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Simulation study of GaAsP/Si tandem solar cells

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ABSTRACT

A model, adapted from the Shockley–Queisser detailed balance model to tandem solar cells with a monolithically grown $GaAs_xP_{1-x}$ top junction on a Si bottom junction, has been developed. Updated data have been used for the absorption spectrums. Two surface geometries, flat and ideally textured, have been investigated. As an important improvement over existing models, the effects of threading-dislocations-related Shockley–Read–Hall recombinations in the $GaAs_xP_{1-x}$ cell, due to the lattice mismatch between the $GaAs_xP_{1-x}$ epilayers and the Si substrate, have been taken into consideration. Auger recombinations in the Si bottom cell and luminescent coupling between the cells have also been considered. For a dislocation-free 2-μm-thick top cell, maximal theoretical efficiencies of 41.6% and 39.1% have been calculated for a textured and a flat surface, respectively. For threading dislocation (TD) densities below 10^4 cm^{-2}, the impact of TDs in the $GaAs_xP_{1-x}$ layers on the solar cell performances is very limited. With TD densities over 10^5 cm^{-2}, the top cell open-circuit voltage is reduced, hence the overall efficiency. For TD densities over 4×10^6 cm^{-2}, as the diffusion length of minority carriers in the base gets smaller than the base thickness, the short-circuit current in the top $GaAs_xP_{1-x}$ cell is also reduced, resulting in a decrease in the optimal top cell bandgap. Using non-ideal EQEs and surface recombination rates from published experimental data, the long-term efficiency potential of the investigated technology has been estimated to be ~35.1% for an ideally textured $GaAs_xP_{1-x}$/Si tandem cell with a TD density of 10^5 cm^{-2} (~33.0% with a flat surface).

1. Introduction

The photovoltaic industry has seen a remarkable development in the recent years, largely fueled by a continuous reduction of costs along the entire value chain. Nevertheless, further improvements are needed in order to keep this sustained pace of cost reduction and further expand the adoption of the technology. Among the multiple levers for cost reduction, improving the efficiency plays a very significant role as it impacts the cost of the whole system.

With 25.6% record efficiency and 25.0% efficiency achieved with processes used for industrial production of solar cells [1,2], the low-cost market-dominant crystalline silicon-based solar cell technology is already very close to its theoretical maximal efficiency, and the margin for further improvement is very small. On the other hand, III–V based multi-junction solar cells have been able to achieve efficiencies close to 40% without concentration [3,4]. However, the need for expensive substrates makes their high scale development unlikely. Although epitaxial Lift-Off (ELO) process is a solution pathway to overcome this issue [5], uncertainties remain regarding the costs and limits of substrate reuse.

The combination of III–V single- or multi-junction solar cells integrated on a comparatively low-cost silicon substrate are promising alternative candidates for cost-efficient fabrication of high efficiency solar cells. Wafer bonding circumvents issues arising from polar-on-nonpolar integration and difference in lattice constant between materials and has resulted in high efficiency devices [6]. However, the fabrication of III–V cells on distinct substrates involves a step of separation in a process akin to ELO. Challenges pertaining to this technology are thereby still a concern for wafer bonding pathways. On the other hand, direct epitaxial growth of a III–V top cell on a silicon bottom cell acting as a substrate is a very elegant and potentially industrially relevant way to produce high-efficiency tandem solar cells on a low-cost substrate. Following the initial developments by Hayashi et al. in the 1990's [7] and the work carried out by Geisz et al. [8,9] in the 2000's, the technology has seen substantial progress in the recent years with the contributions of Grassman et al. [10,11] and Lang et al. [12].

In order to prove the concept and the feasibility of high-quality III–V devices grown on Si substrates, we focus our present work on the development of a dual-junction cell, comprising a Si bottom cell and a III–V top cell. In this case, multiple generic dual-junction

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Table 1
Formulas used for the calculation of the electronic parameters of the materials investigated with the respective sources.

Electronic parameter	Formula	Source
Bandgap [eV]	$E_g(GaAs_xP_{1-x}) = 1.42x + 2.78(1-x) - 0.19x(1-x)$	[18]
Density of states in the conduction band [cm^{-3}]	$N_c(GaAs_xP_{1-x}) = 5.6 \times 10^{19}(0.08 - 0.039x)^{\frac{3}{2}}$	Extrapolated from [19] and [20]
Density of states in the valence band [cm^{-3}]	$N_v(GaAs_xP_{1-x}) = 2.9 \times 10^{19}(0.6 - 0.18x)^{\frac{3}{2}}$	Extrapolated from [19] and [20]
Diffusion coefficient of electrons [$cm^2.s^{-1}$]	$D_n(GaAs_xP_{1-x}) = 39 - 57x + 108x^2$	Extrapolated from [19] and [20] with corrections from [21]
Diffusion coefficient of holes [$cm^2.s^{-1}$]	$D_p(GaAs_xP_{1-x}) = 5 - 10x + 12.5x^2$	Extrapolated from [19] and [20]
Relative permittivity	$\varepsilon_r(GaAs_xP_{1-x}) = 12.9$	Extrapolated from [19] and [20]

models [13–15] have shown that the top cell bandgap should lie between 1.6 and 1.8 eV. As there is no nitrogen-free III–V material lattice-matched to silicon in this bandgap window, a lattice-mismatched architecture is needed. In order to achieve the highest crystal perfection, the lattice mismatch should be as small as possible. Among the III–V materials, $GaAs_xP_{1-x}$ is the nitrogen-free ternary compound material in the targeted bandgap window exhibiting the smallest lattice-mismatch with silicon. Moreover, GaP is nearly lattice-matched with silicon, and therefore offers an ideal pathway for the integration of a 1.6–1.8 eV $GaAs_xP_{1-x}$ top cell on silicon. However few material-specific and architecture-specific detailed models of such structures have been developed so far to determine the exact bandgap needed for the top cell and the parameters influencing the efficiency of the dual-junction cell. Most of the modeling work on dual-junction solar cells, including the aforementioned contributions, suffers from the lack of architecture-specific features and relies on theoretical absorption spectrums, infinite cell thickness hypothesizes or dark-current calculations based on theoretical electronic parameters or empirical relations built on outdated cell performances. Moreover the impact of crystal imperfections on dual-junction III–V/Si solar cells performances has not been considered in the modeling works reported in the literature, although the formation of defects is inevitable for 1.6–1.8 eV III–V materials monolithically grown on silicon substrates.

The main hurdle in accurately simulating bandgap-dependent, material-specific and architecture-specific dual-junction solar cells lies in the lack of data regarding the chosen material ($GaAs_xP_{1-x}$ in the present work). In order to approximate the expectable behavior of the real material without using an extensive number of electronic parameters, we simulate the device performances as a result of the flow equilibrium in the cells, adapting the detailed balance model developed by Shockley and Queisser [16]. We consider the radiative limit as the upper thermodynamic boundary on the cells performances and use simple models to calculate non-radiative recombination rates, such as Auger and Shockley–Read–Hall. The need for specific electronic parameters is thus limited to its minimum as the main input in the model is the absorption spectrum of the top cell material.

As an important improvement over already existing models, the impact of threading dislocations (TDs), the main source of inefficiencies for lattice-mismatched III–V solar cells, has been integrated in the model. Additionally, the luminescent coupling between the cells due to photons from radiative recombinations in the top cell cascading to the bottom cell has also been taken into account. The impact of two geometrical architectures for the front surface (flat and ideally textured) has also been investigated. Finally, other sources of non-idealities such as non-perfect EQE and surface recombinations are added in Section 3.4 in order to give an evaluation of the long-term potential performances of the technology. This comprehensive model allows for quantitative insights in the design of $GaAs_xP_{1-x}$/Si dual-junction solar cells such as the ones currently developed [10–12], highlighting the processes limiting the efficiency of the investigated architecture. Moreover, targets are set regarding the maximum threading dislocation density (TDD) needed in order to achieve very high efficiency devices ($> 35\%$).

2. Method

The model presented hereafter has been developed using MATLAB® R2014a. All the calculations are wavelength-dependent with rectangular integration on the wavelength between 280 and 1450 nm with a 0.5 nm step. The efficiencies were calculated for air mass 1.5 global (AM1.5G) without concentration using data from the ASTM G173-03 reference spectrum [17]. The percentage of arsenic x in the top $GaAs_xP_{1-x}$ cell can vary from $x=0.55$ to 1, representing the direct bandgap domain of $GaAs_xP_{1-x}$ [18]. The main challenge in accurately simulating a bandgap-dependent $GaAs_xP_{1-x}$/Si dual-junction solar cell lies in the lack of data regarding the electronic parameters of $GaAs_xP_{1-x}$ for varying percentages of arsenic x. Using the blackbody theory applied to semiconductors and the flow equilibrium in the cells, our model reduces the amount of electronic parameters needed to a very limited number, namely the bandgap $E_g(GaAs_xP_{1-x})$, the densities of states in the conduction and valence bands $N_c(GaAs_xP_{1-x})$ and $N_v(GaAs_xP_{1-x})$, the diffusion coefficient of electrons and holes $D_n(GaAs_xP_{1-x})$ and $D_p(GaAs_xP_{1-x})$ and the relative permittivity $\varepsilon_r(GaAs_xP_{1-x})$. The formulas used for the calculation of these electronic parameters and their sources are summarized in Table 1. The five last electronic parameters are moreover solely used for the modeling of the impact of TDs. Hence the bandgap is the single parameter needed for the determination of the perfect crystal theoretical maximal efficiency.

This is possible through the use of a thermodynamic approach exclusively based on the absorption spectrum of the material for the calculation of the radiative recombination rate. In order to determine the absorption spectrum of $GaAs_xP_{1-x}$ for different percentage of arsenic x, we make the hypothesis that the main consequence of the incorporation of arsenic is a blue-shift from the absorption spectrum of GaAs equal to the difference in bandgap between $GaAs_xP_{1-x}$ and GaAs. Given the very similar shape of absorption spectrums of III–V materials, this is a rational hypothesis. The GaAs absorption reference spectrum has been extrapolated based on data from Ref. [22] between 280 and 826.5 nm and from the fitted model from Ref. [23] based on experimental data from Ref. [24] above 826 nm. For the bottom Si solar cell, the absorption spectrum has been extrapolated from Ref. [25].

2.1. Cell architecture

The cell architecture investigated here is detailed in Fig. 1. We have concentrated our efforts on a 2-terminal contact architecture, which is the most established solar cell device architecture in practice. In this structure, the two cells are series-connected through a high bandgap buffer such as a $GaAs_xP_{1-x}$ metamorphic buffer on a GaP nucleation layer, as presented in Refs.