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An analytical model for optimizing the performance of graphene based silicon Schottky barrier solar cells

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ABSTRACT

In this paper, a model taking into account the effects of carrier loss mechanisms has been developed. The model simulates the photovoltaic properties of the graphene/n-type silicon Schottky barrier solar cells (G/n-Si_SBSC), and it can reproduce the experimentally determined parameters of the G/n-Si_SBSC. To overcome the low efficiencies of G/n-Si_SBSC, their performances have been optimized by modifying the work function of graphene and Si properties, accounted for variation of its thickness and doping level. The obtained results show that the work function of graphene has the major impact on the device performance. Also, the temperature dependence of the G/n-Si_SBSC performance is investigated.

1. Introduction

Graphene has been studied as a promising electrode material in organic and inorganic solar cells [1–3] due to its transparency [4], high conductivity[5], flexibility [6], low cost, and large-scale manufacturing properties [7,8]. Graphene also possesses excellent chemical and physical stability with a tunable work function [9–11]. Furthermore, graphene/silicon (G/Si) structure has been studied and shows diode characteristics as a Schottky junction [12]. In particular, Schottky barrier solar cells (SBSC) obtained by deposition of graphene sheets on n-Si wafer has been reported [3,13]. The major process for the fabrication of G/Si solar cells can be accomplished *via* a solution transfer process at room temperature in air. Therefore, G/Si-SBSC has emerged as a promising candidate for high-performance and cost-effective photovoltaic applications. Furthermore, G/Si solar cells have potentials to deliver higher efficiencies through oxidating the Si surface and modifying graphene with using of chemical dopants such as bis(trifluoromethanesulfonyl)amide [14], $SOCl_2$ [15,16], HNO_3 [15–17] and 1-pyrenecarboxylic acid (PCA) and $AuCl_3$ [18], introducing Au nanoparticles onto the graphene [19], introducing a colloidal antireflection coating onto a G/Si solar cell [20], introducing a graphene oxide interlayer to engineer the G/Si interface [21], performing appropriate surface passivation [22] or introducing a polymer electron blocking layer [23].

It was pointed out that these structures were not optimized, and could potentially be optimized by considering the effect of the temperature, doping concentration, Si thickness, and graphene work function. Until now, there are rare works on modeling of graphene based solar cells. Thus, a deep insight into G/Si solar cells is highly needed. Herein, through the optical conductivity calculation of graphene, the optical transmittance spectrum of graphene is obtained. Then, using transmittance of graphene and the drift and diffusion charge transport equations taking into account Shockley–Read–Hall, Auger, radiative and surface recombinations, an optoelectronic analytical model is presented to optimize the performance of G/Si solar cells.

2. G/n-Si_SBSC structure

One of the earliest efforts towards developing graphene-based solar cells is reported by Li et al. [3], whereby graphene sheet transferred onto n-type Si wafer, produced G/n-Si_SBSC.

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Thus, all the used parameters of the G/n-Si_SBSC employed in this study, shown in Fig. 1, are taken from Ref. [3]. The work function of graphene is 4.8 eV and n-Si wafer has a thickness of $t_{Si}=200$ nm and doping of $N_d=3\times10^{15}$ cm^{-3} unless otherwise stated.

3. An analytical model

The conversion efficiency (η) of a solar cell is calculated as follows:

$$\eta=\frac{J_{sc}V_{oc}FF}{P_{in}} \tag{1}$$

where $P_{in}=100$ mW/cm^2 is the input power from the sunlight for 1-sun under AM1.5G condition, FF is the fill factor and shows the squareness of the J–V curve of solar cell expressed as follows:

$$FF=\frac{J_mV_m}{J_{sc}V_{oc}} \tag{2}$$

where V_m and J_m are the voltage and current density respectively corresponding to the maximum power output, V_{oc} is the open circuit voltage defined as follows:

$$V_{oc}=\frac{nkT}{q}\ln\left(\frac{J_{sc}}{J_0}-1\right) \tag{3}$$

and n is the diode ideality factor, k is Boltzmann's constant, T is the temperature of solar cell, q is the electron charge, J_0 is the saturation reverse current density, and J_{sc} is the short-circuit current density calculated at $V=0$ of J–V curve of G/Si_SBSC defined by

$$\begin{aligned}J&=-J_D+J_L\\ J_D&=J_0\left(e^{qV/nkT}-1\right)\\ J_L&=J_{ph}-J_{SRH}-J_{Aug}-J_{surf}-J_{rad}\end{aligned} \tag{4}$$

where J_D and J_L are the dark and light-generated current densities, respectively. In the following we briefly discuss about every part of J_L:

– J_{ph} is the current density from the sum of photo-excited carriers in the depletion (J_d) and neutral (J_p) regions of Si. J_d is given by [24]

$$J_d=q\Phi(\lambda)[1-R_G(\lambda)]Q_Ee^{-\alpha(\lambda)W} \tag{5}$$

$$\mu_p\left(\frac{\text{cm}^2}{\text{Vs}}\right)=54.3\left(\frac{T}{300}\right)^{-0.57}+\frac{1.36\times10^8T^{-2.23}}{1+0.88(T/300)^{-0.146}\left[N_d/(2.35\times10^{17}(T/300)^{2.4})\right]} \tag{13}$$

where $\Phi(\lambda)$ is the number of incident photons per unit area per time per wavelength in AM1.5G condition, λ is the wavelength of incident photons, Q_E is the quantum efficiency, $\alpha(\lambda)$ is the absorption coefficient of Si, W is the width of depletion region, and $R_G(\lambda)$ is the reflectivity of the graphene defined by [25,26]

$$W=\sqrt{\frac{2\varepsilon_{Si}}{qN_d}\left(\frac{\varphi_B-(E_C-E_{Fn})}{q}-\frac{k_BT}{q}\right)} \tag{6a}$$

$$\varphi_B=\varphi_G-\chi \tag{6b}$$

$$R_G(\omega)=\frac{\left|\sqrt{\varepsilon_1\varepsilon_{Si}}\varepsilon_0+\sqrt{\varepsilon_1}\sigma(\omega)/c-\varepsilon_1\varepsilon_0\right|^2}{\left|\sqrt{\varepsilon_1\varepsilon_{Si}}\varepsilon_0+\sqrt{\varepsilon_1}\sigma(\omega)/c+\varepsilon_1\varepsilon_0\right|^2} \tag{7}$$

where ε_1 and ε_{Si} are the relative permittivities of the air and Si, respectively, and $\sigma(\omega)$ is the optical conductivity of graphene given by [27,28]

$$\sigma(\omega)=\sigma^{\text{intra}}(\omega)+\sigma^{\text{inter}}(\omega) \tag{8}$$

where σ^{intra} corresponds to the intraband electron–photon scattering processes given by the following:

$$\sigma^{\text{int ra}}(\omega)=\frac{2iq^2T}{\pi\hbar(\omega+(i/\tau))}\ln[2\ \cos\ h(\mu/2T)] \tag{9}$$

where τ corresponds to the electron-disorder scattering processes, and μ is the chemical potential.
The second term in Eq. (7) is related to the direct interband electron transitions calculated by

$$\sigma^{\text{int er}}(\omega)=\frac{q^2}{4\hbar}\left[G(\omega/2)-\frac{4\omega}{i\pi}\int_0^{+\infty}dE\frac{G(E)-G(\omega/2)}{\omega^2-4E^2}\right] \tag{10}$$

where the function of G is the difference of the Fermi functions, $G(E)=f_0(-E)-f_0(E)$, and for numerical calculations it is given by

$$G(E)=\frac{\sin\ h(E/T)}{\cos\ h(\mu/T)+\ \cos\ h(E/T)} \tag{11}$$

The current density from photo-excited carriers in the neutral region, J_p, is obtained from the minority-hole density, p, in the neutral region of n-Si. It can be calculated from the one-dimensional steady-state continuity equation as follows:

$$D_p\frac{d^2p}{dx^2}-\mu_p\frac{dp}{dx}-\left(\frac{p-p_0}{\tau_p}\right)=-\Phi(\lambda)(1-R_G(\lambda))\alpha(\lambda)e^{-\alpha(\lambda)x} \tag{12}$$

where x is the distance from the interface between graphene and Si, D_p is the diffusion constant which depends on carrier mobility through the Einstein relation, μ_p is the hole mobility which is dependent upon the doping level and temperature as given by the empirical relationship [29]

The boundary conditions for solving Eq. (11) are

$$\begin{cases}p=p_0, & \text{at } x=W\\ D_p\frac{d(p-p_0)}{dx}=S_p(p-p_0), & \text{at } x=t_{Si}\end{cases} \tag{14}$$

Finally, the minority current density is obtained as follows:

$$J_p=q\mu_pp-qD_p\nabla p \tag{15}$$