



Design of $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{In}_y\text{Ga}_{1-y}\text{As}$ triple junction solar cells with anti-reflective coating

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ABSTRACT

Multi-junction solar cells (SC) made from III–V compound semiconductors are still in the development phase. Here, we perform calculations for multi-junction cells: $\text{Al}_x\text{Ga}_{1-x}\text{As}$ top junction, GaAs middle junction and $\text{In}_y\text{Ga}_{1-y}\text{As}$ bottom junction (all of these materials with band-gaps between 2.1 and 0.8 eV) in order to obtain the optimal band gap and thickness for each junction under the AM1.5 solar radiation spectrum. The ideal photo-current density is around 15.5 mA/cm^2 . In order to reduce the natural reflectivity, an anti-reflective coating (ARC) was chosen, based on a MgF_2/ZnS double layer, allowing for a significant increase of the current density with respect to a cell without it. Calculations of external quantum efficiency (QE) were also performed for the three cases mentioned above: ideal one, taking into account the total reflection and with the ARC double layer. Finally, when more realistic calculations are done, taking into account the carrier recombination at each sub-cell, and the light reflection for a tandem cell with the designed ARC on top, the expected conversion efficiency (η), under the AM 1.5 spectrum (without concentration), was determined to be around 38.5%, making this an attractive III–V compound tandem cell to be investigated in the near future.

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1. Introduction

Tandem solar cells formed by AlGaAs alloys (1.9 eV)/GaAs (1.4 eV)/InGaAs (1 eV) are very promising for concentrator terrestrial and space applications. The main advantage of this design is the possibility to be fabricated based on a single III–V semiconductor family (AllnGaAs in this case), which would provide a monolithic (simplified epitaxial) growth for the entire solar cell, avoiding interconnection losses and maximizing the efficiency. Another relevant aspect of this design is that germanium is not

used as substrate, and although Ge is now a conventional material for three junction solar cells, it is less abundant than Ga, so that solar cells made from Ga compounds are an important alternative to the present technology [1].

Some of the most studied systems at present are triple junctions (TJ) of InGaP/GaInAs/Ge and InGaP/GaAs/InGaAs. In the latter case, a high efficiency close to 37.7% (measured under the AM 1.5 spectrum) was reported in 2013 [2]. Other less studied systems today are the AlGaAs/GaAs double junctions (DJ), which has been dismissed due to structural defects and crystalline quality which cause low conversion efficiencies [3,4]. However, researchers from Hitachi Cable's Advanced Research Center have reported $\text{Al}_{0.36}\text{Ga}_{0.64}\text{As}/\text{GaAs}$ cells with efficiencies around 27.6% (in 2001) and 28.5% (in 2007). Then, these materials are again

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of interest for tandem solar cells [5,6]. A more recent paper reports the design of a triple junction $\text{Al}_{0.36}\text{Ga}_{0.64}\text{As}/\text{Al}_{0.18}\text{Ga}_{0.82}\text{As}/\text{GaAs}$ in order to reduce resistive power losses affecting the performance of the cell system [7]. These solar cells were obtained by techniques such as Molecular beam epitaxy (MBE) and metal organic chemical vapor deposition (MOCVD).

Today there are only few reports for solar cells based on $\text{AlGaAs}/\text{GaAs}/\text{InGaAs}$ triple junctions, and therefore our interest in this investigation. We do simple analytical calculations and optimization of the anti-reflective coating which allows for a higher efficiency, as has been done for single junction solar cells [8]. In this article, we focus on the design of a triple junction $\text{AlGaAs}/\text{GaAs}/\text{InGaAs}$ solar cell, under the standard AM 1.5 solar spectrum, including the design of an anti-reflective coating (ARC) formed by MgF_2/ZnS double layers. We show results of quantum efficiency (QE) in three cases: (i) ideal carrier generation and collection, (ii) considering the total light reflection and (iii) a double ARC layer. Finally, the open circuit voltage (V_{oc}), fill factor (FF) and power conversion efficiency (η) of this three junction solar cell is determined from the three-diode equivalent circuit model.

2. Theoretical considerations

The calculations for the determination of the appropriate parameters (band-gap and thickness) of a multi-junction solar cell formed by a top AlGaAs junction (1.9 eV), a middle GaAs junction (1.4 eV) and a bottom InGaAs junction (1.0 eV) were performed as is explained in the following sections. The junctions were assumed to be connected in series, so that the photo-current must be the same for each junction. This fact determines the thickness d required for each of the junctions.

2.1. Photocurrent

Calculations of the photocurrent for each junction were performed first considering an ideal case where the collection efficiency of the generated carriers is 100%, i.e. each photon with $E > h\nu$ is absorbed generating one electron-hole pair which is collected at the respective junction, producing the cell photo-current. In other words, we have a quantum generation yield of 100% and a carrier collection efficiency of 100%. In this ideal case, for which the reflectance $R(\lambda)$ is assumed to be zero, the photocurrent expression is given by:

$$J_i = \int_{\lambda_{\min}}^{\lambda_{\text{gap}i}} j(\lambda) e^{-\left(\sum_{k=1, \dots, i-1} \alpha_k d_k\right)} d\lambda \quad (1)$$

$$\alpha \approx A \left(\frac{hc}{\lambda} - E_{\text{gap}} \right)^{1/2} \text{ and } A \approx 10^5 \text{ (cm}^{-1}\text{)} \quad (2)$$

q is the electron charge, α_k is the absorption coefficient ($k=1,2,3\dots$), d_k is the thickness of each junction, λ_{gap} is the wavelength corresponding to the band gap of each material ($\lambda_{\text{gap}} = hc/E_{\text{gap}}$ where h is the Planck's constant and c is the velocity of light in air); $j(\lambda) = qN_0(\lambda)$ is the spectral electron

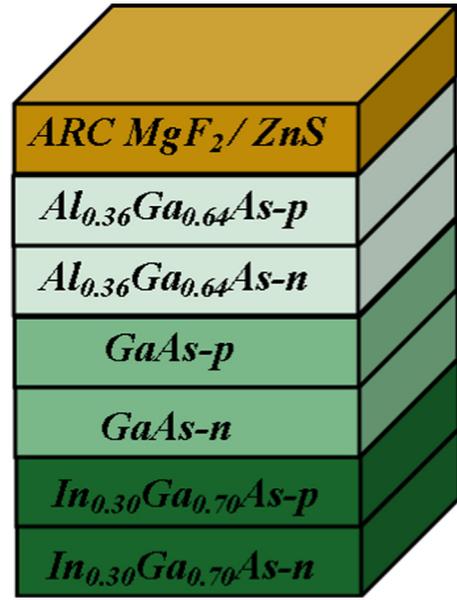


Fig. 1. Schematic of the three-junction solar cell structure with double-layer anti-reflection coating.

current density for N_0 photon flux density under the standard global AM 1.5 solar spectrum (1000 W/m^2).

An improved calculation, for a better design of the solar cell, requires that the overall reflectance and transmittance in the cell system shown in Fig. 1, is taken into account, as assessed by the optical transfer matrix model [9]. Normal incidence ($\varphi=0$) was considered on the air/top-junction/middle-junction/bottom-junction system, with the absorbing layers having complex refractive index $\tilde{n}_j^* = n_j - ik_j$ and thickness d_j . Then, for the optical matrix of the j th material we have

$$(C_j) = \begin{pmatrix} e^{i\delta_j} & r_j e^{i\delta_j} \\ r_j e^{-i\delta_j} & e^{-i\delta_j} \end{pmatrix} \quad (3)$$

where $\delta_j = 2\pi n_j \cos(\varphi)/\lambda$ and r_j are the Fresnel reflection coefficients. The recurrence relation may be written as

$$\begin{pmatrix} E_{j+1}^+ \\ E_{j+1}^- \end{pmatrix} = \begin{pmatrix} e^{i\delta_j} & r_j e^{i\delta_j} \\ r_j e^{-i\delta_j} & e^{-i\delta_j} \end{pmatrix} \begin{pmatrix} E_j^+ \\ E_j^- \end{pmatrix} \quad (4)$$

where E_j are the components of the electric vectors E . For a system with n layers, we have

$$\begin{pmatrix} E_0^+ \\ E_0^- \end{pmatrix} = (C_1)(C_2) \dots (C_{n+1}) \begin{pmatrix} E_{n+1}^+ \\ E_{n+1}^- \end{pmatrix} \quad (5)$$

The product of these matrices is:

$$(C_1)(C_2) \dots (C_{j+1}) = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad (6)$$

Then the total reflectance is given by

$$R = \frac{(E_0^-)(E_0^-)^*}{(E_0^+)(E_0^+)^*} = \frac{cc^*}{aa^*} \quad (7)$$

Table 1

Main parameters of double ARC layers: refractive indices and thickness.

ARC system	Layers	Refractive index ($\lambda=650$ nm)	Thickness (nm)
MgF ₂ /ZnS	MgF ₂	1.4	103
	ZnS	2.4	65

Table 2

Values for the parameters used in the calculations of the 3-junction solar cell.

	Al _{0.36} Ga _{0.68} As	GaAs	In _{0.3} Ga _{0.7} As
Bandgap (eV)	1.9	1.4	1.0
Thickness (cm)	6*10 ⁻⁵	2.4*10 ⁻⁴	3*10 ⁻⁴
$n+ik$ ($\lambda=650$ nm)	3.6+i0.1	3.8+i0.2	3.9+i0.3
D_n (cm ² s ⁻¹)	34.4	200.0	188.0
D_p (cm ² s ⁻¹)	2.9	10.0	7.5
N_c (cm ⁻³)	7.1*10 ¹⁷	4.7*10 ¹⁷	2.8*10 ¹⁷
N_v (cm ⁻³)	1.2*10 ¹⁹	9.0*10 ¹⁸	4.9*10 ¹⁸
n_i (cm ⁻³)	2.1*10 ³	2.1*10 ⁶	4.7*10 ⁹
L_n (cm)	1.8*10 ⁻³	6.0*10 ⁻³	4.0*10 ⁻³
L_p (cm)	1.7*10 ⁻⁴	5.0*10 ⁻³	2.7*10 ⁻³
X_n (cm)	5.0*10 ⁻⁵	2.0*10 ⁻⁴	2.5*10 ⁻⁴
X_p (cm)	1.0*10 ⁻⁵	4.0*10 ⁻⁵	5.0*10 ⁻⁵
S_n (cm s ⁻¹)	1.0*10 ³	1.0*10 ³	1.0*10 ³
S_p (cm s ⁻¹)	1.0*10 ³	1.0*10 ³	1.0*10 ³
N_d (cm ⁻³)	1.0*10 ¹⁷	1.0*10 ¹⁷	1.0*10 ¹⁷
N_a (cm ⁻³)	1.0*10 ¹⁸	1.0*10 ¹⁸	1.0*10 ¹⁸

D_n =diffusion coefficient of electrons, D_p =diffusion coefficient of holes, N_c =Conduction band effective density of states, N_v =Valence band effective density of states, S_n =electron surface recombination velocity, S_p =hole surface recombination velocity, L_n =diffusion length of electrons, L_p =diffusion length of holes, X_n = n layer thickness, X_p = p layer thickness, N_d =donor atoms density, N_a =acceptor atoms density.

2.2. Design of a double anti-reflection layer

In order to maximize the photo-current density of the solar cell, a two-layered anti-reflective coating system can be designed. This can be done by depositing layers with a refractive index intermediate between that of the top junction cell material (n_s) and that of the air ($n_0=1$). In our case, the optimum refraction index for each layer should be

$$n_m = n_0^{\left(\frac{M+1-m}{M+1}\right)} n_s^{\left(\frac{m}{M+1}\right)} = n_s^{\left(\frac{m}{M+1}\right)} \quad (8)$$

where m corresponds to the m th layer and M is the total number of layers in the anti-reflective coating system [10]. For a double layer system, the ideal refractive index values for each of the two layers at $\lambda=650$ nm are $n_1=1.539$ and $n_2=2.371$. Then, a possible appropriate double layer is MgF₂/ZnS. Table 1 shows the optimum thickness and refractive index for each of the materials.

3. I–V Curves taking into account volumetric and surface recombination

An even more realistic calculation for the photo-current can be made if we take into account, both volumetric and surface recombination of the photo-generated carriers at each junction. The dark characteristics of the cell will also depend upon the recombination phenomena at each

junction. Hence, for calculating the I – V curve for each junction we have used the conventional expressions for the photo-current and dark current reported in many textbooks [see reference [11], for example]. The following sections describe such calculations, assuming the material properties [12] given in Table 2. The total thickness (X_n+X_p) for each junction was adjusted so that the photo-current density was the same for all junctions.

3.1. External quantum efficiency

Calculations of the external quantum efficiency at each junction were made from the total generated photocurrent at a given wavelength

$$j(\lambda) = j_n(\lambda, -w_p) + j_p(\lambda, w_n) + j_{gen}(\lambda) \quad (9)$$

where j_n and j_p are minority carrier currents from the n and p neutral regions and j_{gen} is the generated current in the space charge region with total width w_n+w_p . The external quantum efficiency was obtained from the ratio between the photocurrent and the incident spectral photocurrent:

$$QE(\lambda) = \frac{j(\lambda)}{qN_0(\lambda)} \quad (10)$$

The depleted space-charge region widths w_n and w_p were calculated according to the dielectric constant for each material.

3.2. Efficiency

Calculations for the efficiency associated to each junction are performed from the characteristic J – V curves for each sub-cell. Additionally, a three junction model (see Fig. 4) was also used for calculating the values of J_{sc} , FF and V_{oc} for the full tandem solar cell.

4. Results

4.1. Photocurrent

Photocurrent density values were obtained taking into account the parameters shown in Table 2. The total thickness (X_n+X_p) for each junction was adjusted so that the photo-current density was the same for all junctions. The results given in Table 3, as ideal, assume the total reflection of the system to be zero and all the generated electron–hole pairs collected with 100% efficiency. It can be seen that the illumination current density in this ideal case is around 15.5 mA/cm². However, since the real reflectance $R(\lambda)$ is different from zero, it can be shown that there is a decrease for the illumination current density that is approximately 40% (Table 3).

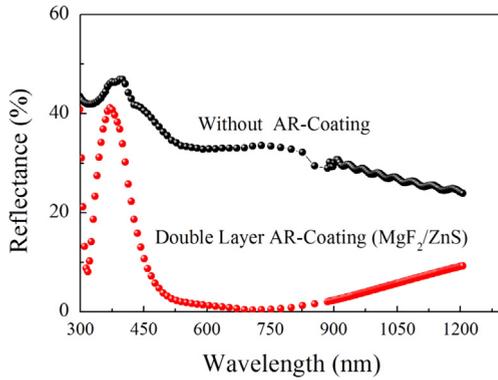
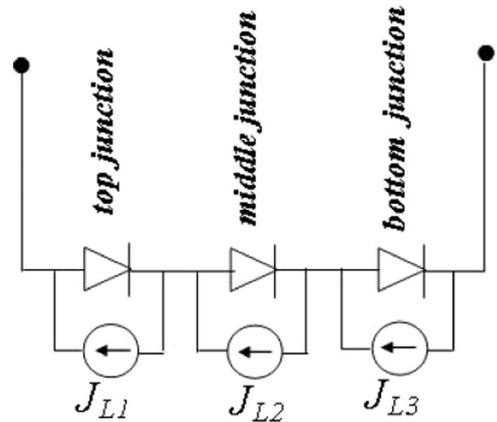
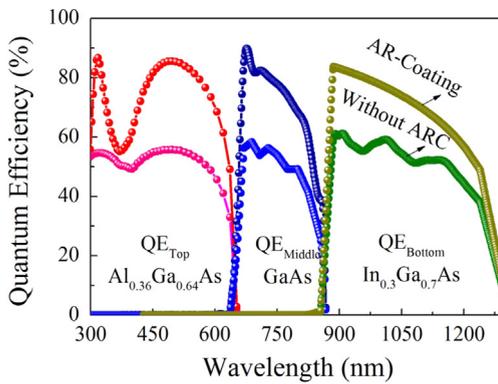
4.2. Double ARC design

In order to reduce the effect of the high reflectance, as discussed previously, a double ARC layer was designed, as explained above. The appropriate choice for our tandem cell was the MgF₂/ZnS double ARC. Fig. 2 shows the difference between the reflectance spectra of a solar cell without ARC and with the mentioned double ARC. It is clearly seen that

Table 3

Calculated current densities for each of the cases discussed in the text.

3 Junction cell	J_L (mA/cm ²)		
	Ideal	Without AR-coating	With double AR-coating
Al _{0.36} Ga _{0.64} As/GaAs/In _{0.3} Ga _{0.7} As	15.5	9.6	13.7

**Fig. 2.** Shows a comparison of the reflectance in the SC with and without MgF₂/ZnS ARC system.**Fig. 4.** Electrical equivalent circuit for the three junction solar cell.**Fig. 3.** Comparison of the external quantum efficiency of cells with a double ARC and without ARC.

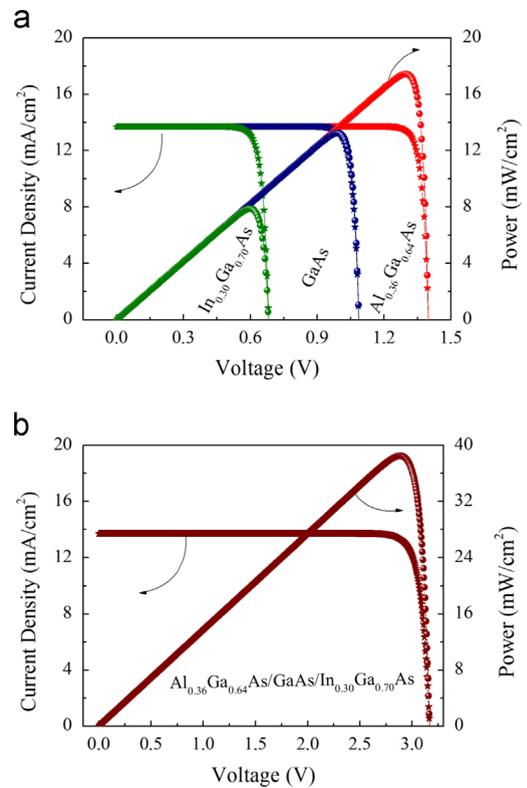
the reflectance in average is decreased by about 30%, causing a sharp increase in the current density as indicated in Table 3 itself.

4.3. External quantum efficiency

Fig. 3 shows the external quantum efficiency (QE_{Top} , QE_{Middle} and QE_{Bottom}) using expression (10) for each junction. First, the calculation of the ideal QE is considered; the second case involves the reflection due to all the layers (as was already discussed), causing a drop in quantum efficiency of about 40% in average. The third case determines the QE using a double ARC, allowing the QE to be recovered by about 30%, as shown in Fig. 3.

4.4. Conversion efficiency

For the case of a cell with double ARC and with volumetric and surface recombination taken into account,

**Fig. 5.** Power and current versus voltage curves for (a) each sub-cell and (b) the composite tandem solar cell.

J_{sc} , V_{oc} , FF and conversion efficiency η were determined for each of the junctions. Fig. 5(a) shows the J - V and P - V curves for each of the sub-cells. A more realistic calculation of

Table 4

Calculated current densities, open circuit voltage, fill factor, and power conversion efficiency for each of the sub-cells and for the full cell with a 3 junction model. The calculations include carrier volumetric and surface recombination, and light reflection for a cell using the designed double AR-coating.

Solar cell	J_{sc} (mA/cm ²)	V_{oc} (V)	FF	η (%)
Al _{0.36} Ga _{0.68} As	13.7	1.4	0.91	17.4
GaAs		1.1	0.89	13.2
In _{0.3} Ga _{0.7} As		0.7	0.84	7.9
3-junction model		3.2	0.89	38.5

these curves for the full tandem cell was made using the equivalent circuit for 3 cells in series (see Fig. 4), with $J_{L1}=J_{L2}=J_{L3}=13.7$ mA/cm² (J_{L1} – J_{L3} are the photo-current densities for each junction). The resultant J – V and P – V curves are shown in Fig. 5(b). These results are summarized in Table 4. For the proposed tandem solar cell: $J_{sc}=13.7$ mA/cm², $V_{oc}=3.2$ V, $FF=0.9$ and $\eta=38.5\%$. This is an expected high conversion efficiency under the AM 1.5 solar spectrum, comparable to current technology three junction solar cells, and therefore the AlGaAs/GaAs/InGaAs solar cell studied here is an attractive alternative for high efficiency solar energy conversion.

5. Conclusions

In this work, we have reported the design of an Al_{0.36}Ga_{0.64}As/GaAs/In_{0.30}Ga_{0.70}As triple junction solar cell by determining its photo-current density J_{sc} , the open-circuit voltage V_{oc} and the filling factor FF . We also report the design of the anti-reflective layer to maximize the illumination current density, based on MgF₂/ZnS ARC system. A conversion

efficiency of 38.5%, under 1 sun (Global AM 1.5 solar spectrum) radiation, can be achieved for this kind of solar cell, making this an attractive alternative to other 3 junction solar cells.

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