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Modeling of dual-metal Schottky contacts based silicon micro and nano wire solar cells

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ABSTRACT

We study solar cell properties of single silicon wires connected at their ends to two dissimilar metals of different work functions. Effects of wire dimensions, the work functions of the metals, and minority carrier lifetimes on short circuit current as well as open circuit voltage are studied. The most efficient photovoltaic behavior is found to occur when one metal makes a Schottky contact with the wire, and the other makes an Ohmic contact. As wire length increases, both short circuit current and open circuit voltage increase before saturation occurs. Depending on the work function difference between the metals and the wire dimensions, the saturation length increases by approximately an order of magnitude with a two order magnitude increase in minority carrier length. However current per surface area exposed to light is found to decrease rapidly with increase in length. The use of a multi-contact interdigitated design for long wires is investigated to increase the photovoltaic response of the devices.

1. Introduction

One dimensional nanomaterials like nanowires and nanotubes hold great potential for many applications such as electronics [1,2], sensors [3,4], and photovoltaics [5–7]. Nano engineered materials like nanowires and nanotubes are considered to be potential candidates for low cost and high efficiency solar cells. There have been many studies on solar cells based on single as well as multiple nanowires [8–11]. Tsakalakos et al. [8] studied p–n junction based silicon nanowire solar cells on metal foils, and found large current density and low optical reflectance. Sivakov et al. [9] fabricated silicon nanowire solar cells by electroless wet chemical etching of micro crystalline silicon layer on glass and achieved a high power conversion efficiency of 4.4%. Tian et al. [10] studied single p-i-n coaxial silicon nanowires and measured open circuit voltage (V_{OC}) of 0.26 V and short circuit current (I_{SC}) of 0.503 nA. Experimental study on Schottky solar cells comprising multiple SiNWs bridging two different metals with different work functions was carried out by Kim et al. [11]. They obtained a low V_{OC} of 0.167 V but high I_{SC} of 91.1 nA. Kelzenberg et al. [12] studied single-nanowire solar cells with one rectifying junction created by electrical heating of the segment of the nanowire beneath it. For a nanowire of diameter 900 nm, they achieved a V_{OC} of 0.19 V and a short circuit current density of 5.0 mA cm^{-2}. Hybrid Schottky diode solar cells [13] with poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS) film deposited on metal-assisted chemically etched SiNW arrays produced V_{OC} of ~0.48 V and J_{SC} of ~30 mA cm^{-2}. These works on nanowire based solar cells primarily focus on experimental investigations to demonstrate their potential in realizing the next generation of solar cells. However, a detailed study on the influence of various parameters like nanowire dimensions and work function of the metal contacts in modifying the photovoltaic behavior of the nanowires is lacking. In this work, we present results from simulation studies on Schottky junction based microwire and nanowire solar cells, and investigate the dependence of their photovoltaic properties on metal work functions, wire dimensions as well as minority carrier lifetimes.

2. Device structure, problem statement

Fig. 1 is a sketch of the device structure under study. There are two dissimilar metal pads, with dissimilar work functions, bridged by a rectangular cross-section wire. *L*, *W* and *H* represent the wire length, width and height, respectively. The array of downward pointing arrows represents vertically downward incident light beam. Only the top surface (of area $L \times W$) of the wire is

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illuminated. The effect of substrate is not considered in this work. Performance enhancing features such as an antireflection coating or back reflector have not been included so as to keep the focus on the role of the silicon wire and metal contacts.

The work focuses on understanding how device dimensions and minority carrier lifetimes affect the photovoltaic properties (short circuit current, open circuit voltage, *I*–*V* characteristics) of the solar cell. The work also investigates the effects of the metal work functions on the solar cell performance. It explores ways to improving the efficiency of the solar cells, including the selection of metals. Simulation is done with Silvaco Atlas software [14]; details are given in Appendix A.

3. Simulation versus analytical solutions

We start with a simulation that can be verified against a one dimensional (1D) analytical solution. For this we assume that the contacts are Ohmic. For the simulation part, a microwire with $L=6.8\ \mu m$, $W=1.0\ \mu m$, $H=0.85\ \mu m$ was 2D simulated using the approach described in the previous section. For the analytical solution, we consider the one dimensional (1D) minority carrier diffusion equation along wire length in the presence of an electric field [15]

$$D_n\frac{\partial^2\Delta n}{\partial x^2}+\mu_n\frac{\partial}{\partial x}(E[n_0+\Delta n])-\frac{\Delta n}{\tau_n}+G_L=0 \qquad (1)$$

where D_n is carrier diffusion coefficient, μ_n is carrier mobility, E is the electric field, n_0 is equilibrium carrier density, Δn is photo-generated (excess) electron density, τ_n is electron lifetime, and G_L is photo-generation rate. Note E constant along length for Ohmic contacts.

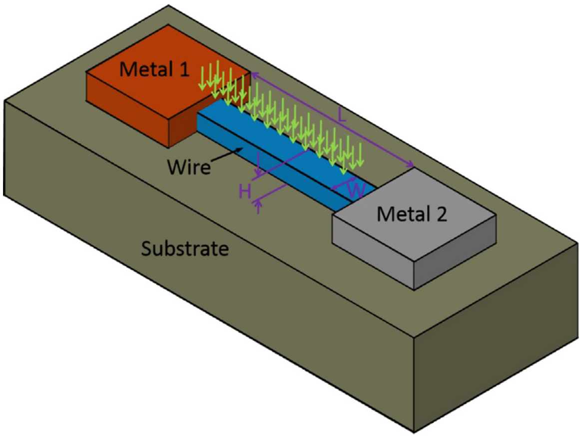

Fig. 1. Schematic representation of a single nanowire between two metal pads. Wire dimensions are indicated, and the downward pointing array of green arrows represents the incident light. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Then excess minority carrier concentration, Δn, is found by solving Eq. (1), which is a linear second order differential equation having a solution of the form

$$\Delta n=Ae^{m_1x}+Be^{m_2x}+C \qquad (2)$$

where

$$m_{1,2}=-\frac{\mu_nE}{2D_n}\pm\sqrt{\left(\frac{\mu_nE}{2D_n}\right)^2+\frac{1}{D_n\tau_n}}.$$

The constants A–C are found from the boundary conditions, $\Delta n(x=0)=0$ at the left contact and $\Delta n(x=L)=0$ at the right contact, and are given by

$$A=C\left(\frac{1-e^{m_2L_x}}{e^{m_2L_x}-e^{m_1L_x}}\right),\quad C=G_L\tau_n\quad\text{and}\quad B=-A-C. \qquad (3)$$

here G_L along the 1D line for analytical calculation is extracted from two dimensional (2D) G_L generated by Atlas simulator. Eq. (2) along with Eq. (3) represents the analytical expression of the excess minority carrier density. Analytical expression for current can be calculated by first finding the current densities as given below

$$J_n=q\mu_nnE+qD_n\nabla n$$
$$J_p=q\mu_ppE-qD_p\nabla n\quad[\text{as }\nabla p=\nabla n] \qquad (4)$$

where E is the electric field, $D_{n(p)}=kT\mu_{n(p)}/q$ is electron (hole) diffusion constant. Then total current, I, is found by multiplying the total current density by the cross sectional area, A, of the wire, or $I=A(J_n+J_p)$.

Fig. 2 presents the comparison between the results from simulation (line with symbols) and analytical calculation (solid line) for our microwire with a uniform p-type doping density of 10^{15} cm^{-3}. Fig. 2(a) compares excess electron (minority carrier) density for different applied biases between the contacts. The photo generated minority electron density is symmetric with

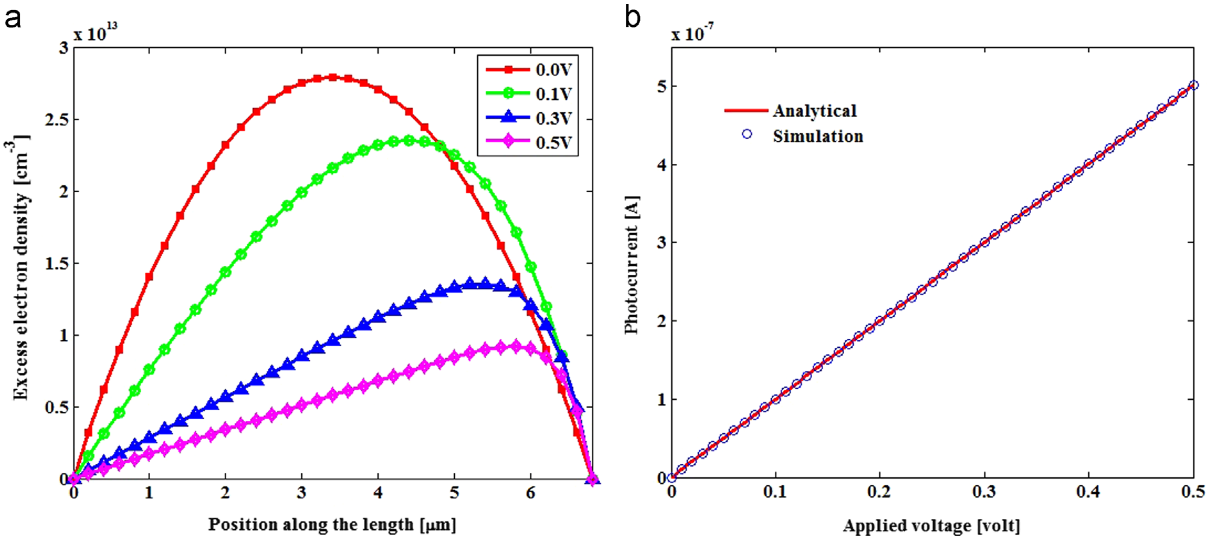

Fig. 2. Comparison of (a) excess electron density and (b) photocurrent from analytical calculation (solid line) and simulation (symbol).