set at 3 and 10 nm respectively. The number of quantum wells however within the GaAs solar cell was varied to examine the change on performance it had on the overall device. Carrier lifetime was calculated to be approximately 17.2 ns as per the parameters obtained from our DTFT simulations and similar calculations done by Arakawa et. Al on similar MQW structures [16].

Table 2: GaTIAs electronic properties calculated for our device simulations

Material	Electronic Bandgap	Effective Electron Mass	Electron Mobility	Lattice Parameter
GaAs	1.43 eV	0.063m ₀	8500 cm ² /Vs	5.6353 Å
Ga _{0.93} Tl _{0.23} As	0.99 eV	0.048m ₀	6176.2 cm ² /Vs	5.6941 Å
TlAs	-1.35 eV	0.003m ₀	1723.5 cm ² /Vs	6.1827 Å

DEVICE SIMULATIONS

Our devices were simulated using the commercial package, Sentaurus TCAD, to measure its performance compared to a standard single junction GaAs, and how it improved its efficiency and overall absorption, the latter of which can be more readily observed through the different devices' simulated External Quantum Efficiency (EQE). The 1-D modelling of the devices was optical by nature while incorporating tunnelling effects caused by minor dislocations at the interface of the barrier and well structures for the MQW solar cells. By varying the number of quantum wells within the structure, and changing the incident input to a monochromatic source of light at a given wavelength, we were able to obtain and plot the change of the EQE vs wavelength for a control GaAs cell, and GaAs/Ga_{0.93}Tl_{0.7}As cells with 10, 15, 30 and 50 QWs, the results of which are plotted below in Figure 3.

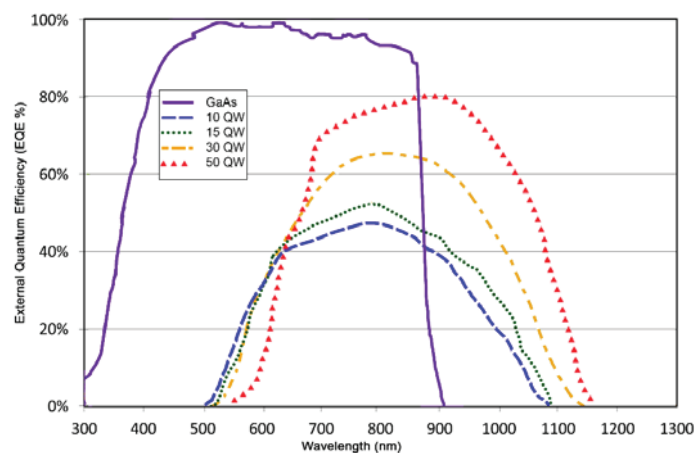


Figure 2: External Quantum Efficiency Plots for GaAs/Ga_{0.93}Tl_{0.7}As MQW Solar Cells normalized to the EQE of a single junction GaAs solar cell.

As is demonstrated by the results, adding as little as 10 QWs to the structure extends the absorption band from 900 nm to approximately 1085 nm, with the 50 QW structure extending it even further to 1168 nm, along with a peak photon conversion at 900 nm allowing for these lower energy photons that would have passed through GaAs to be absorbed and converted into electrical carriers. This is further illustrated in Figure 4 where the structures are illuminated under a standard AM 1.5 G spectrum and their respective J-V curves plotted against a standard single junction GaAs for comparison.

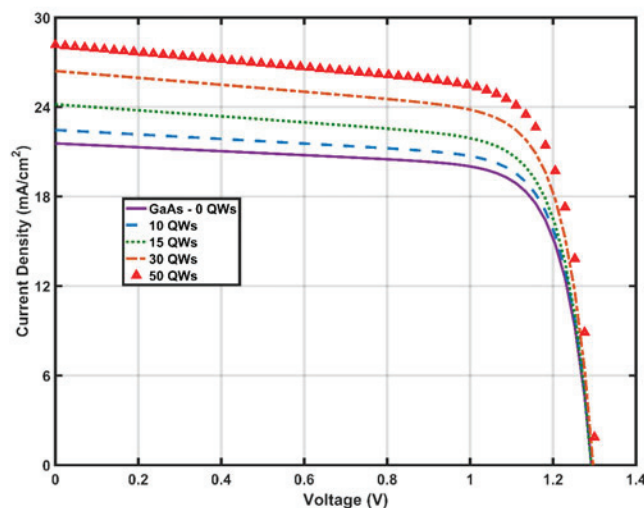


Figure 3: J-V curves of $\text{Ga}_{0.93}\text{Tl}_{0.07}\text{As}$ MQWs with varying numbers of QW structures. As noted, parameters like the short circuit current and the overall efficiency rise with increasing QWs.

The J-V curves show that the addition of QWs improves the short circuit current, and overall power generation from the device, with the power conversion increasing by 3.87% on an absolute scale for the 50 QW structure. The increase in efficiency is attributed to the improved photon absorption in the active region within the structure but also increases the carrier recombination within the device. This is in agreement with similar testing on InGaN/GaN MQW solar cells, which showed a performance saturation beyond 40 QWs [17]. Albeit not shown, we observe the same saturation at a QW count of 70, while being able to notice a decrease in some of the performance parameters between 10 and 50. The Fill Factor, for example, falls as a result of increasing shunt resistances in the model. The additional QWs create a longer path for the carriers to go through the device before being collected by the contacts at either end. Additionally, the higher the number of QWs, the more complex, and by extension expensive, the growth of these structures become, making it imperative that a cost-benefit analysis is carried through on the available options prior to committing to one device structure over the other. Table 2 shows the numerical values for some of the key performance parameters of these devices.

Table 3: Performance parameters of Ga₉₃Tl₇As/GaAs MQW Solar Cell under AM 1.5G for a selection of N QWs.

N, Number of Quantum Wells	Rated Efficiency	J_{sc} mA/cm ²	V_{oc} V	Fill Factor	Power Converted W/m ²
0	13.99 %	21.56	1.28	81.2 %	13.99
10	14.47 %	22.46	1.28	79.7 %	14.47
15	15.26 %	24.17	1.28	77.3 %	15.26
30	16.63 %	26.41	1.29	74.7 %	16.63
50	17.86 %	28.16	1.30	70.9 %	17.86

CONCLUSIONS

This analysis enclosed herewith lays a solid foundation for the future development and growth of GaAs/GaTlAs MQW solar cells that can be considered for solar energy harvesting purposes into the near infra-red. While limited to dilute concentrations, the significant drop in bandgap at concentration levels as low as 7%, allow for the implementation of these MQWs solar cells, with relative efficiency improvements going up to 21.7% (or an absolute efficiency gain of 3.87%) for the 50 QW solar cell device.

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