A performance optimization and analysis of graphene based schottky barrier GaAs solar cell

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Abstract. Performance optimization of Graphene-GaAs schottky barrier solar cell have been performed by considering variables such as substrate thickness, Graphene thickness, dependence between graphene work function and transmittance. The optimized parameter was extensively used to numerically model the design using TCAD Atlas. The results show the enhanced performance of the design with the optimized thickness of Graphene (0.3µ m) and GaAs (10µ m), resulting in significant increase in power conversion efficiency from 0.732% to 2.581% and reasonable fill factor up to 70%. It was further analysed that maximum potential was developed in the vicinity of the anode, which results in better charge collection hence improving the overall performance of the solar cell. The results are validated with the reported experimental work.

1. Introduction
The widely used Indium tin oxide (ITO) and fluorine tin oxide (FTO) as window electrodes in optoelectronic devices appear to be increasingly problematic mainly due to the limited availability of indium. Thus, a new unique material with a single atomic layer of carbon hexagon, Graphene have attracted lots of research in the last few years. This transparent single atomic layer has great potential application to replace high cost ITO and FTO as a window layer in solar cell [1]. The flexibility, robustness, environmental stability and optical transparency of Graphene with high mobility and near zero bandgap [2] is believed to have a great potential in optoelectronics and photonics application. Few layer graphene and single layer graphene have been produced by Chemical vapor deposition (CVD) [3]. Graphene sheets have also been produced by mechanical exfoliation via repeated peeling of highly ordered pyrolytic graphite (HOPG) or by chemical oxidation of graphite [4]. Graphene based solar cells have been recently fabricated on various substrate such as Si [5], CdS [6] and GaAs [7]. Wenjing et al. successfully transferred single and bilayer graphene on n-type GaAs to form Schottky junction yielding a power conversion efficiency of 1.95% [8]. GaAs in comparison with most commonly used Si Substrate, GaAs being highly resistant to radiation [9] and having direct band gap [10] makes it suitable for highly efficient solar cell both for terrestrial and space application, but it is necessary to study the band parameter and optimize various thickness of the structure of solar cell to make it more efficient. Hence,
in this paper we have optimized the thickness of the GaAs substrate with graphene layer in SILVACO TCAD, and the result obtained have been validated with published experimental data.

2. Optimization of GaAs and graphene thickness

The illuminated AM 1.5 spectrum is plotted using Silvaco Atlas in Figure 1, which shows the wavelength corresponding to the peak solar spectrum is 0.473 µm, this value has been precisely extracted using HP4151 Tonyplot tool in Silvaco, hence the absorption coefficient of GaAs corresponding to the wavelength is approximately calculated as 152086.1014706021 (cm⁻¹).

The Beer-Lambert’s equation \( \frac{dI}{dx} = -\sigma N dx \), where \( I_x \) intensity of the incoming wave in x direction, \( \sigma \) is the lattice vibration/absorption per unit area, which gives the equation (1)

\[
I = I_0e^{-\sigma t}
\]  

(1)

where \( I \) is the intensity of the transmitted wave and \( I_0 \) is the intensity of the incoming light, and \( t \) is the thickness of the material in which the light is illuminated, obtaining a fitness function using equation (1), the different optimized GaAs thickness is plotted in Figure 2 for different transmittance of graphene. Kostya S. et al [11] gives experimentally obtained the transmittance and thickness for different number of graphene layer, using this experimental value and curve fitting, Figure 3 gives the plot of different transmittance of graphene layer with corresponding graphene thickness.

![Figure 1. The illuminated AM 1.5 spectral irradiance varying with the wavelength, absorption coefficient of GaAs and wavelength.](image1)

![Figure 2. Graphene transmittance vs GaAs thickness.](image2)
Using this values from published experimental data in Figure 3 and the calculated optimized GaAs thickness in Figure 2, we obtain a noble optimized thickness of the GaAs corresponding to different thickness of graphene which is given in Figure 4, which can be used for modeling of optimized structure of Graphene-GaAs solar cell.

![Figure 3](image1.png)

**Figure 3.** Plot of different transmittance of graphene for different thickness of graphene.

![Figure 4](image2.png)

**Figure 4.** Optimised GaAs thickness for different layer of graphene.

### 3. Device structure and modelling

Figure 5 shows the proposed structure of the graphene, the device consists of three regions. The top area is covered with multilayer graphene followed by SiO$_2$ window layer which have been grown upon GaAs substrate. The first step in the modelling of device in any TCAD is the definition of mesh, the mesh must be defined in such a manner that it doesn’t not take much unnecessary simulation time at the same time it must give high accuracy, thus Figure 6 shows the meshing of the modelled structure, it can be seen that the density of mesh is high in the top portion of the device as it consists of Graphene GaAs junction and also Graphene, SiO$_2$ junction. Any semiconductor could form schottky junction with certain metal provided that the semiconductor has a moderate carrier density and the difference of workfunction between the metal and the semiconductor is big enough which would give rise to a schottky barrier.

![Figure 5](image3.png)

**Figure 5.** Structure of the proposed schottky barrier graphene GaAs solar cell.

![Figure 6](image4.png)

**Figure 6.** Generated finer mesh model of the design.

The I-V characteristics of the schottky-barrier solar cell is given by [12] which is expressed in equation (2)
\[ I_o = \alpha A^{**} T^2 \exp(-e\phi_{Bn} / kT) \]  

(2)

where \( \alpha \) is the cell area, \( A^{**} \) the effective Richardson constant (which depends on the current–transport mechanism considered), and \( \phi_{Bn} \) the metal-semiconductor (taken here to be n-type) barrier height as expressed in equation (3). \( T \) is absolute temperature and \( B \) is the Boltzmann’s constant. And barrier height for p-type semiconductor \( \phi_{Bp} \) is expressed in equation (4)

\[ \phi_{Bn} = \phi_G - \chi, \text{ for an n-type semiconductor} \]  

(3)

And, \( \phi_{Bp} = E_G - \phi_G + \chi, \text{ for p-type semiconductor} \]  

(4)

where, \( \phi_G \) is the workfunction of graphene, \( \chi \) is the electron affinity of the semiconductor and \( E_G \) is the semiconductor energy gap. The major parameters used in the modelling and simulation in the Graphene GaAs are given in Table 1, which have been obtained from various literature reviews, when sunlight is illuminated in the Graphene GaAs solar cell, electron hole pair are formed this electron hole pairs are separated by the built in electric field at the schottky junction, thus electrons are collected at the electrode, Figure 7 shows the energy band diagram and the photovoltaic action of Graphene n-GaAs solar cell.

![Energy band diagram of graphene n-GaAs solar cell.](image)

**Figure 7.** Energy band diagram of graphene n-GaAs solar cell.

**Table 1.** Major parameter for Graphene GaAs solar cell.

| Materials                                      | GaAs          |
|------------------------------------------------|---------------|
| Band gap \( E_g \) (eV) at 300 K              | 1.42          |
| Lattice constant \( \alpha \) (Å)             | 5.653         |
| Affinity (eV)                                 | 4.07          |
| e-mobility, MUN (cm²/V × s)                   | 8000          |
| h+ mobility, MUP (cm²/V × s)                  | 400           |
| Conduction band effective Density of state, \( N_c \) (cm⁻³) | 4.35×10¹⁷ |
| Valance band effective Density of state, \( N_v \) (cm⁻³) | 8.16×10¹⁸ |
| Nature of Energy Gap                          | Direct        |

Since Graphene is a new material, it is currently unavailable in the material library of SILVACO Atlas, thus in order to create an acceptable and accurate model of Graphene layer, initially Graphene layer have been defined with material as 4H-SiC and then the material properties of 4H-SiC were modified to give the material metallic characteristics while also matching experimental sheet resistance values [13]. Without altering the optical properties of 4H-SiC material model, firstly it was made to be
completely transparent, than the transmittance of the Graphene is input by constructing an .nk file for graphene using the experimental value from [14]. Thus, graphene is modeled as a semimetal, with carrier mobility of 15,000 cm²/Vs. The carrier densities were calculated by Fermi distribution and by adjusting the values of effective masses, a thickness of 10 nm, and band gap such that the carrier densities agree with experimental results.

4. Results and discussion

4.1. Effects of GaAs substrate thickness

The modelled device was illuminated with AM1.5G solar spectrum to simulate the global terrestrial sunlight, the LUMINIOUS 3D takes into account for the simulation of sunlight in SILVACO Atlas. The GaAs crystal substrate is acts as the absorption area hence it can be seen in that the photogeneration is maximum on GaAs as shown by the contours in Figure 3, on the other hand Graphene layer acts as a transparent electrode, for the intensity of photogenerated carriers and the workfunction difference between Graphene-GaAs junction is the built in Schottky junction. Figures 8 and 9 show the photogeneration rates of GaAs solar cell under AM1.5 illumination with depth for absorption layer were maintained at 5μm, 10μm respectively. The light could be absorbed in barrier layer and inside the semiconductor. The photogeneration rate is given by 
\[ G = \eta_0 \frac{P \lambda}{h c} e^{-\alpha y}, \]
where \( P \) is the cumulative effect of reflection, transmission and loss due to the absorption over the ray path, \( y \) the relative distance for the given ray, \( h \) the Planck’s constant, \( \lambda \) the wavelength, \( c \) the speed of light and \( \alpha \) the absorption coefficient calculated for each set of (n,k) values, \( \eta_0 \) internal quantum efficiency, which represents number of carrier generated per photon per pair. Both results show the most effective absorption area located in the surface attachment about 0.1 μm. For a graphene thickness of 0.5 μm the optimized GaAs thickness is approximately 10 μm, hence Figure 9, which is the optimized structure shows better photogeneration rate which validates our optimization data.

4.2. Analysis of \( I_{sc} \), \( V_{oc} \)

Short circuit current (\( I_{sc} \)) & open circuit voltage (\( V_{oc} \)) are very important parameter in the analysis of the performance of the solar cell as the output power of the solar cell depends on these two factors, \( I_{sc} \) is the maximum current that can flow, whereas the maximum voltage in open circuit is called the \( V_{oc} \). The expression for open circuit voltage is given equation (5)

\[
V_{oc} = \frac{kT}{q} \ln \left[ \frac{q \phi_h + J_0 (1 + r_s \beta)}{J_0 (1 + r_s \beta)} \right]
\]
where $r_g$ is the generation enhancement ratio, and the field factor can be calculated using equation (6) as

$$FF = \frac{V_{OC} - \frac{Ln(V_{OC} + 0.72)}{V_{OC} + 1}}{V_{OC} + 1}$$

Table 2 gives the output result of the modelled solar cell for different GaAs substrate thickness, it must be noted that for the substrate thickness of 10 um, maximum $J_{SC}$, $V_{OC}$ and FF is obtained, giving maximum efficiency of 2.581%. Figure 10 shows the overlay of I-V curve of various GaAs thickness for 0.3 µm graphene thickness. The potential developed is shown in Figure 11, which shows that maximum potential is developed at the anode vicinity, which implies in better charge collection.

Table 2. Performance output from various GaAs substrate thickness cell.

| GaAs substrate thickness | Short circuit current, $J_{SC}$ (mA/cm²) | Open circuit Voltage, $V_{OC}$(V) | Field Factor, FF (%) |
|--------------------------|------------------------------------------|----------------------------------|----------------------|
| 1 um                     | 1.555e-009                               | 0.337566                         | 63.9252              |
| 2 um                     | 1.917e-009                               | 0.351637                         | 65.9488              |
| 5 um                     | 2.091e-009                               | 0.356200                         | 69.0916              |
| 10 um                    | 2.141e-009                               | 0.357314                         | 69.7376              |

5. Conclusion
A novel optimization has been performed using result from published experimental data and generating fitness function for the thickness of GaAs and Graphene in schottky barrier graphene GaAs solar cell. These optimised values have used for numerically modelling of the solar cell in SILVACO TCAD Atlas, and it was verified that the performance of the solar cell increases significantly with the obtained optimised parameter. It was further analysed that maximum potential was developed in the vicinity of the anode, which results in better charge collection hence improving the overall performance of the solar cell. This remarkable optimization technique as well as data can be used in the study, design and development of different structure of graphene based solar cell.

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