

Modelling and Optimization of GaAs used in mechanically stacked solar cells

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Abstract: Different approaches have been made in order to reach higher 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 modelling and predict their maximum performance. The structures of solar cells are based on the single junction Si, Ge and GaAs cells. We have simulated each cell individually and extracted their optimal parameters (thickness, concentration, the recombination velocity.....), 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 physical parameters giving the best current of short-circuit and voltages of open circuit as well high conversion efficiency have obtained for the two solar materials and tandem.

I. Introduction

The drive for higher photovoltaic efficiency has led from single-junction to multiple band gap (tandem) cells, which can be better matched to the solar spectrum. In this approach, cells of different band gaps are placed optically in series, either during the growth process or joined together after individual processing. One promising combination of materials is GaAs and Ge, with energy band gaps of 1.42 and 0.66 eV. Although not the theoretically optimum combination of band gaps, this system has the advantage of being lattice matched. Mechanically stacked tandems of GaAs and Ge have been reported [1, 2, 3].

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 [4]. 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.

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, and possibly Silicon (1.12 eV). Silicon as a substrate material is on it self interesting because it is inexpensive and a lot of knowledge of solar cell processing on this material is available. The band-gap is a little too high to be ideal for use in multijunction solar cells. Of all the low band-gap materials germanium is used in most commercial triple-junction cells [5]. Several principal parameters that influence the operation of a solar cell are emitter and base doping, junction depth and base thickness...

The purpose of this work comes to contribute to the optimisation of the performance of Si and Ge (n^+p) 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 two solar materials.

II. Theoretical approach

Modelling and optimization of a conventional solar cell performance n^+p 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, open-circuit 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...) are included in the program.

The structures of our study are shown on the Fig. 1.

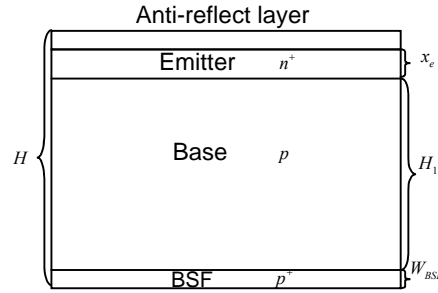


Fig. 1: Structure of the solar cell

Numerical simulations were performed with a FORTRAN program. The two layer model uses a 2 to 50 μm range thick base, a 0.1 to 0.6 μm range thick emitter and the doping densities are 10^{16} to $5 \cdot 10^{16} \text{cm}^{-3}$ range in the base and 10^{17} to $5 \cdot 10^{19} \text{cm}^{-3}$ range in the emitter. We take the recombination velocity of the front and the back surfaces varying between 0 to 10^5cm.s^{-1} .

Collecting a photocarrier for each photon is given for the emitter region by [6, 7]:

$$J_p(\lambda) = \frac{q(1-R(\lambda))\alpha^2 L_p^2 F(\lambda)}{\alpha^2 L_p^2 - 1} \times \left\{ \frac{1 + \frac{S_p}{\alpha D_p}}{ch \frac{x_e}{L_p} + \frac{S_p L_p}{D_p} sh \frac{x_e}{L_p}} - \left[1 + \frac{1}{\alpha L_p} \frac{sh \frac{x_e}{L_p} + \frac{S_p L_p}{D_p} ch \frac{x_e}{L_p}}{ch \frac{x_e}{L_p} + \frac{S_p L_p}{D_p} sh \frac{x_e}{L_p}} \right] \exp(-\alpha x_e) \right\} \quad (1)$$

$R(\lambda)$ is the reflectivity as a function of the wavelength λ , α the absorption coefficient and $F(\lambda)$ the illumination flux at the wavelength λ .

Similarly, the probability of collecting a photocarrier from the base is given by:

$$J_n(\lambda) = \frac{q(1-R(\lambda))\alpha^2 L_n^2 F(\lambda)}{\alpha^2 L_n^2 - 1} \exp(-\alpha(x_e + W)) \times \left\{ \alpha L_n - \frac{sh\left(\frac{H_1}{L_n}\right) + \frac{S_n L_n}{D_n} ch\left(\frac{H_1}{L_n}\right) - \left(\frac{S_n L_n}{D_n} - \alpha L_n\right) \exp(-\alpha H_1)}{ch\left(\frac{H_1}{L_n}\right) + \frac{S_n L_n}{D_n} sh\left(\frac{H_1}{L_n}\right)} \right\} \quad (2)$$

In the depleted layer, the electric field aids the collection of photocarriers, resulting in collection of every photocarrier generated there, as calculated by:

$$J_{SRC}(\lambda) = q(1-R(\lambda))F(\lambda) \exp(-\alpha x_e)(1 - \exp(-\alpha w)) \quad (3)$$

Passivation of the solar cell also decreases the dark current of the solar cell, and, therefore, increases the open circuit voltage, Voc. Assuming ideal material, the transport equations can be solved to give the dark current associated with the base and emitter regions (first two terms in eq. 4) [8,9]. An estimation of the dark current in the depleted layer is included as the third term [9] and is given below:

$$J_{Dark} = \frac{q D_n n_i^2}{N_a L_n} \frac{sh\left(\frac{H_1}{L_n}\right) + \frac{S_n L_n}{D_n} ch\left(\frac{H_1}{L_n}\right)}{ch\left(\frac{H_1}{L_n}\right) + \frac{S_n L_n}{D_n} sh\left(\frac{H_1}{L_n}\right)} \left(\exp\left(\frac{qV}{kT}\right) - 1 \right) + \frac{q D_p n_i^2}{N_d L_p} \frac{sh\left(\frac{x_e}{L_p}\right) + \frac{S_p L_p}{D_p} ch\left(\frac{x_e}{L_p}\right)}{ch\left(\frac{x_e}{L_p}\right) + \frac{S_p L_p}{D_p} sh\left(\frac{x_e}{L_p}\right)} \left(\exp\left(\frac{qV}{kT}\right) - 1 \right) \quad (4)$$

$$+ \frac{\pi n_i q^2 W}{kT \tau_0 (U_d - U_a)} sh\left(\frac{qU_a}{2kT}\right)$$

Where n_i is the intrinsic carrier concentration, N_a and N_d are the concentrations of acceptors and donors, U_a is the built-in voltage, and τ_0 is the nonradiative carrier lifetime, given by $\frac{1}{N_T \sigma v_{th}}$, the reciprocal of the product

of the trap density, the capture cross section, and the thermal carrier velocity [9].

We calculate the currents $J_B(\lambda)$ in the base, $J_E(\lambda)$ in the emitter and $J_{SCR}(\lambda)$ in the depletion region for each wave length, i. the characteristic current-voltage, the maximum power and the efficiency of conversion, by using the parameters of device.

For a wavelength λ the total current crossing the cell is the sum of all those current compounds. The light generated current of the cell is the result of integration on all solar spectrums.

$$\begin{cases} J_L(\lambda) = J_E(\lambda) + J_{SCR}(\lambda) + J_B(\lambda) \\ J_{SC} = \int_{\lambda_{min}}^{\lambda_{max}} J_L(\lambda) d\lambda \end{cases} \quad (5)$$

To do this integral extending from λ_{min} to λ_{max} , we have divided the total current into N intervals the steps variable and by numeric integration (Simpson's method), we calculated the all current crossing the cell, the model that we will use takes into account the following concepts: the diffusion and conduction currents, the generation-recombination in different regions, the variations of lifetime with concentration, the coefficient of reflectivity, the recombination velocity in front and back surface. The data used in the simulation of efficiency are the wavelength λ in μm ($0.3 \mu m \leq \lambda \leq 2 \mu m$), the absorption coefficient $\alpha(\lambda)$ in (cm^{-1}) and the v flux. The accuracy of numeric simulation depends strongly on the choice of physics model used to describe the function of the solar cell. To determine the maximum power P_{max} , the current-voltage characteristic for a single-junction solar cell has to be considered $J = J_{SC} + J_{DARK}$ the efficiency is determined normalizing the power by the total incident

$$\text{power of the spectrum } \eta = \frac{P_{max}}{P_{inc}}.$$

To obtain the maximum conversion efficiency, optimized top and bottom cells are required simultaneously. A low-quality top cell with a high-quality bottom cell can significantly deteriorate the performance of the device since the primary

contribution to the output of a tandem cell is derived from the top cell.

In this work, we optimize the GaAs cell, to form GaAs / Si and GaAs / Ge tandem cells. Then, we compare their efficiency in other to choose the best one.

III. Modelling and Simulation of a GaAs Top Cell Using AM1.5G

Whatever the structure of a solar cell optimization of its parameters is necessary to have a good efficiency. Usually, the parameters to optimize are the thickness of the cell, the level and doping profiles. Optimization of solar cell thus includes the study of the influence of these parameters on the performance to obtain a structure leading to maximum efficiency. The numerical simulation is commonly used for optimization of solar cell.

Figure 1 shows the influence of the base thickness on the cell efficiency with varying back surface recombination ($S_p = 0 \text{ cm/s}$), where the base doping level is 10^{17} cm^{-3} . With increasing thickness, first the photocurrent increases due to enhanced absorption. The V_{oc} decreases with increasing thickness due to an increase in the saturation current density J_0 . With decreasing substrate thickness the cell efficiency is more influenced by the surface recombination. For a very low surface recombination the optimum thickness is around $10 \mu m$, for increased recombination velocity (above 1000 cm/s) at least $10 \mu m$ is required to reach the highest efficiency.

Figure 2 shows that there is an optimum doping of the base that corresponds to the maximum efficiency of the cell. This value is within the range $5 \cdot 10^{16}$ to $5 \cdot 10^{17} \text{ cm}^{-3}$. Increased doping of the base causes the degradation of the lifetime of carriers and mobility. This causes a significant decrease in performance. If the base is low doped ($< 10^{16} \text{ cm}^{-3}$) height of the potential barrier of the p-n junction is reduced. In this case, the electric field of the p-n junction is weaker and conditions of collection carriers are bad.

We showed that the velocity of surface recombination is one of the parameters that most influence the performance of the cell. The high rear recombination velocity of the cell can completely degrade performance. In contrast, the effect on the efficiency is negligible if the rate of recombination at the surface is less than 10^3 cm.s^{-1} .

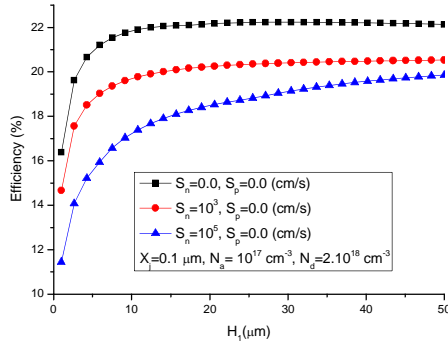


Figure 1: Influence of the thickness of the base on the efficiency conversion

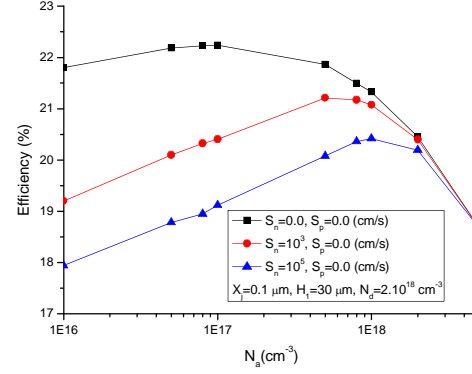


Figure 2: Influence of the doping of the base on the efficiency conversion

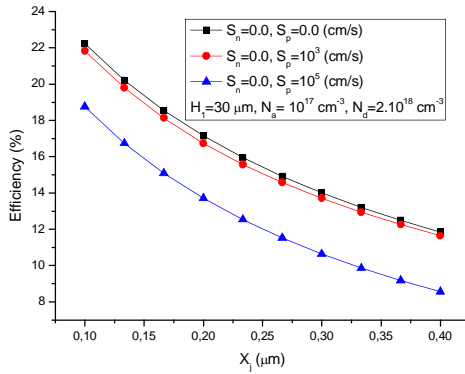


Figure 3: Influence of the thickness of the emitter on the efficiency conversion

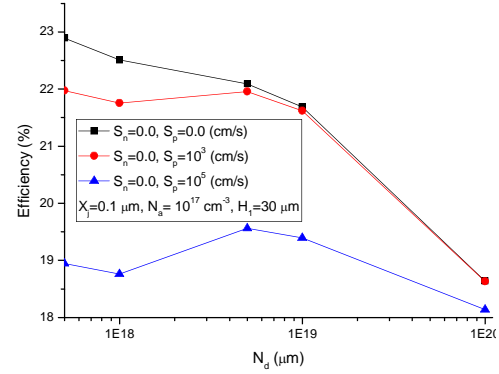


Figure 4: Influence of doping of the emitter on the efficiency conversion

In the figure 3, the efficiency decrease rapidly when increasing the thickness of the emitter. In this figure the efficiency takes its high value when the recombination velocity S_p varies from 0 to 1000 cm.s^{-1} and a thickness of the emitter is low. This range of thickness allows to the generated carriers near the surface.

Figure 4 show that to have a better efficiency one may use a doping level of the emitter higher. Indeed, the thickness of the *emitter* is less than that of the base causing recombination in the emitter is negligible in comparison to the recombination in the base. In contrast by rising doping level of the *emitter* increases the height of the potential barrier of the p-n junction. This causes the growth *efficiency* of the cell.

As illustrated above a too high emitter doping level results in an increased efficiency loss due to Auger recombination and band-gap narrowing. Moreover a higher emitter doping will result in increased front surface recombination. As a result, ideally the doping level of the emitter is between 10^{18} and 10^{19} cm^{-3} . The influence of the surface recombination is especially present at lower doping levels, as is shown in Figure 4.

The optimum GaAs solar cell parameters that have been determined by the described simulations are:

$$H_b : 10 \text{ to } 20 \mu\text{m}, N_a : 10^{17} \text{ to } 10^{18} \text{ cm}^{-3}, x_j : 0.1 \text{ to } 0.2 \mu\text{m}, N_d : 10^{18} \text{ to } 10^{19} \text{ cm}^{-3}.$$

The results obtained are in good agreement with those of Liou and al [10].

IV. Simulation Results of a Mechanically Stacked GaAs/Si and GaAs/Ge tandem Cell

Two main reasons for the limitation of solar cell efficiency are losses by thermalisation and non-absorption of low-energy-photons.

In the case of thermalisation, the excess energy of absorbed photons is transferred to the active material via phonons. This energy is then a pure loss for the photovoltaic conversion. However, photons with energy smaller than the band gap cannot be absorbed. Therefore, in single cell device, a trade-off has to be found between thermalisation losses, and the usage of a too large band gap.

The idea of a tandem cell is to achieve better absorption efficiency by using materials having

different band gap. One material should then collect the higher energetic photons and the other, with a lower band gap than the first one, should absorb photons with lower energy.

In tandem cells, two (or more) junction solar cells are deposited on top of each other. Two methods are available to stack these cells: parallel or serial connections. Serial connection is much likely to be realizable, since it does just require thin, non-continuous, non-absorbing metallic layers to separate the different cells and act as recombination layer. When two cells are serial - connected, the same current has to flow through the entire device. This current is dictated by the lowest current of the two cells. In the case of serial connection, the voltage of a tandem cell is determined by the addition of the voltages of the individual cells.

The calculations are based directly on the available spectral data sets. Starting with the irradiance data point at the highest energy, the efficiency was calculated for the upper solar cell. The remaining part

of the spectrum was taken to calculate the efficiency of the lower solar cell: The highest added efficiencies of the top and the bottom solar cells were drawn dependent on the different spectra.

The total efficiency is [11, 12] :

$$\eta_{GaAs/Si} = \eta_{GaAs} + \eta_{Si} \quad \text{and} \quad \eta_{GaAs/Ge} = \eta_{GaAs} + \eta_{Ge} \quad (6)$$

A mechanically stacked tandem cell was modelled as a GaAs top cell mounted on top of a Ge or Si bottom cells. The two cells were connected externally to form a two-terminal device. This approach allows the fabrication of individual cells and their operation to be independent.

To obtain the maximum overall conversion efficiency, optimized top and bottom cells are required simultaneously. A low-quality top cell with a high-quality bottom cell can significantly deteriorate the performance of the device since the primary contribution to the output of a tandem cell is derived from the top cell.

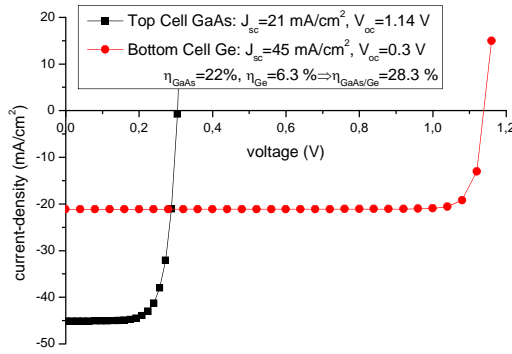


Figure 5: Simulated J-V curves for a GaAs/Ge tandem with a total AM1.5G efficiency of 28.3%.

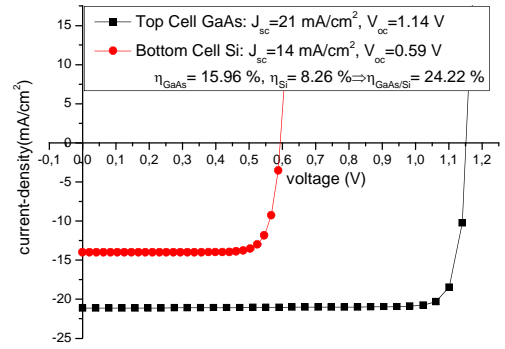


Figure 6: Simulated J-V curves for a GaAs/Si with A total AM1.5G efficiency of 24.22%.

Figure 5 shows the J-V characteristics of the GaAs top and Ge bottom cells. According to equation (6), the efficiency is $\eta_{GaAs/Ge} = 28.30\%$ for GaAs/Ge tandem cell with a 22% GaAs top cell and a 6.30% Ge bottom cell.

Figure 6 shows the J-V characteristics of the GaAs top and Si bottom cells. The efficiency obtained is $\eta_{GaAs/Si} = 24.22\%$ for GaAs/Si tandem cell with a 15.96% GaAs top cell and an 8.26% Si bottom cell.

We remark that the efficiency of GaAs/Ge is higher than to GaAs/Si one. This is due to the difference between the gap energy of the materials (Ge and Si). The value of band gap of Si is near of the value of GaAs and allows the absorption of the same range of wavelength. This reflects low efficiency of tandem

GaAs/Si. In contrast, the gap value of Ge is very low compared to the gap value of the GaAs, which allowed him to absorb beyond the infrared range and thus giving a best efficiency but much lower than the highest efficiency 3J cell [13].

For Tandem cell the GaAs / Ge in reference [14], the authors found an efficiency of 35.7% in a configuration with two-terminal with the AM0 spectrum.

For Tandem cell the GaAs / Si in the reference [15], the authors found an efficiency of 29.6% with four-terminal. They used a concentrator and the AM1.5 spectrum.

V. Conclusion

Device modelling and numerical simulations for a mechanically stacked GaAs/Ge and GaAs/Si tandem cells have been performed using a numerical simulations program. These simulations reveal that a 28.30% GaAs/Ge conversion efficiency with a high-efficiency GaAs top cell and an optimized Ge bottom cell structure can be achieved. This efficiency is superior to the efficiency of the GaAs/Si tandem cell (24.22%) due to the difference between the gap energy of the materials (Ge and Si).

Increased efficiency can be obtained for multijunction solar cells (three or more junctions).

VI. References

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