Performance Analysis of AlxGa1-xAs/epi-Si(Ge) Tandem Solar Cells: A Simulation Study

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Performance analysis of $Al_xGa_{1-x}As$/epi-Si(Ge) tandem solar cells: a simulation study.

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Abstract

A new strategy for the development of III-V/Si tandem solar cells has recently been proposed consisting in low temperature PECVD epitaxy of silicon or silicon-germanium on gallium-arsenide. This paper thus gives first insights about theoretical but realistic maximum performance of such tandem cells by means of full numerical simulations considering perfect layers and interfaces. The consequences of using a thin epi-Si bottom cell instead of a thick silicon substrate are investigated. In case no light trapping scheme is considered, a minimum epi-layer thickness of 20µm is mandatory for the tandem to exhibit higher conversion efficiencies than a single GaAs solar cell. The epi-Si can yet be advantageously replaced by an epitaxial silicon-germanium alloy to increase the bottom cell optical absorption and thus decrease the minimum required thickness by a factor of ~4 (~5µm). Finally, simulations show that over 33% efficiency can be obtained for $Al_xGa_{1-x}As$/epi-$Si_{0.63}Ge_{0.27}$, which confirms that this is a promising new concept.

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Keywords: tandem solar cells; III-V on silicon; silicon on III-V; modeling; simulation

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1. Introduction

Multijunction solar cells based on III-V compounds have by far the highest conversion efficiency. However, the fabrication cost remains very high. An attractive solution to lower the cost while maintaining high efficiencies is to design multijunctions on cheaper substrates such as silicon [1-2]. Different routes have been proposed to deal with lattice mismatch issues between Si and III-Vs: epitaxial growth of GaAs on Si with or without buffer layers or non-epitaxial techniques such as mechanical stacking [3-7]. A novel approach has been recently reported by Cariou et al. [8-9] consisting in direct epitaxial growth of thin Si or SiGe layers on GaAs by low temperature plasma enhanced chemical vapor deposition (PECVD). This reversed approach has many advantages compared to the classical ones, which opens a new way for making III-V/Si tandem solar cells: (i) A high crystal quality has been demonstrated: interface issues due to lattice and thermal mismatch seem to be highly reduced. (ii) The silicon or silicon-germanium epitaxy is done at low temperature (below 200°C) preventing from the degradation of the underlying III-V layers and interfaces.

However, one critical aspect still has to be carefully investigated to evaluate the potential benefits of this novel concept. Indeed, due to the low deposition rate, the high quality epi-Si layers are still rather thin (~10µm), which leads to a reduced optical absorption in the bottom cell compared to the classical approaches that consider a thick Si wafer (>200µm). This thickness constraint has a direct consequence on the short circuit current density value (Jsc) and on the current matching, which has so far only been calculated in literature for a thick bottom cell.

In this paper, we present a first simulation study aimed at facilitating the future design of III-V/epi-SiGe tandem solar cells. Actually, the conventional efficiency calculations of III-V/Si tandem cells are generally based on the ideal radiative limit and suffer from too limiting assumptions in case thin epi-Si layers are used, e.g. complete absorption in the sub-cells [1,10-11]. Therefore, we propose to simulate these novel structures using TCAD tools [12], in which physical models are known to be well adapted for realistic multijunctions simulation [13]. The maximum efficiencies achievable at 1sun will be investigated, without any particular light trapping scheme, considering perfect materials and interfaces.

2. Modeling of the AlGaAs/epi-Si(Ge) tandem cells

The tandem structure we propose to simulate is inspired from literature and from the work of Cariou et al. on GaAs and epi-Si single cells [9, 14-15]. A simplified schematic of the solar cell is depicted in Fig. 1. It is composed of an $Al_xGa_{1-x}As$ top cell and a epi-Si(Ge) bottom cell both connected in series using a tunnel junction. The Al composition (x) can be varied in order to tune the band gap of $Al_xGa_{1-x}As$ from 1.42eV (x=0) to above 2eV (x>0.45) [16]. The detailed layers information concerning thicknesses, doping levels and compositions are given in Table 1. Note that the tunnel junction optimization is out of the scope of this paper. For the sake of simplicity, we have chosen a rather simple tunnel junction, which does not limit the operating current under 1sun illumination (high peak current and low resistivity).

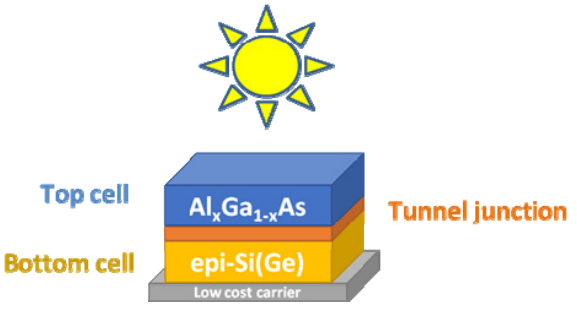

Fig. 1. Simplified schematic of the novel concept of the AlGaAs/epi-Si(Ge) tandem solar cells. More detailed information on each layer can be found in Table 1.

Simulations of current density versus voltage curves (J(V)) have been performed with Silvaco's ATLAS 2D simulator [12]. Band structure, electrical transport and recombination parameters for III-V materials and amorphous and crystalline silicon were chosen in agreement with literature values [12,16,18] and are composition and doping dependent. To simulate the illuminated J(V), realistic photogeneration profiles have been calculated through the entire structure thanks to the Transfert Matrix Method (TMM) using the optical indexes of the various layers as input. The latters are composition dependent and are obtained by interpolation of experimental data found in literature, mainly coming from ellipsometry measurements [12, 16]. Note that the optical shading due to the opaque metal contacts at the front side is not taken into account.

Table 1. Structure of the simulated AlGaAs/epi-Si(Ge) tandem cell based on literature and on our own developments [9, 14-15]. E_C-E_F is the a-Si:H activation energy i.e. the energy difference between the Fermi level (E_F) and the bottom of the conduction band (E_C) in the hydrogenated amorphous silicon layer.

	Material	Role	Thickness (µm)	Net doping (/cm^3)
Top cell	SiO_2/TiO_2	Anti-Reflective Coating (ARC)	0.104/0.05	-
	$Al_{0.85}Ga_{0.15}As$ (p)	Window	0.035	$2x10^{18}$
	$Al_xGa_{1-x}As$ (p)	Emitter	0.2	$2x10^{18}$
	$Al_xGa_{1-x}As$ (n)	Base	Variable (0.1-4)	$2x10^{17}$
	$Al_{0.3}Ga_{0.7}As$ (n)	Back Surface Field (BSF)	0.1	$2x10^{18}$
Tunnel junction	GaAs (n++)	n++ layer	0.03	$3x10^{19}$
	GaAs (p++)	p++ layer and emitter of the bottom cell	0.03	$3x10^{19}$
Bottom cell	epi-Si or epi-$Si_{1-y}Ge_y$ (n)	Base	Variable (5-500)	$1x10^{14}$
	a-Si:H (n)	BSF	0.012	E_C-E_F~0.2eV
	Aluminum	Flat metal contact	0.4	-

3. Results and discussion

In order to evaluate the potential of these tandem cells in terms of maximum achievable efficiencies, we first performed simulations without introducing defective layers and interfaces. This way, it is possible to investigate the sole effect of reducing the bottom layer thickness from a few hundreds of microns to a few microns, corresponding respectively to the classical approach of making III-V on a Si substrate and the hereinabove presented novel concept.

Actually, thinning the bottom cell significantly modifies the optimum design of the top cell. Indeed, because the two sub-cells are connected in series one has to carefully match the current of each individual cell. This is classically done by tuning the band gap of the top base: the optimum is ~1.7eV for a silicon band gap of 1.12eV [1-2]. This value is only valid for a complete light absorption in each sub-cell i.e. for thick top and bottom bases. Yet, if the top cell is partially absorbing, lower optimum band gap values can be found [1].

Our simulations are fully consistent with this literature results as shown by the contour plot in Fig. 2 (a), which represents the simulated Jsc values for different top cell thicknesses and Al compositions, for a thick bottom cell. The maximum Jsc values (>18mA/cm^2) are found in the red region which shifts from x~0.22 (Eg~1.7eV) to x=0 (Eg=1.42eV) as the top absorber thickness is reduced from 4µm to 0.1µm.

If the Si bottom absorber is now reduced to an extreme value of 5µm, our simulations on Fig. 2 (b) indicate that the Al composition has this time to be increased (~0.4<x<~0.6) to keep matching the current. This is a consequence of the steep reduction of the external quantum efficiency (EQE) of the bottom cell, as it is illustrated on Fig. 3. Note that for x values over 0.45 the AlGaAs ternary band gap becomes indirect, which also reduces the optical absorption and the EQE of the top cell. Furthermore, high contents of Al are reported to increase the number of defects inside this layer, which would decrease the minority carrier lifetime experimentally [17]. In this case, other III-V compounds with similar band gaps could be advantageously considered. Nevertheless, the best Jsc value is still rather low: Jsc~9mA/cm^2 for a 1.24µm $Al_{0.56}Ga_{44}As$ top cell. Despite higher values of open circuit voltage

(Voc~2.2V), this tandem cell with 5µm epi-Si exhibits a conversion efficiency of only η~17%, which is even lower than that of a single GaAs cell: Voc~1V and η~24% [14]. We can thus wisely wonder what the minimum epi-Si thickness to achieve reasonable efficiencies (at least over 25%) could be.

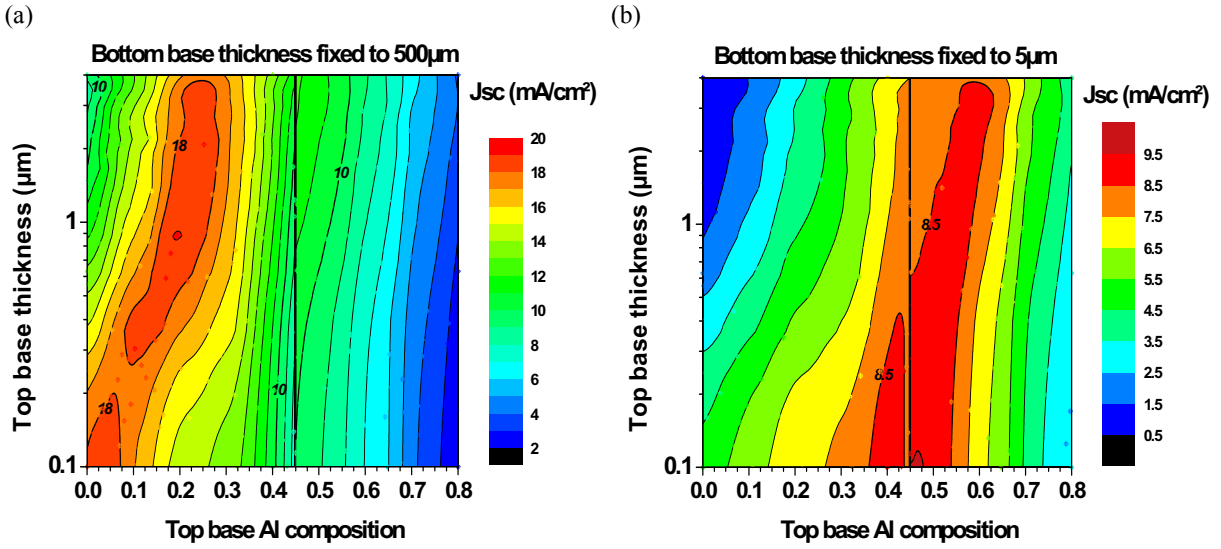

Fig. 2. Maps of tandem cell short circuit densities (Jsc) simulated for different combinations of Aluminum compositions and thicknesses of the top base: (a) for a thick Si bottom cell (500µm) and (b) for a thin Si bottom cell (5µm). The solid lines for x=0.45 represent the border between direct and indirect band gap for AlGaAs.

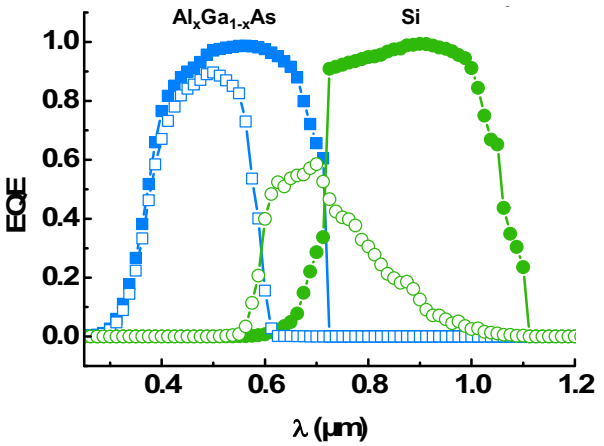

Fig. 3. External Quantum Efficiency (EQE) versus photon wavelength of two current matched AlGaAs/Si tandem cells. The blue square and green circle symbols represent the individual EQE of the top and the bottom cells respectively. Jsc~19mA/cm^2 is obtained for a 1.16µm $Al_xGa_{1-x}As$ top cell with x=0.24 and for a 500µm Si bottom cell (full symbols). Jsc~9mA/cm^2 is obtained for a 1.24µm $Al_xGa_{1-x}As$ top cell with x=0.56 and for a 5µm Si bottom cell (open symbols).

For this study, we fixed the top base thickness to 1µm and simulated the AlGaAs/epi-Si tandem efficiency for various bottom base thicknesses and top base Al compositions. As seen on Fig. 4 (a), 25% efficiency can be reached if the bottom base is at least 20µm thick. At this stage, it is important to keep in mind that no particular light trapping scheme is used at the back side, meaning that there is still room for improving this tandem cell

performance. However, without considering a complex and expensive light trapping scheme, we can more easily change silicon by a more absorbing material, such as SiGe. Indeed, as seen on Fig. 4 (b), replacing the epi-Si bottom base by a $Si_{0.63}Ge_{0.27}$ layer allows one to use 4 or 5 times less thickness for the same resulting efficiency. Namely, 25% efficiency can still be reached with only 5µm of epi-$Si_{0.63}Ge_{0.27}$ and 33% with 20µm.

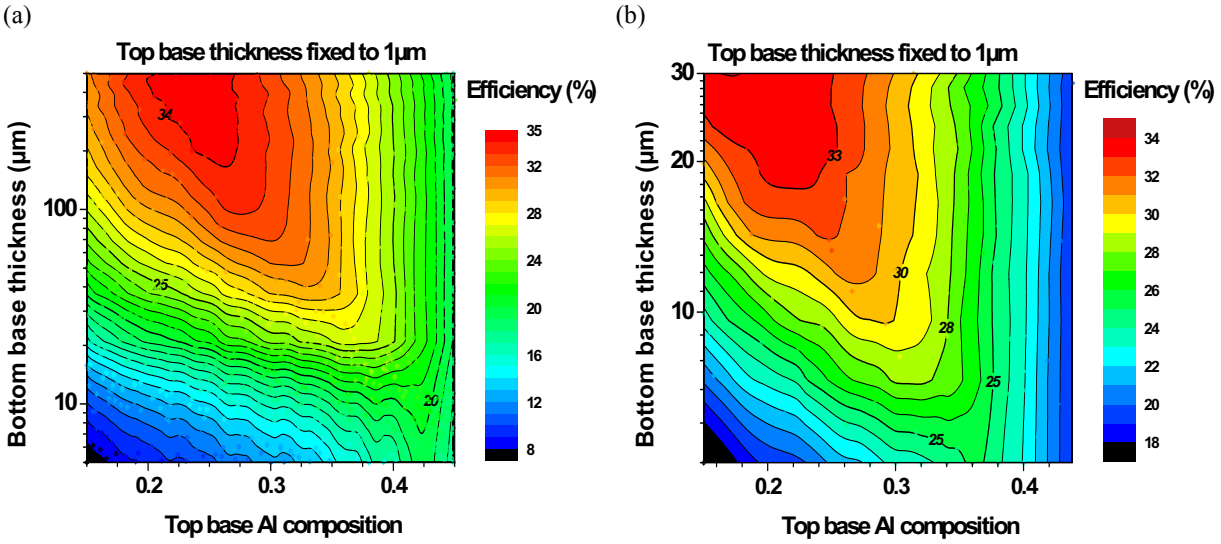

Fig. 4. Maps of tandem cell efficiencies simulated for different combinations of top base Aluminum compositions and bottom base thicknesses: (a) for a bottom cell in epi-Si and (b) for a bottom cell in epi-$Si_{0.63}Ge_{0.27}$.

4. Conclusion and perspectives

This first simulation study was aimed at evaluating the recently reported concept of III-V/epi-SiGe tandem cells in terms of maximum achievable efficiencies. Rather thin Si bottom cells are present in these structures, which modifies the III-V optimum band gap and thickness that has been so far calculated in literature for III-V/Si tandem cells. Our simulations also reveal that the minimum thickness for the epi-Si bottom cell is ~20µm. This value could be difficult to achieve experimentally. Though the development of light trapping schemes could help relax this thickness constraint, the solution consisting in a replacement of the epi-Si layer by epi-SiGe is already very satisfying and has to be considered in future designs. Without light trapping, 25% efficiency can still be reached with only 5µm of epi-$Si_{0.63}Ge_{0.27}$ and over 33% efficiency can be obtained with a 20µm thick epi-$Si_{0.63}Ge_{0.27}$ bottom cell.

Although epitaxial silicon layers are of good crystalline quality, there are inevitably some defects either at the interface or in the bulk. Those energetically located within the band gap of the semiconductor can increase the Shockley-Read-Hall recombination in the bottom cell and can therefore decrease tandem cell performance. As a consequence, it is of crucial importance to find a way to precisely evaluate the defect density inside the epitaxial layer. Our ongoing studies are thus aimed at investigating both experimentally and theoretically the impact of the epi-layer defects on the tandem cell performance. The benefits of light trapping are also being evaluated.

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