

DESIGN AND OPTIMIZATION OF A HETERO-JUNCTION SOLAR CELL USING SILVACO SOFTWARE PACKAGES

Muhammad Fairuz Osman
B.Eng. (Hons) Electrical Engineering
Faculty of Electrical Engineering
Universiti Teknologi MARA
40450 Shah Alam, Selangor.
Email: fross@streamyx.com
Supervisor: Assoc. Prof. Dr. Mohamad Rusop
Co-Supervisor: Mr. Uzer Mohd. Noor

Abstract: In this paper, the design and optimization of a hetero-junction solar cell, utilizing a simulation using Silvaco software packages have been demonstrated. In this study, a hetero-junction of GaAs/AlGaAs solar cell and a single p-n junction Si solar cell were simulated. Firstly, fundamentals of solar cell operation, performance and designs issues have been presented. The simulation of the solar cells using Silvaco TCAD Tools consisted of processes simulation of constructing solar devices in ATHENA and simulation of electrical characteristics of solar devices in ATLAS. The results from both simulations of the hetero-junction of GaAs/AlGaAs solar cell and a single p-n junction Si solar cell were analyzed to compare their performances. Then, the paper was concluded with an argument that the hetero-junction solar cell would provide better performance and efficiency over the single junction Si solar cell. Finally, the future design improvements have been suggested.

Keywords: Solar Cell; Heterojunction; Photovoltaics; Efficiency; Photogeneration; Bandgap Energy

1.0 Introduction

One of the today's biggest challenges is how to supply our increasing need for energy. With the shortage of fossil fuels these days, it is needed to consider renewable energy sources such as photovoltaics. When exposed to light, solar cells are capable of producing electricity for many years while requiring only minimal maintenance and operational costs. Currently, the wide-spread use of photovoltaics over other energy sources is limited by the relatively high cost and low efficiency of solar cells.

Hetero-junction solar cells offer higher efficiencies compared to traditional solar cells made of a single layer of semiconductor material. Depending on the particular technology, hetero-junction solar cells are capable of generating approximately more power under the same conditions than single junction solar cells made of silicon.

Hetero-junction solar cells are composed of two layers of materials that have different bandgaps. The top layer has a larger bandgap while the bottom layer has a smaller bandgap. This design allows less energetic photons to pass through the upper layer and be absorbed by a lower layer, which increases the overall efficiency of the solar cell.

1.1 Fundamental Solar Cell Concepts

Solar cells are semiconductor devices that are designed to generate electric power when exposed to electromagnetic radiation. The spectrum of light given off by the sun is shown as in Figure 1.

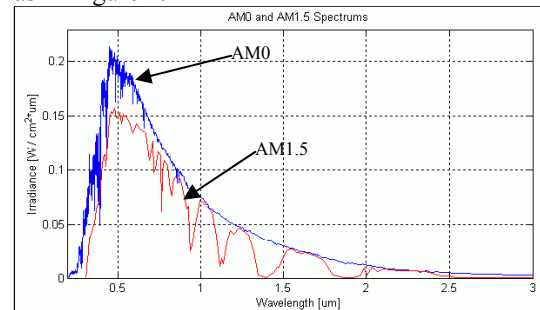


Figure 1: Spectrum of solar radiation in space, AM0 (blue) and on earth, AM1.5 (red) [2].

Solar cells consist of one or more p-n junctions. Light enters the semiconductor material through the n region and generates an electron-hole pair (EHP) in the material due to the photoelectric

effect. The n region is designed to be thin while the depletion region is thick. If the EHP is generated in the depletion region, the built-in electric field drifts the electron and hole apart. The result is a current through the device called the photocurrent. If the EHP is generated in the n or p regions, the electron and hole drift in random directions and may or may not become part of the photocurrent [1].

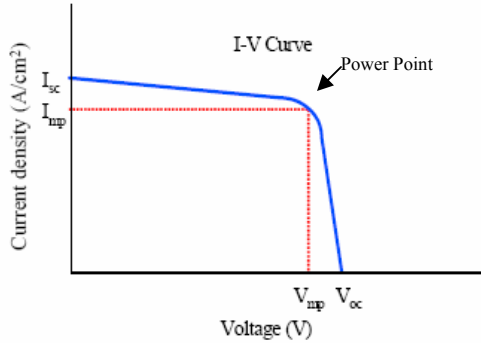


Figure 2: Current versus voltage curve (I-V curve) for a typical solar cell [3].

The following terms determine the performance of a solar cell:

- **Short-circuit Current, J_{sc} :** The current of a solar cell when the top and bottom (negative and positive leads) are connected with a short circuit. This is the horizontal intercept on the I-V curve shown in Figure 2.
- **Open-circuit Voltage, V_{oc} :** The voltage between the top and bottom of a solar cell. This is the vertical intercept on the I-V curve shown in Figure 2.0.
- **Power Point:** The point on the I-V curve of a solar cell at (J_{pp}, V_{pp}) that generates the maximum amount of power for the device. This is the point that encloses the most amount of area in the first quadrant when vertical and horizontal lines are drawn from the point. This represents power since the area is equivalent to the current times voltage of the cell. The power point is shown in Figure 2.
- **Fill Factor, FF:** A percentage given by Equation 1 that describes how close the I-V curve of a solar cell resembles a perfect rectangle, which represents the ideal solar cell.

$$\text{Fill Factor} = \frac{V_{pp} * J_{pp}}{V_{oc} * J_{sc}} \quad (\text{Eq. 1})$$

- **Quantum Efficiency:** The number of EHPs that are created and collected divided by the number of incident photons [1]. This is a percentage since each photon can produce at most one EHP.
- **Overall Efficiency:** The percent of incident electromagnetic radiation that is converted to electrical power. Often the overall efficiency for a given solar cell depends on many factors including the temperature and amount of incident radiation.

1.2 Basic Concept of Hetero-junction Solar Cells

In a normal single layer solar cell, much of the energy of incident light is not converted into electricity. If an incident photon has less energy than the bandgap of the semiconductor material, the photon cannot be absorbed since there is not enough energy to excite an electron from the conduction band to the valence band. Therefore, none of the light with less energy than the bandgap is converted in the solar cell. If an incident photon has more energy than the bandgap, the excess energy will be converted into heat since the electron can only absorb the exact amount of energy required to move to the valence band.

Hetero-junction solar cells can make better use of the solar spectrum by having different semiconductor layers with different bandgaps. Each layer is made of a different material, which usually is a group III-V semiconductor, and absorbs a different portion of the spectrum. The top layer has a larger bandgap so that only the most energetic photons are absorbed in this layer. Less energetic photons have to pass through the top layer since they are not energetic enough to generate EHPs in the material. The bottom layer has a smaller bandgap than the previous. Therefore, each layer absorbs the photons that have energies greater than the bandgap of that layer and less than the bandgap of the higher layer.

1.3 Design Considerations Bandgaps

How much energy can be obtained from each photon is determined by the bandgaps. Ideally the difference between adjacent layers of the solar cell is approximately constant so that each layer can absorb an equal amount of the

spectrum of incident light shown in Figure 1. The difference between bandgaps should be made as small as possible since the amount of excess energy from light converted to heat is equal to the difference between the photon energy and the bandgap of absorbing material. Furthermore, the solar cell should take advantage of as much of the spectrum as possible so the top layer should have a high bandgap and the bottom layer should have a small bandgap that most part of the spectrum can be absorbed as possible.

Lattice Constant

In monolithic hetero-junction solar cells, the different semiconductor layer is grown directly on top of the other layer using the same substrate. As a result of this method, the lattice constant, which describes the spacing of the molecules of a crystal structure, must be the same for all of the layers.

Current Matching

Since the current flows through a solar cell from the top to the bottom, the layers of a hetero junction solar cell are in series. Therefore, the current passing through each layer must be the same and the current produced by the solar cell is limited by the layer that produces the least amount of current. For maximum efficiency, the cell must be designed so that each layer produces the exact same current. The current is proportional to the number of photons absorbed in each layer. The two most important factors in determining the thickness of each layer is the number of photons in the spectrum that the layer should absorb and the absorption constant of the material. The light intensity decreases exponentially with penetration depth into a material where the exponential constant is called the absorption constant [1:221]. A layer with a low absorption constant must be made thicker since on average a photon must pass through more of the material before it is absorbed. Properly designing the thickness of each semiconductor material based on these factors will match the current produced by each layer.

2.0 Methodology

The solar cells were simulated in ATHENA and ATLAS. The simulation consisted of:

- construction of solar cell doping and geometry
- simulation of short circuit current
- simulation of open circuit voltage
- simulation of spectral response

2.1 The first part of the simulation was to create a hetero-junction solar cell structure, using ATHENA. The hetero-junction solar cell presented in this paper was constructed of two layers different band gap material, GaAs and AlGaAs in p-n-n configuration. The junction of n type was grown over p type GaAs. Then, a layer of n⁺ was grown over the GaAs layer. Finally, an n⁺ type of AlGaAs was layered on top of n type of GaAs. A single contact was placed in the center of the structure. The process consisted of an implant and diffusion followed by electrode formation. The electrode statement was then used to define the electrodes for ATLAS.

2.2 The first simulation run in ATLAS simulated the response of the device to illumination by the solar spectrum. At the start of the file, the material parameters for the structure were set. The imaginary refractive index (which was directly related to the absorption coefficient) of the metal was defined to a high value to ensure it was opaque to the incident radiation.

2.3 The Illumination by solar spectrum was defined by the beam statement. The origin and angle of incidence needed to be defined. An angle of 90 degrees means normal incidence from the top. The parameter power.file points to an external file that contains a list of wavelength vs. intensity. The file 'optoex08.spec' contained data for the Air Mass Zero Solar Spectrum. The intensity in the file was considered just as relative intensity between the wavelengths. The actual power in Watts/cm² was set by the b1 parameter of the solve statement. The photo-generation rate would appear in the solution structure file.

2.4 Anode and cathode was shorted to obtain short circuit current. This was simulated by illuminating the device with zero voltage on all contacts. The B<n> parameter of the solve statement sets the power of the light defined as beam <n>. An extract statement was used to measure the short circuit current.

2.5 The system was reset using the command 'solve init' for the second test to simulate open circuit voltage. The current through the device was forced to be zero. The device is illuminated and then the voltage across the device was measured. To set the current to zero it was first necessary to set one electrode to have current boundary conditions.

This was done on the cathode using the current parameter of the contact statement Simulating with the device illuminated and $icathode=0$ gives the open circuit voltage. This voltage was measured using the extract statement Note the use of the syntax `vint."cathode"` as opposed to `v."cathode"`. This was necessary when it needed to extract the voltage directly on the semiconductor contact as opposed to the applied bias. The structure stored at this point was plotted to show contours of photogeneration, carrier concentration or potential.

2.6 The second ATLAS run in this simulation was used to simulate the spectral response of the solar cell. At the start, the definition of material parameters and opaque metal contact is repeated. For this test a different light beam was required. A beam origin and angle of incidence were set as before. The wavelength or spectrum file was not set since the wavelength was to be varied in this simulation. The short circuit case was considered so zero biases were set on both electrodes. The parameter `lambda` of the solve statement was used to set the wavelength of the incident light. The range of wavelength used was 300 nm to 1000 nm.

2.7 Plotting the resulting log file, it was possible to see how the cathode current varied with wavelength. Setting a plot versus wavelength of source photocurrent (current available in the light beam), available photocurrent (current available for collection) and actual cathode current showed how the device behaved. This simulation has produced all the data needed to create a plot of efficiency versus optical wavelength.

3.0 Results and Discussion

3.1 The hetero-junction solar cell presented in this paper was constructed of two layers of GaAs and AlGaAs in p-n-n configuration. The n^+ layer was grown over p-type of GaAs. Then, the n^+ layer of AlGaAs was then layered over the p-n junction of GaAs to form p-n-n heterojunction solar cell. The physical structure of the cell is shown as in Figure 3.

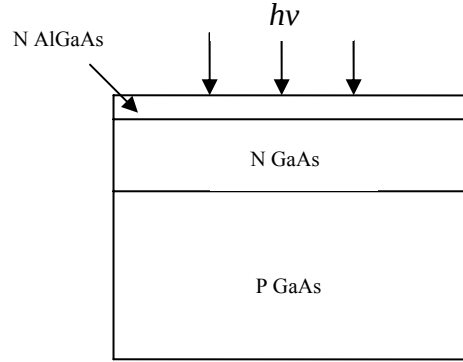


Figure 3: Heterojunction of AlGaAs/GaAs

The structure of GaAs/AlGaAs hetero-junction solar cell was modeled in Athena and it was then simulated in Atlas to determine its performance characteristics. The device was simulated under light illumination of Air Mass Zero (AM0) of solar spectrum.

3.2 The photogeneration rate of a hetero-junction solar cell of AlGaAs/GaAs is shown in Figure 4. The maximum photo-generation rate is about 21.2 /scm^3 . The rate is decreasing drastically from the top surfaces through the bottom of the structure as the light intensity decreases as it penetrates deep into the structure. The minimum value of the photo-generation rate is 2.65 /s.cm^3 .

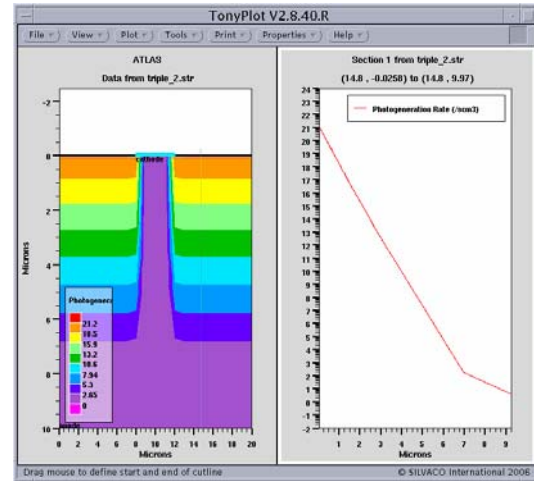


Figure 4: Photo Generation Contour

3.3 When photons with energy higher than the bandgap are incidents, it becomes absorbed to photogenerate a free EHP that is an electron in the conduction band and a hole in valence band. The photo generation takes place in the depletion layer. The electric field in the depletion layer then separates the EHP and drifts them in opposite directions until they reach the neutral region. The drifting carriers generate a current called photo current [4].

3.4 Since the photogeneration determines photo-current, as the photo-generation rate decreasing, the current density of device is consequently decreasing from the surface through the bottom. The total current density according to the depth of the structure is shown in Figure 5. The maximum current density generated is approximately 0.0775 A/cm^2 . Even though, the current density only peaks at near the surface of the cell due to a higher concentration of electrons at this point.

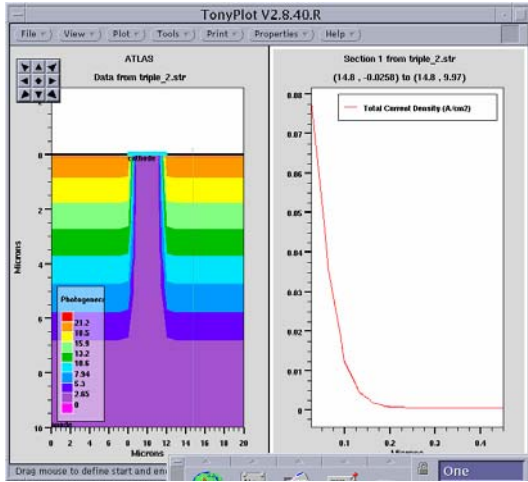


Figure 5: Current Density

3.5 Furthermore, the potential of the region in the solar cell's structure is described as shown in Figure 6. At the surface, the potential is about -0.225 V . The maximum negative potential, which is -0.5 V generated after 1.0 micron from the surface and the potential is leveled off after this level. The potential is developed through the device structure due to electric field formed from the positive space charge site to the negative space charge site.

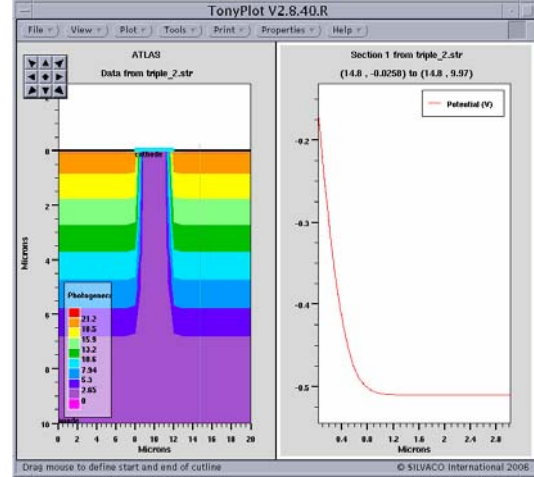


Figure 6: Potential in Device Structure

3.6 The spectral response is shown as in Figure 7. From the Figure 7, the maximum cathode current produced is $0.125 \mu\text{A}$, when the optical wavelength is about $0.85 \mu\text{m}$. However, the cathode current drops drastically after optical wave length of $0.87 \mu\text{m}$. This is the point what is called the cutoff wavelength for GaAs, where the GaAs can not absorb the photons anymore and can not generate EHP [1]. The figure also shows the available photo current produced by the AM0 radiation and photo-current generated in the solar cell. From the spectral response simulation, it can be seen that the heterojunction of GaAs/AlGaAs covers more range optical wavelength of light spectrum than the single p-n junction of Si.

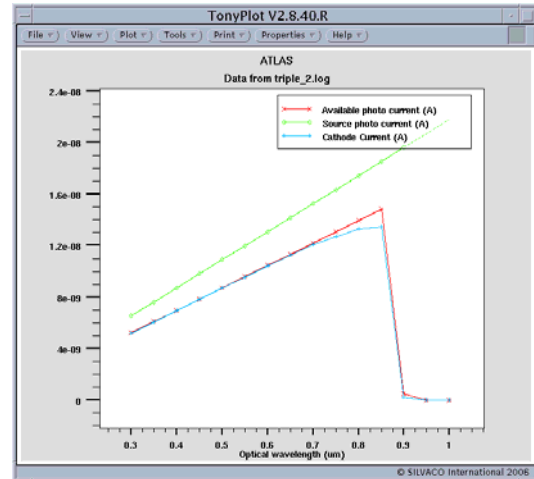


Figure 7: Spectral Response. Current versus Optical Wavelength.

3.6 The quantum efficiency of the hetero-junction solar cell is portrayed in the Figure 8. The efficiency is decreasing gradually after the optical wavelength of about $0.7\mu\text{m}$ as the optical wavelength increases. The maximum quantum efficiency found in the simulation is about 0.8 compared to 0.78 found in the single p-n junction Si solar cell. However, the efficiency of the device drops suddenly after the optical wavelength of $0.87\mu\text{m}$, where it is the cutoff wavelength for GaAs. Therefore, beyond this point, the cell cannot convert the light energy into electrical anymore.

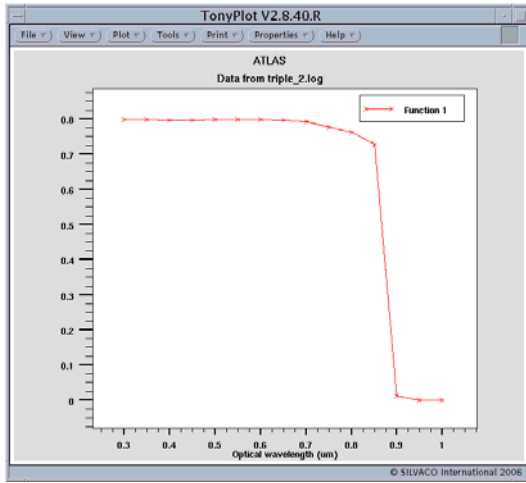


Figure 8: Quantum Efficiency

Configuration	Isc (A)	Voc (V)
Si p-n	4.81931e-10	0.309712
GaAs/AlGaAs p-n-n	4.75013e-10	0.840744

Table 1.0: Comparison Isc and Voc between a single p-n junction of Si solar cell and a heterojunction GaAs/AlGaAs solar cell.

3.7 From the comparison as in Table 1.0, it is shown that the value of Isc for hetero-junction of p-n-n of GaAs/AlGaAs is smaller than that of a single p-n junction of Si. It thus proves that a leakage current in the hetero-junction is smaller than the one found in the single junction of Si. On the other hand, the open circuit voltage, Voc for the hetero-junction of p-n-n of GaAs/AlGaAs is greater than the one found in the single p-n junction of Si. This implies that the hetero-junction of GaAs/AlGaAs has a higher electrical potential energy.

4.0 Future Improvements

The current use of AlGaAs and GaAs for the layers of a hetero junction solar cell can be improved. The GaAs layer absorbs too much of the spectrum, since the difference between the bandgap of the top two layers is 0.37eV. Using a new semiconductor layer that has a bandgap of 1.25 eV will make the cell more efficient since the bandgaps will differ by a constant 0.18 eV. Another possible design improvement keeps the three AlGaAs and GaAs, layers but adds another layer of a material with a bandgap of between 1.43eV and 1.8 eV. This new three junction solar cell will have a difference of lower bandgap energy between each adjacent layer

5.0 Conclusions

Using Silvaco's Software packages, Athena and Atlas is an innovative approach to design and simulate solar cells. In this simulation, all the parameters can be set according to the desired values and condition. Using Silvaco's software packages, heterojunction GaAs/AlGaAs solar cell was successfully built and simulated. In conclusion, from the simulation results, hetero-junction GaAs/AlGaAs solar cell offers better performance and efficiency over single p-n junction Si solar cell.

6.0 Acknowledgement

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