Improved design of InGaP/GaAs//Si tandem solar cells

Santiago Torres-Jaramillo, Roberto Bernal-Correa, and Arturo Morales-Acevedo

1 Grupo de Investigación en Ciencias de la Orinoquia, Universidad Nacional de Colombia Sede Orinoquia, Arauca, Colombia
2 Centro de Investigación y de Estudios Avanzados del IPN, Electrical Engineering Department-SEES, Ciudad de México, México

Received: 19 June 2020 / Received in final form: 16 January 2021 / Accepted: 19 January 2021

Abstract. Optimizing any tandem solar cells design before making them experimentally is an important way of reducing development costs. Hence, in this work, we have used a complete analytical model that includes the important effects in the depletion regions of the III-V compound cells in order to simulate the behavior of two and four-terminal InGaP/GaAs//Si tandem solar cells for optimizing them. The design optimization procedure is described first, and then it is shown that the expected practical efficiencies at 1 sun (AM1.5 spectrum) for both two and four-terminal tandem cells can be around 40% when the appropriate thickness for each layer is used. The optimized design for both structures includes a double MgF2/ZnS anti-reflection layer (ARC). The results show that the optimum thicknesses are 130 (MgF2) and 60 nm (ZnS), respectively, while the optimum InGaP thickness is 220 nm and GaAs optimum thickness is 1800 nm for the four-terminal tandem on a HIT silicon solar cell (with total tandem efficiency around 39.8%). These results can be compared with the recent record experimental efficiency around 35.9% for this kind of solar cells. Therefore, triple junction InGaP/GaAs//Si Silicon tandem solar cells continue being very attractive for further development, using high efficiency HIT silicon cell as the bottom sub-cell.

Keywords: III-V/Si tandem solar cells / hybrid tandem/multi-junction solar cells / anti-reflecting coating

1 Introduction

Over the last decades, photovoltaic energy has become one important contributor to the current energy production, around 1.7% of the world power supply [1]. Thin film solar cells based on CdTe, copper indium gallium selenide (CIGS) or amorphous silicon have been developed as a cheaper alternative to crystalline silicon cells [2–7]. On the other hand, tandem cells, or multi-junction cells, as they are also called, were originally used for spacecrafts, where materials such as gallium-arsenide (GaAs) and germanium (Ge) substrates were combined for the first time to achieve high efficiencies [8–10]. In order to create cost-effective tandem cells, the most obvious way is to add new materials on top of conventional single-junction cells based on silicon or thin film materials such as CIGS. Adding an additional junction layer to industrial PV cells can be the cheapest way to further improve photovoltaic efficiency [11]. Specifically, a very attractive alternative for having very high efficiency solar cells is the coupling of different generation solar cells (e.g. Perovskite/CIGS, III-V/Si) [12,13]. Experimentally, the new technologies that couple two or more solar cell junctions based on III-V materials and Si, have exceeded the efficiency limit for a single junction, reaching efficiencies around 36%. This achievement is due to the optimization of parameters such as reflectance and thickness of each junction material [14]. In this regard, the use of HIT (HJ) silicon solar cells, as bottom cells, is important because they have been reported to be the record efficiency silicon cells [1]. Besides, III-V semiconductor multi-junction solar cells are attractive because they have achieved more than 40% under solar concentration [15].

Essig et al. [14] have demonstrated experimental conversion efficiencies of 32.5% and 32.8% (AM1.5) for III-V//Si two-junction solar cells based on mechanical stacking of GaInP-GaAs//Si cells. In addition, they showed a three-junction GaInP/GaAs//Si cells with a record 35.9% efficiency (All of the above was achieved with the use of ZnS/MgF2-based anti-reflective coatings to prevent optical losses in the device [14]. In this work, it is shown that improved designs of two-terminal and four-terminal three-junction InGaP/GaAs//Si tandem solar cells with a double anti-reflection coating (Fig. 1) can achieve even higher efficiencies, around 39.8%, at one sun.
(AM1.5). The model used for the III-V solar sub-cells includes the effects related to the carrier recombination within the space-charge regions which cause the reduction of both the illumination current and the open-circuit voltage of very thin solar cells. Therefore, the calculations and design results are more realistic than those typically reported without considering these space-charge effects.

2 Four-terminal tandem solar cells

In order to determine the expected efficiencies for the tandem cell structures shown in Figure 1, the calculations for each of the III-V sub-cells (n-p homojunctions) were made using reported values for transport parameters such as mobilities and carrier lifetimes, as will be explained below. The parameters assumed for the III-V compounds are given in Table 1[16,17]. The (front and back) surface recombination velocities for each IIIV sub-cell were assumed to be $S = 10^3$ cm/s. This is an intermediate value between passivated and non-passivated surfaces. In addition, previously reported optical parameters such as refraction and extinction coefficients were also taken in account to evaluate the total cell reflectance $R(\lambda)$ at each wavelength of the AM1.5 solar spectrum [18–20]. For this purpose, an optical matrix method [21] was used for the calculation of the spectral reflectance $R(\lambda)$, assuming a MgF$_2$/ZnS anti-reflecting double layer (ARC). Figure 2 shows the results for the spectral reflectance taking in account different thicknesses for the double ARC used for these tandem cells. The thicknesses used for the calculations shown in Figure 2 are the optimized values, as will be explained below, and the thicknesses used for the experimental record efficiency InGaP/GaAs//Si tandem solar cells reported recently [14].

2.1 III-V Top sub-cell optimization

The InGaP and GaAs tandem homojunctions constitute the top (two-terminal) sub-cell, and they were assumed to be connected in series (through a tunnel junction), so that the photo-current (short-circuit) density for each junction should be the same. The thickness for each material is designed to satisfy this condition.

The optimization proceeded using a two-step process. In the first step, a first order approximation for the photocurrent of each sub-cell was calculated using the following equation:

$$J_{Li} \approx \int \frac{\lambda_{gap}^i}{\lambda_{min}} \exp \left( -\sum_{k=1}^{i-1} \alpha_k d_k \right) (1 - \exp(-\alpha_i d_i)) d\lambda \quad (1)$$

with direct bandgap absorption coefficients calculated by

$$\alpha_k \approx A \sqrt{\frac{hc}{\lambda} - E_{gap}}$$

where $A \approx 10^7$ (cm$^{-1}$) and $E_{gap} = 1.9 \text{ eV}$ for InGaP and $E_{gap} = 1.43 \text{ eV}$ for GaAs.

Table 1. Parameters used for the calculations [16,17].

| Respective III-V Sub-cell | InGaP | GaAs |
|---------------------------|-------|------|
| Lifetime n $\tau_n$ (s)   | $10^{-9}$ | $10^{-9}$ |
| Lifetime p $\tau_p$ (s)   | $10^{-9}$ | $2 \times 10^{-8}$ |
| Diffusion coefficient of electrons $D_n$ (cm$^2$/s) | 29 | 200 |
| Diffusion coefficient of holes $D_p$ (cm$^2$/s) | 1.0 | 9.2 |
| Band gap (eV)             | 1.9   | 1.43 |
| Dielectric permittivity   | 11.6  | 13.1 |
| Donor density Nd (cm$^{-3}$) | $10^{17}$ | $10^{17}$ |
| Acceptor density Na (cm$^{-3}$) | $10^{18}$ | $10^{18}$ |
| Surface recombination velocities (cm/s) | $10^3$ | $10^3$ |

Fig. 1. (a) Schematics of a four-terminal InGaP/GaAs//Si-HJ solar cell. The top sub-cell is formed by the two-terminal III-V tandem. (b) Schematics of a two-terminal InGaP/GaAs//Si-HJ solar cell. In this case, the tunnel junctions are not depicted, nor they are considered for the calculations.

Fig. 2. Reflectance for tandem solar cells with a double layer ARC system.
to our previous approach [23] because now we are also considering the analytical model [22]. This provides an improved design at each junction, accordingly to a previously reported approach [22], a more realistic calculation for the photocurrent density was made considering the calculated spectral reflectance \( R(\lambda) \) in the solar spectrum, where \( R(\lambda) \) takes in account the effect associated to the antireflection coating.

Then, in the second step (See Eqs. (3)–(5)) [22], a more realistic calculation for the photocurrent density was made considering the calculated spectral reflectance \( R(\lambda) \) in the solar spectrum, where \( R(\lambda) \) takes in account the effect associated to the antireflection coating.

\[
J_p(\lambda) = \frac{qN'_0(\lambda)(1 - R(\lambda))\alpha(\lambda)L_p}{((\alpha(\lambda))^2L^2_p - 1)} \times \left\{ \frac{S_pL_p}{D_p} + \alpha(\lambda)L_p - e^{-\alpha(\lambda)(W_n - x_n)} \left( \frac{S_pL_p}{D_p} \cosh \left( \frac{W_n - x_n}{L_p} \right) + \sinh \left( \frac{W_n - x_n}{L_p} \right) \right) - \alpha(\lambda)L_p e^{-\alpha(\lambda)(W_n - x_n)} \right\} 
\]

\[
J_n(\lambda) = \frac{qN'_0(\lambda)(1 - R(\lambda))\alpha(\lambda)L_n}{((\alpha(\lambda))^2L^2_n - 1)} \times \left\{ \frac{S_nL_n}{D_n} \left( \cosh \left( \frac{W_p - x_p}{L_n} \right) - e^{-\alpha(\lambda)(W_p - x_p)} \right) + \sinh \left( \frac{W_p - x_p}{L_n} \right) + \alpha(\lambda)L_n e^{-\alpha(\lambda)(W_p - x_p)} \right\} 
\]

\[
J_{sc}(\lambda) = qN'_0(\lambda)(1 - R(\lambda))e^{-\alpha(\lambda)(W_n - x_n)} \left[ \left( 1 - e^{-\alpha(\lambda)(x_n + x_p)} \right) \right] 
\]

where \( q \) is the electron charge, \( \alpha \) is the absorption coefficient, \( d \) is the thickness of each junction \((k = 1, 2)\) above the \( i \)th junction, \( \lambda_{\text{gap}} \) is the wavelength corresponding to the band gap of the \( i \)th material \((\lambda_{\text{gap}} = h/c/E_{\text{gap}}\) where \( h \) is the Planck’s constant and \( c \) is the speed of light in the air). \( N_0 \) is the photon flux density due to the AM1.5 solar spectrum. This first order approximation allowed the estimation of the required thickness for each sub-cell.

Then, for each of the junctions, the total current density is calculated by means of the following expressions:

\[
x_p(V) = \frac{1}{N_a} \left( \frac{2\varepsilon(V_{bi} - V)}{q \left( \frac{1}{N_a} + \frac{1}{N_d} \right)} \right)^{\frac{1}{2}} 
\]

\[
x_n(V) = \frac{1}{N_d} \left( \frac{2\varepsilon(V_{bi} - V)}{q \left( \frac{1}{N_a} + \frac{1}{N_d} \right)} \right)^{\frac{1}{2}} 
\]

where \( \varepsilon \) is the dielectric permittivity of the semiconductor, \( V \) is the bias voltage and \( V_{bi} \) is the built-in potential. In other words, there is a variation of depletion layer thickness as a function of the applied voltage which causes a variation of both the generated photocurrent and the generation-recombination dark current densities as a function of the bias voltage. All this affects the optimized thickness for each of the sub-cells, as well as the total efficiency.

Then, for each of the junctions, the total current \( J \) as a function of voltage can be calculated using an equivalent model with two diodes:

\[
J_i = J_{Li} - J_{0i} \left( \exp \left( \frac{qV}{kT} \right) - 1 \right) - J_{0Hi} \left( \exp \left( \frac{qV}{2kT} \right) - 1 \right) 
\]

where \( J_{0i} \) and \( J_{0Hi} \) are the dark saturation currents due to diffusion and generation-recombination in the
space-charge region, respectively. They are given by

$$J_{0i} = q D_p p_0 \frac{S_p L_p}{D_p} \frac{\cosh \left( \frac{W_n - x_n}{L_p} \right)}{cosh \left( \frac{W_n - x_n}{L_p} \right) + \frac{x_n}{L_p}}$$

$$+ q D_n n_0 \frac{S_n L_n}{D_n} \frac{\cosh \left( \frac{W_p - x_p}{L_n} \right)}{cosh \left( \frac{W_p - x_p}{L_n} \right) + \frac{x_p}{L_n}}$$

and

$$J_{00i} = q \left( \frac{x_n}{\tau_p (1 - R)} + \frac{x_p}{\tau_n} \right)$$

where $\alpha$ is the absorption coefficient for crystalline silicon and $d$ is the reported thickness for the assumed high efficiency HIT solar cell (98 $\mu$m) [25]. The full J-V curve for the silicon HIT solar cell, under the III-V compound sub-cell, can be calculated from this photo-current density $J_L$ and the dark saturation current density $J_0$ determined as explained above.

3 Two-terminal tandem solar cells

The use of the model described in the previous section, and the mentioned considerations corresponding to each of the materials involved, enabled the calculation of the output parameters and characteristic contributions of each of the sub-cells of a two-terminal tandem cell. In this case, the appropriate ARC thicknesses were chosen to cause the largest photo-current density for the whole cell. Then, the thickness for each of the III-V compound sub-cells are selected to generate a constant photocurrent density for the whole tandem cell structure.

4 Results

4.1 Optimized four-terminal tandem solar cells

The external quantum efficiencies for each sub-cell as a function of wavelength are shown in Figure 3 for the different ARC thicknesses considered. The thickness of each absorber layer was chosen so that the illumination current densities reach the maximum value for each sub-cell. In this case, the top and bottom junctions were
assumed to have absorber layers with bandgaps of 1.9 eV (InGaP), 1.43 eV (GaAs), and 1.08 eV (Si), respectively. Figures 4 and 5 show the calculated P-V/J-V characteristics for each of the sub-cells. From these, the efficiencies for the sub-cells can be determined. Ideally, the total efficiency will be the sum of the sub-cell efficiencies. Unlike the two-terminal solar cells where the current density of the junctions must be the same, in the four-terminal cell (where the tandem is mechanically made) the maximum possible photocurrent density can be achieved for each sub-cell.

In Table 3, the optimized efficiency for the ARC used for the reported experimental record efficiency cells [14] is also given. Notice that in this case, the calculated efficiency (39.5%) is slightly less as compared to cells with our optimized ARC which gives a total efficiency of 39.8%. The experimental record efficiency for this kind of cells, under the AM1.5 solar spectrum, is around 35.9% [14]. Therefore, in accordance with the above results, we still can expect some improvement for this kind of solar cells in the near future.

4.2 Optimized two-terminal tandem solar cells

The EQE results for the two-terminal tandem cell are shown in Figure 6 for an ARC with respective optimum layers of 130 and 60 nm. The contribution of each sub-cell is also shown in this figure. As explained before, the ARC coating thickness was chosen so that the cell achieves the largest photocurrent density. The J-V curve can be calculated from the two diodes in series model for each of the InGaP/GaAs and Si sub-cells, as shown in Figure 7. The thickness of each absorber layer was chosen so that the illumination current densities are the same for each sub-cell. In this case, the maximum efficiency was obtained when the top and bottom junctions had absorber layers with thicknesses of 166 nm (InGaP), 360 nm (GaAs), and 98 μm (Si), respectively. The total tandem cell conversion efficiency would be 39.6% as given in Table 4. This value is comparable with the expected efficiency for the optimized four-terminal tandem cell.
4.3 Comparison with our previous results

The maximum efficiency expected for the four-terminal tandem cell in our previous work [23] was 41.7%, while the efficiency achieved in this work is 39.8%, as explained above. This difference is explained by the effects due to the space-charge regions in each of the III-V compound sub-cells. In addition, a double anti-reflection coating was used here which allows for a larger sunlight absorption, compensating some of the loss due to the recombination in the depletion regions. However, our calculations suggest that by optimizing the sub-cell layer thicknesses it is still possible to achieve a higher efficiency than the recent record reported [14].

5 Conclusion

By including a double ARC and the effects due to the space-charge regions in the III-V compound sub-cells, InGaP/GaAs/Si-HJ tandem solar cells were optimized for each of the two or four-terminal configurations. The four-terminal tandem cell efficiency at 1 sun should reach around 39.8% when the appropriate thicknesses for each layer, including the anti-reflection coating, are used. In the specific case of MgF₂/ZnS as ARC, the optimum thickness is 130 and 60 nm respectively, while the calculated optimum InGaP thickness is 220 nm and GaAs optimum thickness is 1800 nm. The results shown here can be compared with the experimental record efficiency already achieved (35.9%) for this type of solar cells [14]. Then, it is still possible to improve this record efficiency.

Author contribution statement

S. Torres-Jaramillo made the calculations and wrote the paper draft; R. Bernal-Correa developed the original code and supervised the calculations; A. Morales-Acevedo proposed the research and the methodology, validated the results and wrote the final version of the paper.

Table 4. Calculated illumination current density, open circuit voltage, fill factor and power conversion efficiency for the two-terminal tandem cells.

| Solar cells | Jsc (mA/cm²) | Voc (mV) | FF (%) | Total η (%) |
|-------------|--------------|----------|--------|-------------|
| GaInP_166 nm/GaAs_360 nm//Silicon-HJ | 16.4 | 2560 | 94.3 | 39.6 |

The calculations include light reflection for a cell with MgF₂/ZnS as ARC.

References

1. S. Almosni et al., Sci. Technol. Adv. Mat. 19, 336 (2018)
2. A. Tombak, T. Kilicoglu, Y.S. Oacak, Renew. Energ. 146, 1465 (2020)
3. C. Yang et al., Sol. Energy 195, 121 (2020)
4. I.E. Tinedert et al., Optik 208, 164112 (2020)
5. G. Liyanage et al., ACS Appl. Energy Mater. 2, 5419 (2019)
6. J. Dreon et al., Nano Energy 70, 104495 (2020)
7. H. Sai et al., Prog. Photovolt. Res. Appl. 27, 1061 (2019)
8. O. Höhn et al., IEEE J. Photovolt. 9, 1625 (2019)
9. B. Jeco et al., J. Photon. Energy 8, 022602 (2018) 
10. P. Caño et al., Sol. Energy Mat. Sol. C 205, 110246 (2020) 
11. E.L. Warren et al., in Proceedings 44th PVSC, Washington D.C., USA, 2017, edited by A. Reinders (IEEE Xplore, 2018), p. 2488 
12. M. Feifel et al., IEEE J. Photovolta. 8, 1590 (2018) 
13. Q. Han et al., Science 361, 904 (2018) 
14. S. Essig et al., Nat. Energy 2, 17144 (2017) 
15. J.F. Geisz et al., Nat. Energy 5, 326 (2020) 
16. R. Ganouni, M. Talbi, H. Ezzaouia, J. Fundam. Appl. Sci. 9, 756 (2017) 
17. G. Lin et al., III-V Multi-Junction Solar Cells, edited by S. Pyshkin, J. Ballato, (Optoelectronics, Intech, 2013) 
18. https://www.pvlighthouse.com.au/refractive-index-library (2020) 
19. https://www.filmetrics.com/refractive-index-database (2020) 
20. https://refractiveindex.info (2020) 
21. R. Bernal-Correa et al., Mat. Sci. Semicon. Pro. 37, 57 (2015) 
22. A. Acevedo-Luna et al., J. Appl. Res. Technol. 15, 599 (2017) 
23. R. Bernal-Correa, S. Torres-Jaramillo, A. Morales-Acevedo, in Proceedings 46th PVSC, Chicago, IL, USA, 2019, edited by S. Kurtz (IEEE Xplore, 2020), p. 0989 
24. M. Taguchi et al., IEEE J. Photovolta. 4, 96 (2014) 
25. https://www.pveducation.org/es/fotovoltaica/dispositivos-semiconductores/coeficiente-de-absorcion (2020)