Solar Energy Materials & Solar Cells 137 (2015) 146–153

Contents lists available at ScienceDirect

Solar Energy Materials & Solar Cells

journal homepage: www.elsevier.com/locate/solmat

Optical and electrical modeling of solar cells based on graphene/Si nanowires with radial *p–i–n* junctions

Zahra Arefinia [a], Asghar Asgari [a,b,*]

[a] Research Institute for Applied Physics and Astronomy, University of Tabriz, Tabriz, Iran
[b] School of Electrical, Electronic and Computer Engineering; University of Western Australia, Crawley, WA 6009, Australia

ARTICLE INFO

Article history:
Received 2 November 2014
Accepted 23 January 2015
Available online 24 February 2015

Keywords:
Graphene
Nanowire
p–i–n radial junction
Solar cell

ABSTRACT

A solar cell based on vertically aligned silicon *p–i–n*, core–shell–shell, nanowires interfacing with graphene film is proposed to exploit the benefits of short carrier collection lengths of radial *p–i–n* junction nanowires and transparency of graphene. A physical device model incorporated with optical characteristics taking into account all recombination processes is established to optimize its electrical performance by modifying nanowires density, filling ratio and thickness. Also, the dependence of the proposed structure to temperature variations and the number of graphene layers on its performance is investigated.

1. Introduction

Graphene has extreme electrical conductivity [1,2], high optical transmittance within the visible-infrared region [3], outstanding flexibility and stability [4,5], while being inexpensive and nontoxic. This makes it a perfect candidate material for creating photovoltaic solar devices. In particular, graphene-based solar cells are the most reputable because of their remarkable performances as transparent electrodes [6–8], counter-electrodes [9], electron acceptors [10,11], hole collectors,[12] and photoactive promoters [13,14] make them promising solutions for fast-response and energy efficient applications.

Recently, there is a growing interest in developing graphene–silicon heterojunction solar cells, and the power conversion efficiencies have reached 1.6 – 8.6% [15–18]. On the other hand, silicon nanowire arrays (SiNWs), which can enhance the light path length by up to a factor of 73 in comparison with that of bulk silicon, can act as a light trapping layer [19]. Thus, using this structure, it may allow cell fabrication with less Si materials and save the cost by permitting high power conversion efficiencies with relatively low-quality Si. Also, graphene film/SiNWs solar cells have been recently reported and it is found that the SiNWs substrate shows better anti-reflective effect [20–22].

On the other side, core/shell/shell NWs structures with p-type/intrinsic/n-type (*p–i–n*) junctions in the radial direction would enable a decoupling of the requirements for light absorption and carrier extraction into orthogonal spatial directions [23–25]. In the radial NWs structures, photo-excited carriers travel very short distances before being collected by the electrodes, resulting in higher charge collection efficiencies, and this advantage leads to a higher tolerance for material defects. Therefore, In order to achieve benefits of both *p–i–n* junctions NWs and graphene based solar cells, in this paper we propose an alternative implementation of vertically oriented *p–i–n* junctions Si nanowires in the graphene/SiNWs solar cells.

The aim of this paper is therefore to present a model for performance considerations of vertically aligned *p–i–n* Si core/shell/shell NWs in contact with graphene, G/(*p–i–n*)SiNWs. Since monolayer graphene or few-layer graphene (FLG) located at the top plays an important role in optical transmittance, through optical conductivity calculation, the optical transmittance spectra is obtained for the AB-stacked FLG as a function of the layer number. Then, the absorption spectrum obtained from Fermi golden rule using the eigenfunctions and eigenvalues of cylindrical nanowire defines the charge carrier generation profile. This profile is used as the input for the drift-diffusion equations of minority carriers to calculate solar cell efficiency, including Shockley–Read–Hall (SRH), Auger, radiative, and surface recombination mechanisms and degenerately doped Si. Then, the impact of surface recombination velocity and temperature is presented. Also, the G/(*p–i–n*)SiNWs performance as functions of the SiNWs radius, thickness and doping concentration is investigated (Table 1).

2. G/(*p–i–n*)SiNWs structure

The schematic view of G/(*p–i–n*)SiNWs is shown in Fig. 1(a). A monolayer graphene or FLG has been deposited on vertically aligned (*p–i–n*)SiNWs with the height of *L* and cylindrical

* Corresponding author at: Research Institute for Applied Physics and Astronomy, University of Tabriz, Tabriz, Iran. Tel.: +98 41 33393005; fax: +98 41 33347050.
E-mail address: asgari@tabrizu.ac.ir (A. Asgari).

http://dx.doi.org/10.1016/j.solmat.2015.01.032
0927-0248/

Table 1
Si characterization parameters.

Parameters of Si	Value	Reference
Band gap, E_g	$(E_g)_{Si}=1.17-\frac{4.73\times10^{-4}T^2}{T+636}$(eV)	[51]
Dielectric constant, ε_{Si}	11.9 ε_0	[28]
Electron effective mass, m_e^*	0.2 m_e	[52]
Hole effective mass, m_h^*	0.49 m_e	[52]
Refractive index	$3.38\times(1+3.9\times10^{-5}\,T)$	[28]

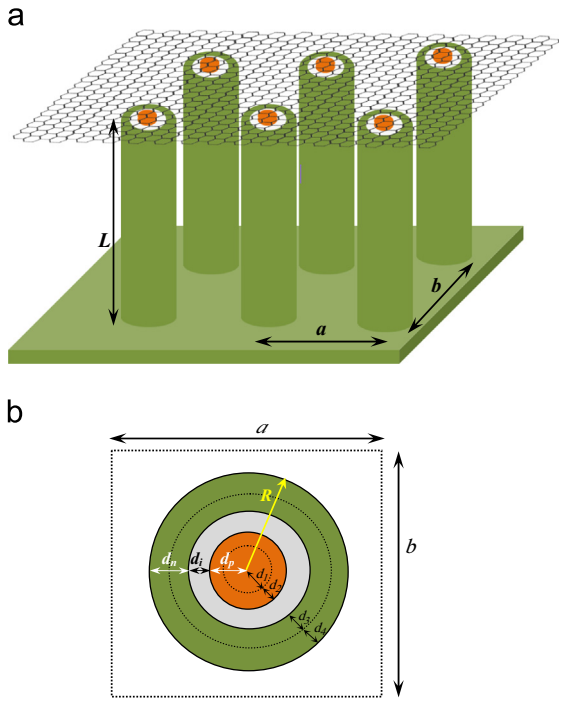

Fig. 1. Schematic of (a) the proposed G/(p–i–n)SiNWs with the height of L and periodicity of a and b. Light is incident on graphene. The external shell of wires with green color is n-type, the middle shell with light gray color is intrinsic and the internal core with orange color is p-type. (b) Cross sectional view of a single nanowire with the total radius of $R=d_p+d_i+d_n$.

geometry. We consider the FLG composed of N layers arranged in the AB (Bernal) stacking. Also, the light is assumed to be normally incident on the top of graphene layer. For more clarity, schematic cross-sectional view of single wire in a unit cell with area of $a\times b$ is shown in Fig. 1(b). Each (p–i–n)SiNW has a diameter of R composed of a p-type core with d_p radius and intrinsic and n-type shells with the thicknesses of d_i and d_n, respectively.

In the vicinity of the junctions of p-type core, and n-type shell with the intrinsic shell, the concentration of mobile charge sharply decreases and the space charge is mainly formed by ionized donors and acceptors. The widths of depletion regions are limited by the p-type core radius and the n-type shell thickness. Therefore, as shown schematically in Fig. 1(b), each SiNW is divided into five regions: the neutral and depletion regions of p-type Si with the width of d_1 and d_2, respectively, the intrinsic Si with the width of d_i, and the depletion and neutral regions of n-type Si with the width of d_3 and d_4, respectively.

We assume that the SiNWs are uniformly distributed in order to have a simple view of the wire density. For cylindrical nanowires, the nanowires density, N_{wr} (the number of nanowires per cross-sectional area, perpendicular to the wire direction) and the filling ratio, F_{wr}, are:

$$N_{wr}=\frac{1}{a\times b} \tag{1}$$

$$F_{wr}=\frac{\pi R^2}{a\times b} \tag{2}$$

Within the frame work of the infinitely deep quantum well approximation, the wave function of electrons in the conduction subbands of a cylindrical wire with radius R in a dielectric medium have the form [26]:

$$\psi_c^{snk}(r,\varphi,z)=\frac{1}{\sqrt{\pi R^2 L}J_{n+1}(\lambda_s^n)}J_n\left(\lambda_s^n\frac{r}{R}\right)\exp(in\varphi)\exp(ikz) \tag{3}$$

where $J_n(x)$ is the Bessel function of the first kind and λ_s^n are its zeros, and $s=1;\ 2;\ldots;\ n=0;\ \pm1;\ \pm2$: are quantum numbers, k is the wave number of the free motion of electron along the wire axis. The corresponding conduction subbands energies are:

$$E_c^{snk}=E_{c_0}+\frac{\hbar^2}{2m_e^*}\left[\frac{(\lambda_s^n)^2}{R^2}+k^2\right] \tag{4}$$

where E_{c_0} is the conduction band edge and equals to E_g, which is measured from the valence-band edge, E_{v_0}. Similarly, the valence subbands wave functions and corresponding energies are:

$$\psi_v^{s'n'k'}(r,\varphi,z)=\frac{1}{\sqrt{\pi R^2 L}J_{n+1}(\lambda_{s'}^{n'})}J_{n'}\left(\lambda_{s'}^{n'}\frac{r}{R}\right)\exp(in'\varphi)\exp(ik'z) \tag{5}$$

$$E_v^{s'n'k'}=E_{v_0}-\frac{\hbar^2}{2m_h^*}\left[\frac{(\lambda_{s'}^{n'})^2}{R^2}+k'^2\right] \tag{6}$$

where m_e^* and m_h^* are Si electron and hole effective mass, respectively.

The band gap of SiNWs is the difference between the first conduction band energy and the first valence band energy as:

$$(E_g)_{wr}=(E_g)_{Si}+\frac{\hbar^2}{2}\left(\frac{2.4}{R}\right)^2\left(\frac{1}{m_h^*}+\frac{1}{m_e^*}\right) \tag{7}$$

where $(E_g)_{Si}$ is the band gap of bulk silicon which depends on doping and can be described empirically as [27]:

$$(\Delta E_g)_{Si}=0.0187\left[\ln\left(\frac{N_d}{7\times10^{17}}\right)+\ln\left(\frac{N_a}{7\times10^{17}}\right)\right] \tag{8}$$

which is valid for $|N_d-N_a|>7\times10^{17}\ \mathrm{cm}^{-3}$.

Using the electron wave function and energy spectrum of cylindrical NWs, the absorption spectrum of a photon with energy of ω is obtained from Fermi's golden rule as [28]:

$$\alpha(\omega)=\frac{\pi q^2}{n_r c\varepsilon_0 m_0^2\omega}N_{wr}\frac{2}{L}\sum_{s,n}\int_{-\infty}^{+\infty}\frac{dk}{(2\pi/L)}\left(\langle\psi_c^{s'n'k}|\hat{r}.\tilde{p}|\psi_v^{snk}\rangle\right)^2\delta(\beta)\left[f_v(\hbar\omega-\beta)-f_c(\hbar\omega-\beta)\right] \tag{9}$$

where $\beta=E_c^{snk}-E_v^{snk}$, n_r is temperature dependent refractive index of Si, $\tilde{p}$ is the momentum operator, $f_{c(v)}$ is the conduction (valence) Fermi distribution function and δ is the Kronecker delta.

Among the other parameters of SiNWs, the electron and hole mobilities play an important role on determining of the performance of G/(p–i–n)SiNWs solar cell. Due to increased surface scattering in NWs with a high surface-to-volume ratio, the mobility is expected to decrease. Kotlyar et al. [29] have shown that, in a cylindrical SiNW, phonon scattering is increased with decreasing diameter due to increased overlap between the electron and phonon wave functions, leading to degradation of the electron mobility. Also, simulations have shown that the surface scattering becomes dominant in NWs smaller than 5 nm × 5 nm, leading to decrease in the electron mobility with decreasing NWs cross-section [30]. But, the measurements of mobility for SiNWs greater than 5 nm × 5 nm have shown that it is close to the mobility in bulk silicon [31–33]. Therefore, we have computed the mobility of SiNWs with an empirical relationship of bulk Si [34].