



Original research article

# Modeling and optimization of core/shell p-i-n Si/Si<sub>0.2</sub>Ge<sub>0.8</sub> nanowire for photovoltaic

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## ABSTRACT

In this work we propose a modeling and simulation of core/shell p-i-n Si/Si<sub>0.2</sub>Ge<sub>0.8</sub> nanowire for photovoltaic. In the first step of this work, we have compared the core/shell p-i-n homo-junction Si and heterojunction Si/Si<sub>0.2</sub>Ge<sub>0.8</sub> Nanowire (NW) solar cell having a length of 3 μm and a radius of 0.19 μm, by studying their current-voltage and external quantum efficiency (EQE). Our results have shown that blending Silicon with 80% of Germanium enhances relatively the short circuit current and efficiency by 3.04% and 8.48% respectively. In other hand, the absorption edge of Silicon NW has extended from 1100 nm to 1200 nm, with a gain of EQE of 15% obtained in this range. In the second part, we have tried to optimize the Si/Si<sub>0.2</sub>Ge<sub>0.8</sub> structure, by varying their radius and length. The corresponding results have indicated that a radius of 0.28 μm and a length of 10 μm are the optimal geometric parameters for any optimization of such structure.

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## 1. Introduction

Solar energy is abundant, clean, and renewable. Solar cells are the devices that convert this energy into electricity. The most inconvenient of photovoltaic energy is their low yield and high cost using conventional solar cell. Nowadays, nanostructure materials are the subject of many researches in goal to overcome the limits of conventional solar cell and to exceed Shockley-Quisser conversion efficiency [1]. Quantum Dot Solar Cell (QDSC) [2–4], Dye-Sensitized solar cell [5] and organic bulk heterojunction devices [6] are one of the examples of such configurations. Despite these promising efforts, no technology has been able to achieve good efficiency and low cost of conventional Silicon p-n junction. This later is formed by planar p-type/n-type homo or heterojunction. Recently, nanowire have been appeared as alternative devices to improve optical absorption and collection efficiency in a planar solar cell [7,8]. Their large surface/volume ratio is useful to enhance the performances of electronic devices. Moreover, they decreasing the density of states in surface which leads to decrease the recombination of photogenerated carriers and reduce distance to collecting junction. Usually, two techniques are used for fabrication of NW: top-down and bottom-up techniques. Top-down technique uses lithography to define the fabricated structure and then transfer it to the substrate by etching or similar way. In bottom-up approach, the material is added to substrate in self-organized way. Bottom-up uses vapor liquid solid (VLS) method to synthesis the nanowire, in this method

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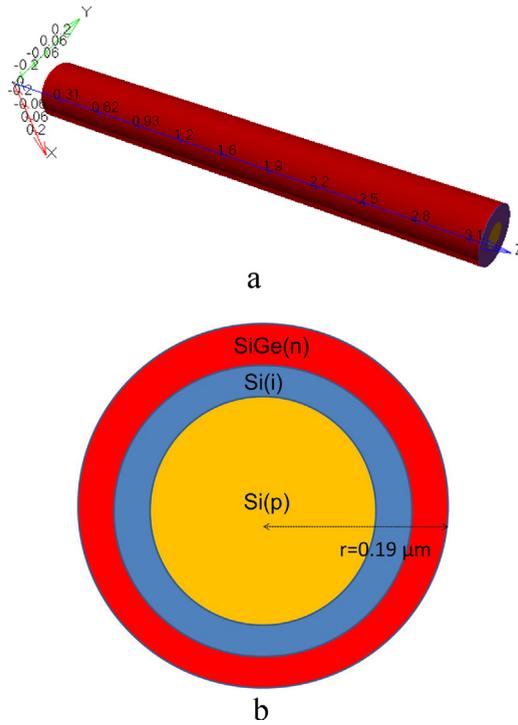


Fig. 1. (a) 3D structure of core/shell p-i-n Si/SiGe. (b) Top view of the structure.

a metallic nanoparticles are employed to growth the nanowire [9]. In addition, the capability to alter the directions of light propagation to the direction of charge separation is one of the most motivations for developing nanowire PV devices. Silicon nanowire is embedded into core/shell solar cell as shown in Fig. 1, creating also a p-i-n radial junction with diameter varying from nanometer to some micrometers. Cutline section of a core/shell nanowire gives a circular core/shell structure which also called Quantum Dot Quantum Well (QDQW) if the diameter is less than 10 nm. Experiments reveal that a single Silicon nanowire exhibits an open circuit voltage of 0.485 V, short circuit of 6.5 mA/cm<sup>2</sup>, fill factor of 70% and an efficiency of 2.2% under 1 sun AM1.5G [10,11]. Because Si is an indirect bandgap semiconductor, a few microns are required to absorb the majority of the photons comprised in the solar spectrum. As a solution to this limitation, Si nanowire (NW) can be allied with others semiconductors to make alloy materials. Among the semiconductors that Silicon can be blended with it is Germanium to create Si<sub>x</sub>Ge<sub>1-x</sub> shell II-V alloy. Thanks to the physicals properties and bandgap of Si<sub>x</sub>Ge<sub>1-x</sub> which is tunable between 1.12 eV and 0.66 eV, this material earns an importance in the field of optoelectronics. In this latter, we are interested on modeling and optimization of core/shell p-i-n Si/Si<sub>0.2</sub>Ge<sub>0.8</sub> NW with radial junction. Many effects are investigated and discussed like influence of radius and length of NW on the main characteristics parameters of a solar cell: current-voltage and external quantum efficiency (EQE). The variation of spatial total density of current in the radial junction is also presented. Fig. 1(a) shows the 3D structure of core/shell p-i-n Si/Si<sub>0.2</sub>Ge<sub>0.8</sub> NW with a total length of about 3 μm and a radius of 0.19 μm. Fig. 1(b) shows the top view of the structure where the red layer represents n-type SiGe shell layer, the bleu one is the intrinsic layer and the brown is the p-type Si core.

## 2. Theoretical model

The following sections describe the physical models that have been used for this simulation. A Low Field Mobility model is used for calculations of the mobility of carriers dependent temperature, and it is given by the following:

$$\mu_{n0}(T_L) = MUN \left( \frac{T_L}{300} \right)^{TMUN} \tag{1}$$

$$\mu_{p0}(T_L) = MUP \left( \frac{T_L}{300} \right)^{TMUN} \tag{2}$$

Concentration dependent model is used for calculations of the mobility of carriers dependent concentration, and it is given by the Masetti model [12].

$$\mu_n = \mu_{nmin} \exp \left( \frac{-P_{c,n}}{N_D} \right) + \frac{(\mu_{nmax} - \mu_{nmin})}{1 + \left\{ \frac{N_D}{C_{r,n}} \right\}^{\alpha,n}} - \frac{\mu_{1,n}}{1 + \left( \frac{C_{s,n}}{N_D} \right)^{\beta,n}} \tag{3}$$

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