Simulation and optimization performance of GaAs/GaAs$_{0.5}$Sb$_{0.5}$/GaSb mechanically stacked tandem solar cells

Y R Tayubi$^*$, A Suhandi$^1$, A Samsudin$^1$, P Arifin$^2$ and Supriyatman$^3$

$^1$Department of Physics Education, Universitas Pendidikan Indonesia, Indonesia
$^2$Department of Physics, Institut Teknologi Bandung, Indonesia
$^3$Department of Physics Education, Universitas Tadulako, Indonesia

*Corresponding author’s e-mail: rachmat@upi.edu

Abstract. Different approaches have been made in order to reach higher solar cells efficiencies. Concepts for multilayer solar cells have been developed. This can be realised if multiple individual single junction solar cells with different suitably chosen band gaps are connected in series in multi-junction solar cells. In our work, we have simulated and optimized solar cells based on the system mechanically stacked using computer simulation and predict their maximum performance. The structures of solar cells are based on the single junction GaAs, GaAs$_{0.5}$Sb$_{0.5}$ and GaSb cells. We have simulated each cell individually and extracted their optimal parameters (layer thickness, carrier concentration, the recombination velocity, etc), also, we calculated the efficiency of each cells optimized by separation of the solar spectrum in bands where the cell is sensible for the absorption. The optimal values of conversion efficiency have obtained for the three individual solar cells and the GaAs/GaAs$_{0.5}$Sb$_{0.5}$/GaSb tandem solar cells, that are: $\eta = 19.76\%$ for GaAs solar cell, $\eta = 8.42\%$ for GaAs$_{0.5}$Sb$_{0.5}$ solar cell, $\eta = 4.84\%$ for GaSb solar cell and $\eta = 33.02\%$ for GaAs/GaAs$_{0.5}$Sb$_{0.5}$/GaSb tandem solar cell.

1. Introduction

Using Tandem solar cells is one of the methods for achieving high efficiency in transforming solar energy into electricity $[1-3]$. In this approach, cells of different band gaps are placed optically in series, either during the growth process or joined together after individual processing $[4]$. The basic idea of high-efficiency multi-junction solar cells is to stack multiple materials, with different band gaps, on top of each other in order to absorb the applied spectrum as efficient as possible. By using multiple junctions a high cell voltage can be realised, which is not possible when using only one broadband absorbing semiconductor. Using an infinite stack of materials, the limiting efficiency of photovoltaic energy conversion is 85 percent $[5]$. A key issue in the design of multi-junction solar cells, with a finite amount of junctions, is to select the right materials with the best possible combination of band gaps. The optimum combination of materials is also influenced by the method of stacking and the amount of terminals. There are two major approaches to the construction of multijunction solar cells. The mechanically stacked approach physically stacks independently-grown layers. The second approach is the monolithically grown, where each semiconductor is sequentially grown on top of the other as one single piece $[4]$. Mechanical tandem solar cell architecture is attractive because two separate devices
could be developed independently targeting a specific part of the incident spectrum and subsequently put together to form a tandem module avoiding tunnel junctions [6]. Solar cells made from III-V semiconductors can be arranged in a cascade architecture which increases their efficiency [7-9].

The single junction solar cells of the gallium arsenide (GaAs) currently have the highest conversion efficiency of 23.4% [6]. However, because of its energy band gap of about 1.4 eV, these solar cells cannot absorb and convert infrared spectra from the sun's. To improve the conversion efficiency that can be achieved, the GaAs solar cells can be paired tandem with other solar cells that have narrow band gap that are sensitive to the infrared spectrum. Suitable materials for application in a bottom cell structure are low band-gap materials, with a band-gap between 0.6 and 0.9 eV [4].

To date we have reported the successful fabrication of GaAs /Si tandem solar cells which achieved 29.6% efficiency and GaAs/Ge tandem solar cells which achieved a 26.1% efficiency with optimized structure [10]. Gallium Antimonide (GaSb) is a III-V ternary alloy semiconductor material that has an energy gap of 0.72 eV so it is potential to be marked with GaAs solar cells. Compared to Ge, GaSb has several advantages; first, the GaSb band gap (0.72 eV) is higher than the Ge band gap (0.66 eV) so that it will generate a higher open circuit voltage (Voc); second, GaSb is a semiconductor material that has a direct band gap while Ge has a the indirect band gap, so that it will be able to generate higher photocurrents. Thus the GaSb solar cell will have greater conversion efficiency than the Ge solar cell.

Because of the difference in band gap between GaAs (1.4 eV) with GaSb solar cells (0.72 eV) is quite large then between the two solar cells can be inserted other solar cells that have a band gap between them. Materials for these solar cells must be selected that are crystalline compatible with GaAs and GaSb solar cells. For that purpose can be selected ternary GaAs0.5Sb0.5. If these three solar cells are arranged into one tandem solar cell, a GaAs/GaAs0.5Sb0.5/GaSb tandem solar cell with triple-junction is obtained.

The purpose of this work comes to contribute to the optimisation of the performance of GaAs, GaAsSb and GaSb solar cells by the determination of physical and technological parameters giving the best photovoltaic conversion efficiency. The optimal values of physical parameters giving the best current of short-circuit and voltages of open circuit as well high conversion efficiency have obtained for the three solar materials. This article describes the theoretical efficiencies that can achieved by each GaAs, GaAs0.5Sb0.5/GaSb, and GaSb solar cells and the conversion efficiency achieved by GaAs/GaAs0.5Sb0.5/GaSb triple-junction tandem solar cells with mechanically stacked structures.

![Figure 1. Structure of GaAs/GaAs0.5Sb0.5/GaSb triple-junction tandem solar cell.](image)
2. Methods

Modelling and optimization of a conventional solar cell performance p-n junction are determined by sequential solving of equations of semiconductors by analytical method. The performances of solar cells can be done by optimization of physical and technological parameters giving the best short-circuit current, opencircuit voltage and efficiency. To reproduce faithfully the shape of solar cell, the models describing the physical parameters of materials necessary for simulation (dielectric constant, gap energy, refractive index, intrinsic concentration, etc.) are included in the program. The tandem solar cells structures of our study are shown on the Fig. 1.

Numerical simulations were performed with a Sigma Plot for Window software. When the p-n junction solar cell is irradiated, then in the solar cell it will be generated photocurrent and dark current. Photocurrent that can be generated in a solar cell is formulated as follows: [11]

\[ J_{ph} = J_{n,ph} + J_{p,ph} + J_{scr,ph} \]  \hspace{1cm} (1)

With

\[ J_{n,ph}(X_1) = K_1 a L_n \exp(-a X_1) + \frac{K_1}{A} x[(S_f L_n / D_n + a L_n) - \exp(-a X_1) \left( (S_f L_n / D_n) + \cosh(X_1 / L_n) \right) + \sinh(X_1 / L_n)]] \]  \hspace{1cm} (2)

\[ J_{p,ph}(X_2) = K_2 a L_p B x\left[(S_b L_p / D_p) \left( \cosh(W_b / L_p) \right) - \exp(-a W_b) \right) + \sinh(W_b / L_p) + a L_p \exp(-a W_b)] \]  \hspace{1cm} (3)

\[ J_{scr,ph} = qF(1 - R) \exp(-a X_1)(1 - \exp(-a W_b)) \]  \hspace{1cm} (4)

Here

\[ A = (S_f L_n / D_n) \sinh(X_1 / L_n) + \cosh(X_1 / L_n) \]
\[ B = (S_b L_p / D_p) \sinh(W_b / L_p) + \cosh(W_b / L_p) \]
\[ K_1 = qF(1 - R) a L_n / (\alpha^2 L_n^2 - 1) \]
\[ K_2 = [qF(1 - R) a L_p / (\alpha^2 L_p^2 - 1)] \exp(-a X_2) \]
\[ W_b = X_b - X_2 \]

\( F(\lambda) \) is a photon flux density that is the number of photons that incident to the front surface of a solar cell per cm² per second per unit of wavelength band width. For the condition of AM1.5 can be approximated by two linear curve equations as follows: [11]

\[ F(\lambda) = C(19.7\lambda - 4.7) \times 10^{15} \] for \( 0.24 \leq \lambda \leq 0.47 \mu m \)
\[ F(\lambda) = C(-2.5\lambda - 5.7) \times 10^{15} \] for \( \lambda \geq 0.48 \mu m \)

C is the sun concentration, \( C = 1 \) for the 1 sun condition.

The above irradiance current density equation applies to a certain wavelength (\( \lambda \)) and is suitable only for very narrow wavelength band width (≈100 Angstrom). Thus the total current density of the irradiation is the sum of current density generated by each of the 100 Angstroms of wavelength bands as follows: [11]

\[ J_{ph} = \sum_{i=1}^{n} J_{ph}(\lambda_i), \hspace{1cm} \lambda_i = 0.24 + 0.01(i - 1) \]  \hspace{1cm} (5)

n is an integer whose magnitude depends on the largest wavelength that can be absorbed by the solar cell.
Dark current consists of injection current and recombination current. Injection current formulated as:

\[ I_{inj} = J_0 \left( \exp(qV/kT) - 1 \right) \]  

while recombination currents are formulated as follows: [12]

\[ I_{rec} = qn_i W \left( \tau_{po} \tau_{na} \right)^{-1/2} \sinh(qV/2kT) \left( q(V_{bi} - V)/kT \right)^{-1} \pi/2 \]  

A solar cell is essentially a p-n junction diode that has a wide cross section. Therefore a solar cell can be characterized by a current-voltage curve (I-V). Taking into account the series resistance (Rs) and shunt resistance (Rsh), the voltage-current characteristics of a solar cell under irradiation can be formulated as follows: [13]

\[ J(V) = J_0 \left( \exp \left( \frac{q(V+Rs)}{kT} \right) - 1 \right) + \frac{qn_i W \sinh(q(V+Rs)/2kT \pi}{q(V_{bi} - (V+Rs))/kT} \left( \frac{V}{Rsh} \right)^{-1} + \frac{V}{Rsh} - J_{ph} \]  

from the equation of I-V characteristic above can be determined the current density of short circuit (Jsc) and open circuit voltage (Voc) as follows:

\[ J_{sc} = -J_{ph} \]  
\[ V_{oc} = n \frac{kT}{q} \ln \left( \frac{I_{ph}}{I_0} \right) \]  

by knowing the Jsc and Voc, then the efficiency of a solar cell can be determined by using the equation:

\[ \eta = \frac{P_{max}}{P_{in}} \times 100\% \]  

here Pmax is the maximum output power (electric) while Pin is the input power (photon). Maximum output power, formulated by:

\[ P_{max} = J_{sc} \times V_{oc} \times FF \]

The parameters of the solar cell material used in the simulation include the value of the band gap energy, the carrier mobility in each material, the electron’s and hole’s life time on each material obtained from various literatures. The band gap energy value of GaAs0,5Sb0,5 of about 1.07 eV [13]

3. Results and Discussion
Figure 2 shows the plot of GaAs solar cell efficiency curve as a function of p-type and n-type thickness for different acceptor doping concentrations (NA = 1 x 1018cm-3, NA = 3x 1018cm-3 and NA = 5x1018cm-3).

![Figure 2](image-url)
There is a considerable increase in efficiency to p-type thickness of 1.2 \( \mu \text{m} \) and n-type thickness of 3.5 \( \mu \text{m} \), more than that relatively small increase. When \( X_j = 1.2 \mu \text{m}, X_B-X_j = 3.5 \mu \text{m}, N_D = 5 \times 10^{17} \text{cm}^{-3} \), and \( N_A = 5 \times 10^{18} \text{cm}^{-3} \) set as optimum value, then will be obtained the value of GaAs solar cell conversion efficiency of about 19.76%.

Figure 3 shows the plot of GaAs\(_{0.5}\)Sb\(_{0.5}\) solar cell efficiency curve as a function of p-type and n-type thickness for different acceptor doping concentrations (\( N_A = 1 \times 10^{18} \text{cm}^{-3}, N_A = 3 \times 10^{18} \text{cm}^{-3} \) and \( N_A = 5 \times 10^{18} \text{cm}^{-3} \)).

![Figure 3: The efficiency of GaAs\(_{0.5}\)Sb\(_{0.5}\) solar cell as a function of p-type and n-type layer thickness.](image)

The trend of increasing the efficiency of GaAs\(_{0.5}\)Sb\(_{0.5}\) solar cell to p-type and n-type thickness similar to GaAs solar cells. When \( X_j = 1.2 \mu \text{m}, X_B-X_j = 3.5 \mu \text{m}, N_D = 5 \times 10^{17} \text{cm}^{-3}, \) and \( N_A = 5 \times 10^{18} \text{cm}^{-3} \) set as optimum value, then will be obtained the value of GaAs\(_{0.5}\)Sb\(_{0.5}\) solar cell conversion efficiency about 8.42%.

Figure 4 shows the plot of GaSb solar cell efficiency curve as a function of p-type and n-type thickness for different acceptor doping concentrations (\( N_A = 1 \times 10^{18} \text{cm}^{-3}, N_A = 3 \times 10^{18} \text{cm}^{-3} \) and \( N_A = 5 \times 10^{18} \text{cm}^{-3} \)).

![Figure 4: The efficiency of GaSb solar cells as a function of p-type and n-type layer thickness.](image)

The trend of increasing the efficiency of GaSb solar cell against p-type and n-type thickness is also similar to GaAs solar cells. When \( X_j = 1.2 \mu \text{m}, X_B-X_j = 3.5 \mu \text{m}, N_D = 5 \times 10^{17} \text{cm}^{-3}, \) and \( N_A = 5 \times 10^{18} \text{cm}^{-3} \) set as optimum values, then will obtained the value of GaSb solar cell conversion efficiency of about 4.84%.

Figure 5 shows the I-V curves for each of individual GaAs, GaAs\(_{0.5}\)Sb\(_{0.5}\) and GaSb solar cells. The efficiency of GaAs /GaAs\(_{0.5}\)Sb\(_{0.5}\)/ GaSb tandem solar cells with mechanically stacked structures can be obtained by summing the efficiency for each of their constituent solar cells. In this way obtained the efficiency of GaAs/GaAs\(_{0.5}\)Sb\(_{0.5}\)/GaSb tandem solar cells about 33.02%.
Figure 5. I-V Characteristic for individual GaAs, GaAs0,5Sb0,5 dan GaSb solar cell.

This theoretical efficiency value is still below the theoretical efficiency value that can be achieved by In0.50Ga0.50P/In0.01Ga0.99As/Ge tandem solar cells that having a theoretical limiting efficiency of 46% [14], but higher than the conversion efficiency achieved by InGaP/InGaAs /Ge tandem solar cells can reach a conversion efficiency of 31.7% under one sun (AM1.5G) [15]. The simulation results are highly probability to be realized due to the deposition techniques for GaAs, GaSb and GaAsSb currently exist.

4. Conclusion
Theoretical conversion efficiency of GaAs/GaAs0,5Sb0,5/GaSb tandem solar cells with mechanically stacked structure can achieve 33.02%. This shows that GaAs/GaAs0,5Sb0,5/GaSb tandem solar cells can be an alternative solution to the problems faced in the development of solar cells today that is the problem of low conversion efficiency.

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