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Technological guidelines for the design of tandem III-V nanowire on Si solar cells from opto-electrical simulations

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ABSTRACT

Effect of geometrical and structural parameters on the efficiency of the tandem solar cell based on the III-V nanowire array on silicon is studied by the means of coupled opto-electrical simulations. A close to realistic structure, consisting of AlGaAs core-shell nanowire array, connected through a tunnel diode to a Si subcell is modelled, revealing the impact of top contact layer, growth mask and tunnel junction. Optical simulation of the tandem structure under current matching condition determine optimal geometrical parameters of the nanowire array. They are then used in the extensive electrical optimization of the radial junction in the nanowire subcell. Device simulations show the necessity of high doping of the junction in order to avoid full shell depletion. The influence of bulk and surface recombination on the performance of the top subcell is studied, exposing the importance of the good surface passivation near the depleted region of the radial $p-n$ junction. Finally, simulations of the fully optimized tandem structure show that a promising efficiency of $\eta = 27.6\%$ with the short-circuit current of $J_{SC} = 17.1$ mA/cm^2 can be achieved with reasonable bulk and surface carrier lifetime.

1. Introduction

Semiconductor nanowires (NW) have recently emerged as promising candidates for a new generation of photovoltaic devices [1], since their excellent antireflection and light-trapping characteristics are superior to those of planar cells [2,3]. In addition, multijunction solar cells present a way to overcome the fundamental Shockley-Queisser efficiency limit, with the current efficiency-record-holding cell being a four junction cell under concentrated sunlight [4]. The outstanding performance of such cells is obtained thanks to selective absorption of different parts of the solar spectrum and minimization of energy losses from thermalization of photogenerated carriers. Combining the benefits of the two structures, III-V nanowires (NW) on silicon tandem cell could be hence considered as potentially one of the most efficient structures within dual-junction solar cells.

The choice of silicon as one of the active layers for a tandem cell is dictated by the element abundance and technological maturity. III-V materials in return have outstanding light absorption properties [5]. Moreover, the use of ternary alloys of III-V materials gives the possibility to continuously fine-tune the band gap of the top cell material to obtain the best possible performance with the given substrate. Particularly, $E_g = 1.7$ eV is known to provide the highest ultimate efficiency with silicon in a tandem cell [6].

In addition to their excellent light absorption properties, nanowires have small substrate-contact area. This leads to a better strain relaxation from the strong lattice mismatches and the formation of antiphase boundaries on the III-V/Si interface [7]. Finally, the use of nanowires introduces another promising concept for the solar cell application, i.e. the radial $p-n$ junction. Indeed, core-shell structure benefits from decoupled effective optical and electrical lengths, allowing to maximize the former and minimize the latter at the same time [8]. Therefore, III-V nanowires allow to significantly reduce material needs without compromising absorption or performance [9].

The complexity of the proposed tandem system, however, implies that an extensive number of parameters influences the performance of the solar cell. Some of them, such as carrier lifetime, cannot be precisely controlled in real devices. Other parameters have a non-monotonic impact on the efficiency, so that the system has to be carefully tailored in order to achieve the highest efficiency. LaPierre in his pioneering theoretical works [10,11] presented a first set of design rules for the perfectly absorbing III-V nanowire on silicon tandem cell. Then, a number of studies with more sophisticated coupled opto-electronic simulations of the system followed [12–14], exploring various aspects of cell design.

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In this work, state-of-the-art numerical techniques are employed to improve the understanding of cell performance dependencies on various internal and external parameters. The main goal of this study hence consists in providing useful and practical guidelines for the complex technological optimization of the III-V nanowire on silicon tandem structure. In this work, $Al_{0.2}Ga_{0.8}As$ ($E_g = 1.7$ eV) is chosen as a top cell material, but the main results are expected to be similar for other alloys with the same band gap, such as $GaAs_{0.8}P_{0.2}$ or $Ga_{0.35}In_{0.65}P$.

From the modelling perspective, the most rigorous approach would imply the coupling of optical and electrical simulation, so that the full characteristic of every possible geometry is simulated, considering each time varying parasitic effects. This approach is however unrealistic from a computational perspective, so an alternative two-step procedure is employed in this work. First, optical simulations are performed by the home-built rigorous coupled wave analysis (RCWA) solver, which is the main methodological feature of this work. The efficiency of our optical tool allows the sampling of the multidimensional parameter space for the self-consistent simulation of a whole complex 3D structure close to the realistic one. Furthermore, in contrast with the Beer-Lambert approximation used in all preceding works for the absorption in the bottom cell, our simulations, are based on the calculation of the spatially-resolved photogeneration rate in silicon. The coupling with electrical simulations of the tandem cell is carried out afterwards using the TCAD commercial simulator Sentaurus, which accounts for a wide variety of electronics effects. Thus, the study of the auxiliary layers effects (top contact, passivation, growth mask) on the current photogenerated in the dual-junction system is reported.

In the first part of the work, optical simulations are carried out to optimize light absorption over the geometrical parameters of the tandem cell under the current-matching condition. In the second part of the paper, charge transport mechanisms are studied and carrier collection efficiency is optimized by the means of electrical device modelling coupled with the optical simulations. Core-shell design of the nanowire subcell requires careful and precise selection of the $p-n$ junction parameters due to the possibility of complete depletion of either core or shell [15,16]. Therefore, a broad numerical study is performed and design rules for radial junctions in the nanowires are proposed. After that, the influence of bulk and surface Shockley-Read-Hall recombination on the junction performance is investigated. Finally, electrical simulations of the fully optimized solar cell consisting of two junctions connected by a tunnel diode are performed. The influence of the NW-Si contact scheme on the overall cell performance is finally discussed.

2. Optical simulations

2.1. Model

The first parameters to be targeted from the technological point of view are the periodicity of the nanowires p, their diameter D and height H. Due to the sub-wavelength structure of the ordered NW array, it is possible to select these geometrical parameters in order to benefit from resonant light trapping. So the first step of the work consists in the light absorption optimization in the tandem cell. Numerical solution of Maxwell's equations in the system is carried out by the home-built RCWA solver [17,18]. This state-of-the-art optical simulation tool enables the study of light, absorbed by complex 3D multilayer structures of arbitrary length, in a reasonable computational time. Our study follows the simulation strategy and choice of parameters, described in detail by Michallon et al. [19].

The investigated system, which replicates a realistic tandem cell, is presented in Fig. 1 (b), with structural parameters summarized in Table 1. The top subcell of the studied tandem features a periodic array of $Al_{0.2}Ga_{0.8}As$ cylindrical nanowires. Their top and side surface is covered with a $t_{pass} = 5$ nm layer of $Al_{0.5}Ga_{0.5}As$. As was shown by Songmuang et al., a few nanometres of $Al_{0.33}Ga_{0.67}As$ can efficiently

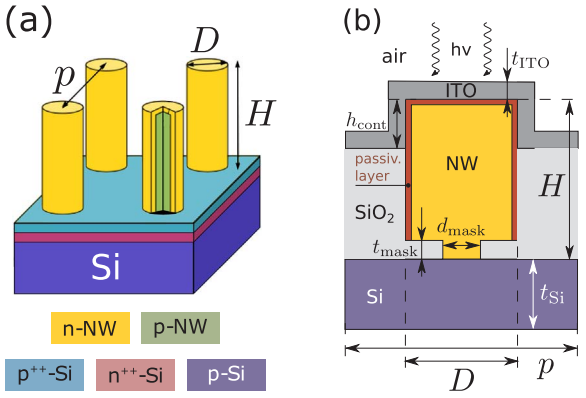

Fig. 1. (a) Schematic of AlGaAs core-shell nanowire on silicon tandem solar cell. (b) Cross-section view of one period of the structure with geometrical and structural parameters of the studied tandem cell, relevant for optical simulations.

Table 1
Geometrical parameters of the studied tandem cell. For H, p and D both variation range and optimal values are given.

Parameter	Description	Value
		0.9 μm − 2.4 μm
H	Height of the nanowire	1.5 μm
		150 nm − 850 nm
p	Nanowire array pitch size	550 nm
		30 nm − 765 nm
D	Diameter of the nanowire	330 nm
t_{Si}	Si subcell thickness	200 μm
t_{ITO}	Thickness of the ITO layer	100 nm
t_{pass}	Thickness of the passivation layer	5 nm
h_{cont}	Vertical extent of top contact	300 nm
t_{mask}	Thickness of the SiO_2 mask	10 nm
d_{mask}	Hole diameter in the SiO_2 mask	50 nm

suppress surface recombination of GaAs nanowires [20]. An alloy with the same band gap difference is therefore chosen as a passivation layer in our study. Nanowires are then encapsulated in SiO_2 for mechanical and chemical stability of the device. An additional 10 nm layer of silica serves as a growth and isolation mask as well as a passivation layer for the bottom subcell. A $t_{ITO} = 100$ nm layer of indium-tin oxide (ITO) is used as a transparent contact, which covers the top and a fraction of the side of the nanowire, labelled h_{cont}. Such thickness is a good trade-off between the optical and electrical properties. Indeed, thinner ITO contacts have reduced conductivity [21], while thicker ITO layers increase optical losses as nonvanishing absorption coefficient of ITO was taken into account in simulations [22].

The studied bottom subcell consists of the Si substrate with a typical thickness of 200 μm. In the optical simulations it is modelled by a semi-infinite silicon slab with absorption calculated in the first 200 μm. Simulations of such system can be conveniently done with RCWA, reflections from the absent back silicon/air interface are not present and cannot yield unphysical interference effects induced by the simulated coherent light. This approach correctly takes into account the diffracted light induced by the nanowire array in contrast with the Beer-Lambert approximation, commonly used for the substrate. However, similarly to the Beer-Lambert approach, our method may somewhat underestimate light absorption in Si due to the absence of back reflection. This point is further discussed among the loss analysis at the end of Section 2.2. The whole structure is illuminated from the air on top by monochromatic planewaves. Optical indices of all the above mentioned materials are taken from the Refractive index database [23].

Geometrical parameters of the array: NW length H, pitch size p, and filling ratio D/p are varied in order to increase photo-generated current in the structure. For each set of parameters, spectral absorption