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Abstract. In this paper, we present a comprehensive study of high efficiencies tandem solar cells monolithically grown on a silicon substrate using GaAsPN absorber layer. InGaAs(N) quantum dots and GaAsPN quantum wells have been grown recently on GaP/Si susbstrate for applications related to light emission. For photovoltaic applications, we consider the GaAsPN diluted nitride alloy as the top junction material due to both its perfect lattice matching with Si and ideal bandgap energy for current generation in association with the Si bottom cell. Numerical simulation of the top cell is performed. The effect of layer thicknesses and doping on the cell efficiency are evidenced. In these structures a tunnel junction (TJ) is needed to interconnect both the top and bottom sub-cells. We compare the simulated performances of different TJ structures and show that the GaP(n+)/Si(p+) TJ is promising to improve performances of the current-voltage characteristic.

Keywords*:* Tandem solar cells, tunnel junctions, numerical simulation, Photonics on silicon

1. Introduction

Nowadays emphasizes is put on environmental protection and energy needs make solar energy become a major energy source in the future. In this context, there is a strong effort underway to lower the cost of the photovoltaic kilowatt-peak toward new material systems. However the concept of a silicon-based single junction solar cell does not lead to an optimal use of the whole solar spectrum. Its high energy part is lost by carrier thermalisation. To overcome this limitation, the concept of multi-junction solar cell has been proposed and efficiency over 40% were reported for GaAs based cells (Geisz *et al.* 2008; Ming-Han and Yuh-Renn 2012; Baudrit *et al.* 2008; Baudrit *et al.* 2010; Friedman *et al.* 2010; Green *et al.* 2010; Green *et al.* 2013).

Recent progress in III-V-N alloys monolithic growth on silicon substrate (Robert *et al.* 2012; Robert *et al.* 2011) led our research team to propose these promising materials for multi-junction solar cells (Almosni *et al.* 2013; Ming-Han and Yuh-Renn 2012; Aho *et al.* 2010). In this paper, we propose a GaAsPN diluted nitride alloy as the top junction material of a Si based tandem solar cell. Its perfect lattice matching with Si and ideal bandgap energy of 1.7 eV, are both appealing for optimal current generation with a 1.1 eV bandgap Si bottom cell. In this work we present numerical simulation results for the top PIN GaP/$GaAs_xP_{1-x}N$/GaP junction. Modeling is performed using the ATLAS device simulator (Silvaco). Optimized layer thicknesses and doping for the top PIN GaP/$GaAs_xP_{1-x}N$ /GaP junction in terms of efficiency are determined. A key factor to achieve efficient tandem solar cells is the tunnel junction (TJ) between top and bottom sub-cells (Baudrit *et al.* 2008; Baudrit *et al.* 2010). We compare the theoretical performances of various TJ structures and show that the GaP(n+)/Si(p+) exhibits the best current-voltage characteristic.

2. GaAsPN absorbing layer

In order to successfully design a multi-junction cell in the pseudomorphic approach, issues of low defects density at the interface (lattice matching) and current matching between the different cells have to be adressed. Efficiency as high as 44% has been recently reported using InGaAsN diluted nitride on GaAs substrate, but the limitation of this approach is the coast of the GaAs substrate. To overcome this limitation we propose to use the $GaAs_{0.1}P_{0.87}N_{0.03}$ diluted nitride system which is expected to have a perfect lattice matching with Si or GaP and a pseudo-direct bandgap energy of about 1.7 eV (Nguyen Thanh *et al.* 2008).

As already shown in previous work (Almosni *et al.* 2013), lattice matching is obtained between GaAsPN grown by Molecular Beam Epitaxy and the GaP (or Si) substrate. The band gap of the GaAsP alloy is indirect for a small As content (less than 10%) (Harris *et al.* 2008; Robert *et al.* 2012). The direct band gap character is enhanced in dilute GaAsP(N) nitrogen alloys, as confirmed experimentally by time-resolved photoluminescence (Almosni *et al.* 2013). Fig. 1 shows the measured variation of the refractive index (real and imaginary part) of a 1 µm thick GaAsPN layer at a 70° angle of incidence and the corresponding absorption, which vanishes below 1.7 eV. The experimental data have been fitted using a dispersion models (Forouhi et al. 1986; Adachi 1989) for the GaAsPN layer and its native oxide respectively.

3. Modeling

Modeling is performed using the ATLAS device simulator by Silvaco which allows to numerically solve Poisson's equation coupled with continuity equations for both electrons and holes under steady state conditions. An important key feature of the tandem solar cell is the TJ interconnecting both top and bottom sub-cells. In this work, the performances of various tunnel junction diodes have been compared. We use the TJ model implemented in the ATLAS simulator which has been widely validated in the literature for Silicon (Lavery 2008) and for III-V semiconductors (Baudrit et al 2008; Baudrit et al 2010; Allen 2010)..

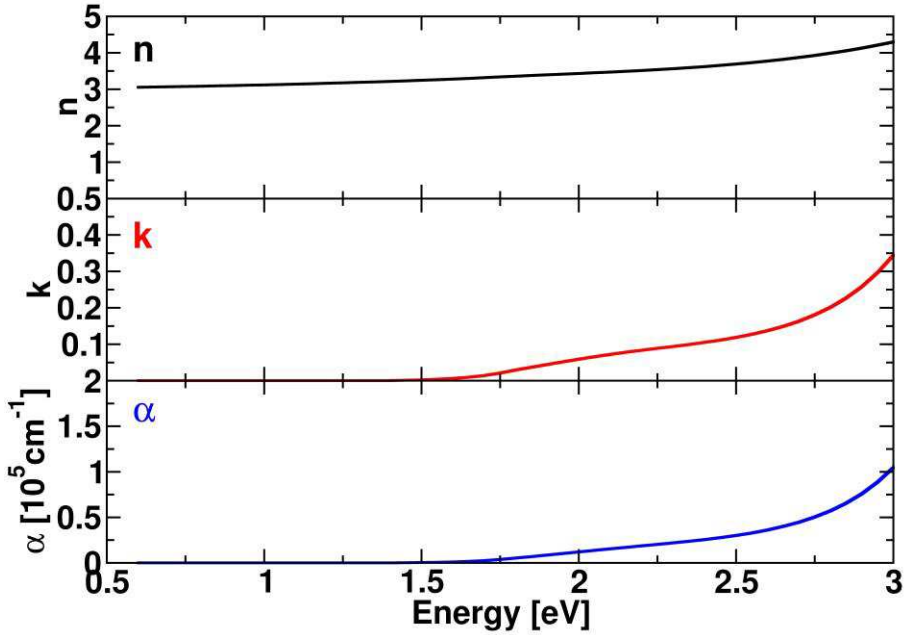

Fig. 1. Real and imaginary part of the GaAsPN refractive index and related absorption coefficient

4. Tunnel junction

Fig. 2(a) shows the schematic structure of the tandem solar cell. Four tunnel junctions configurations have been studied in this work: Si(n+)/Si(p+), GaP(n+)/GaP(p+), GaP(n+)/Si(p+) and GaP(p+)/Si(n+). The layers thicknesses for the simulation were 20 nm. Actually, such thin heavily doped Si layer leads obviously to negligible light absorption.

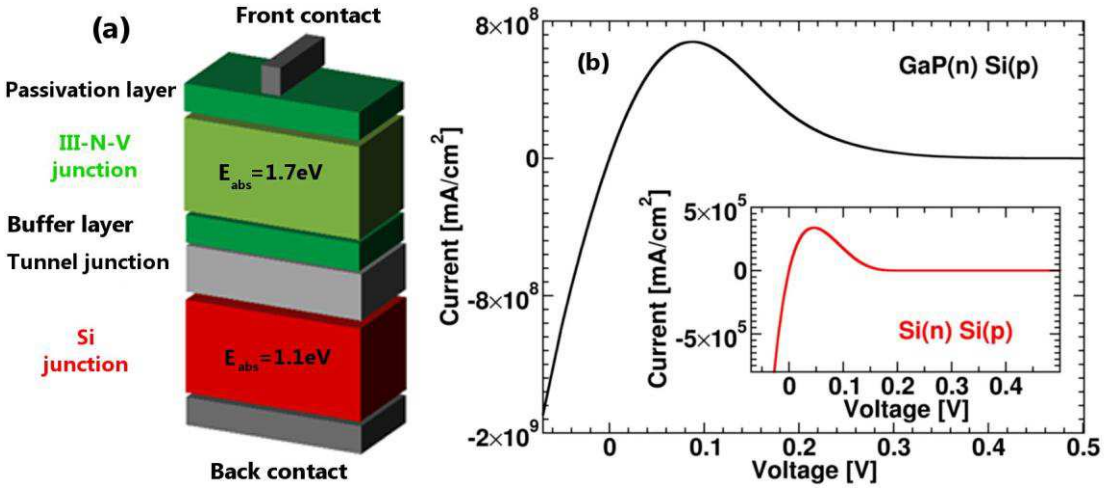

Fig. 2. (a) Schematic of the GaAsPN/Si tandem cell and (b) Simulated current-voltage characteristic of a GaP-n+/Si-p+ and Si-n+/Si-p+ tunnel junctions at uniform doping of 10^{20} cm^{-3}

We used the defaults material parameters provided by the Atlas simulator for the Si (GaP) gap energy 1.08eV (2.26eV) and electron affinity 4.17eV (4.4eV). For a large uniform doping level (10^{20} cm^{-3}), the GaP(n+)/Si(p+) TJ is much more efficient than the Si(n+)/Si(p+) TJ as shown in Fig. 2(b) and Table I because the tunneling barrier thickness is lower for the former case (see Fig. 3).

Parameters	GaP(n+)/Si(p+)	GaP(p+)/Si(n+)	GaP(n+)/GaP(p+)	Si(n+)/Si(p+)
Vp (mV)	92	35	70	45
Ip (mA/cm²)	8.4×10^{8}	$\sim10^{-4}$	$\sim10^{-3}$	3.4×10^{5}
L_B (nm)	3.3	6.9	5.9	4.4

TABLE I: THE VOLTAGE Vp, PEAK CURRENT DENSITIES Ip, AND THE BARRIER THICKNESSES L_B OF THE FOUR TJ AT UNIFORM DOPING OF 10^{20} cm^{-3}

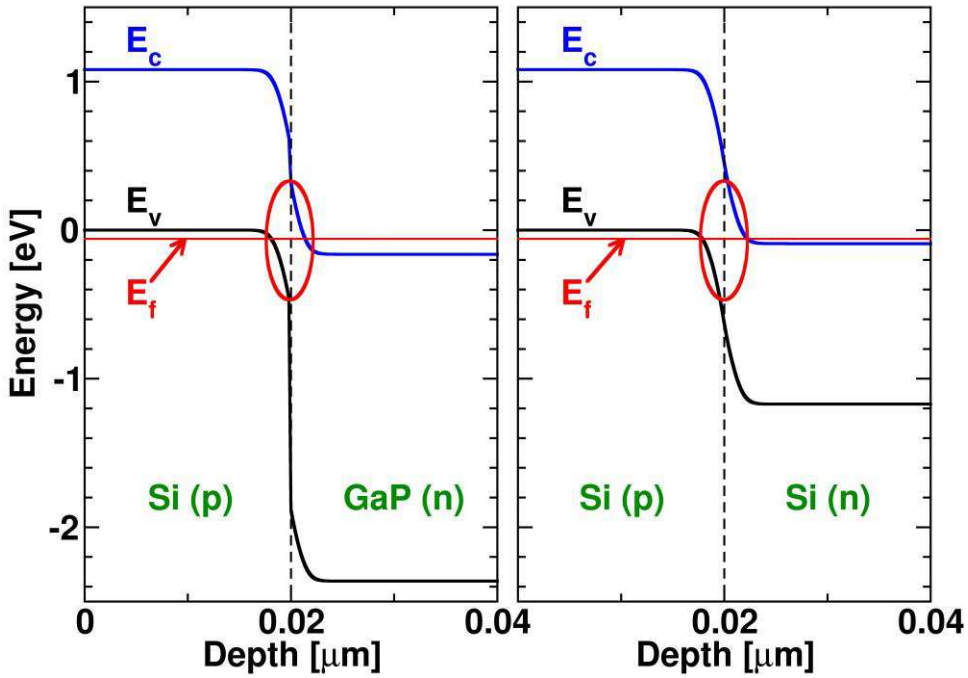

Fig. 3. Simulated Band diagram of a GaP-n+/Si-p+ and Si-n+/Si-p+ tunnel junctions at uniform doping of 10^{20} cm^{-3} at thermal equilibrium. The origin of the energy scale is taken at the top of the valence band of Si(p). In this figure: E_c, E_v and E_f are the bottom of the conduction band, the top of the valence band and the Fermi level of the homo/heterostructure.

5. Top cell structure and material parameters

Table II shows the basic structure of the GaAsPN top cell as well as the doping levels of the various layers, and Table III reports the main material parameters used for the simulation.

GaP	P++	$5x10^{18}$	cm^{-3}	50nm
GaP	P+	$5x10^{18}$	cm^{-3}	200nm
$GaAs_{0.1}P_{0.9}N$	intrinsic	1000nm		
GaP	n+	$1x10^{18}$	cm^{-3}	30nm

TABLE II: LAYER THICKNESSES AND DOPING

Parameters	GaP	GaAsPN
E_g (eV)	2.2	1.7
μ_n ($cm^2V^{-1}s^{-1}$)	150	1000
μ_p ($cm^2V^{-1}s^{-1}$)	80	80
τ_n (s)	10^{-8}	10^{-10}
τ_p (s)	10^{-8}	10^{-10}
χ (eV)	3.8	4.3

TABLE III: MATERIAL PARAMETERS OF GaP AND GaAsPN USED IN THE SIMULATION

Due to the lack of experimental data for the GaAsPN system, carrier mobility and lifetime values reported in table III were chosen according to earlier published results obtained for the GaInAsN material (Geisz *et al.* 2002; Fahy *et al.* 2004; Kashner *et al.* 2001). In these works, electron mobility ranging from 100 to 2000 $cm^2V^{-1}s^{-1}$ and carriers lifetime (at room temperature) ranging from 0.1 to 1 ns were reported.

6. Results

Fig. 4 shows the theoretical effect of the GaAsPN absorber layer thickness on the cell's current-voltage characteristic under AM1.5 solar flux. It can be seen that when increasing the GaAsPN layer thickness from 500 nm to 3000 nm, the open circuit voltage decreases because of the voltage drop due to the parasitic resistance effect, while the short circuit current increases because the density of generated carriers increases. Therefore, an optimum cell efficiency of 9.42% can be obtained for a GaAsPN layer thickness of about 1µm.
This last result can be inferred more accurately from Fig. 5(a) which shows the theoretical variation of the cell efficiency as a function of the wavelength for various GaAsPN layer thicknesses. The simulation was based on experimental values of the absorption coefficient of the GaAsPN material and shows an increase of the cell efficiency around 600 nm with the GaAsPN thickness due to the absorption of GaAsPN material.
First samples have been grown in our laboratory. Fig. 5(b) shows that the measured efficiency variations follow the same trend as the theoretical ones. However, the maximum cell efficiency due to the photo-carriers created in the GaAsPN intrinsic layer of the structure remains quite low. This poor performance could be attributed to low carrier mobility and/or short carrier lifetime. Indeed, in this structure, the intrinsic absorbing layer plays the role of the depletion region which explains that the current increases with the width of the GaAsPN layer. This is especially true for thicknesses which correspond to carrier transit times smaller than the carrier life times (Fig. 4). In fact, Nitrogen-induced defects have been observed in GaAsPN alloys grown on GaP (Jandieri et al 2013) and improvement is still needed to reach a better quality of the materials through growth condition optimization or sample annealing to reduce the influence of these remaining defects on both carrier mobility and lifetime in the GaAsPN layer.

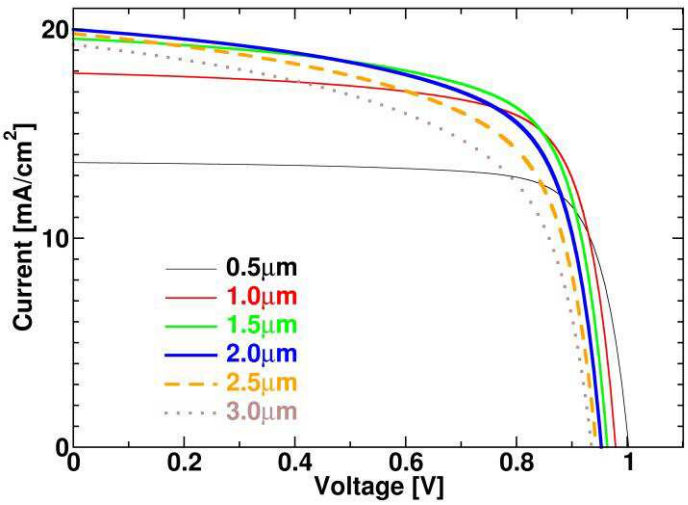

Fig. 4. Current voltage characteristic of the GaP/GaAsPN/GaP cell for GaAsPN layer thicknesses ranging from 0.5 µm to 3 µm.

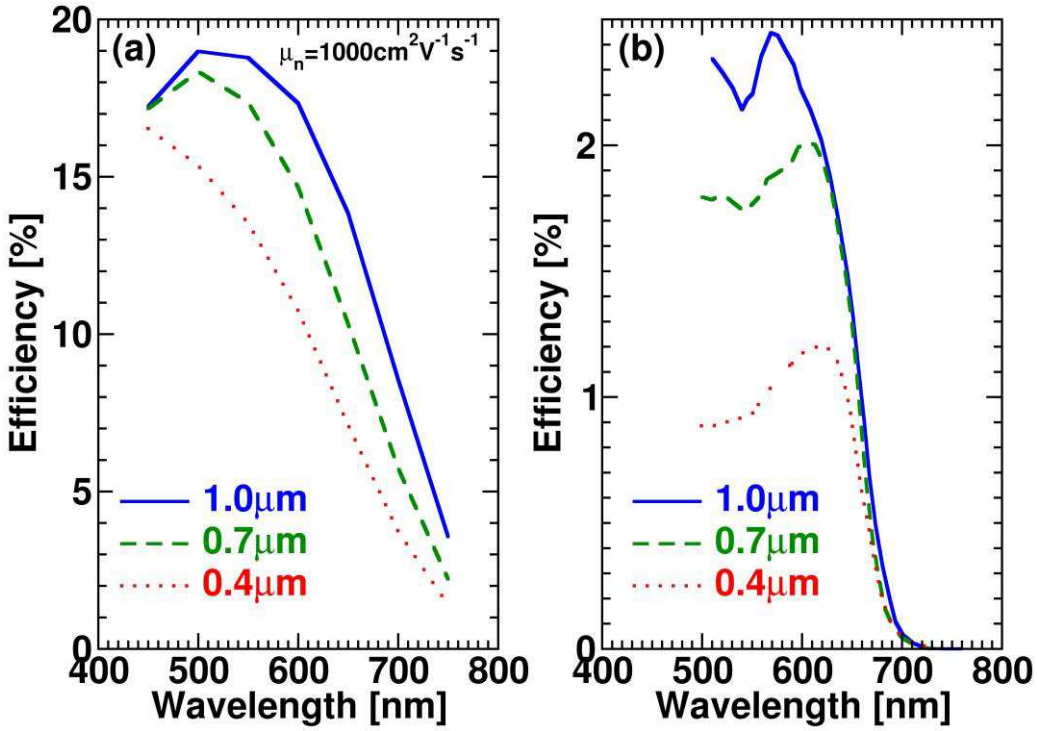

Fig. 5. (a)Simulated efficiency for GaP/GaAsPN/GaP top cell as a function of the wavelength for GaAsPN layer thicknesses ranging from 0.4 µm to 1 µm for μ_n=1000cm^{2}V^{-1}s^{-1}. (b) Measured efficiency for GaP/GaAsPN/GaP top cells as a function of the wavelength for GaAsPN layer thicknesses ranging from 0.4 µm to 1 µm.

7. Conclusion

In summary, we have shown that GaAsPN diluted nitride is a good candidate to play the role of the absorbing layer of the top cell because of its good lattice matching with silicon substrate and its bandgap energy of 1.7 eV. We found that the GaP(n+)/Si(p+) heterostructure is the best tunnel junction configuration to interconnect both top and bottom cells. The correct trend is simulated for the variation of the tandem cell efficiency as a function of the GaAsPN layer thickness. Nevertheless, simulations indicate that there is still room for improvement of the maximum cell efficiency. Material optimization is still needed to improve carrier mobilities and lifetimes. Available material parameters for GaAsPN alloys are scarce. We hope that the present work will stimulate further experimental studies on these materials.

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