The effect of wire diameter on the performance of solar cells based on graphene and silicon quantum wires

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***Abstract*- The effect of silicon quantum wires (SiQWs) diameter of heterojunction solar cells based on SiQWs with rectangular cross sections and graphene (SiQWs/G) is investigated using a coupled optical and electrical model. It is found that SiQWs/G with small cross section area (d^2=4 nm^2) shows high efficiency. because, the band gap of SiQWs obtained from the distance of energy state of wave function of the lowest conduction bands and the highest valence bands increases as the wire diameter decreases. Also, the quantum confinement of SiQWs with small diameter results in a direct band gap of indirect bulk silicon band gap. on the other hand, SiQWs/G with large d^2 also shows high efficiency due to the better light absorption of larger surface area of SiQWs with larger *d*.**

I. Introduction

Tremendous work has been devoted to graphene-based solar cells because of their remarkable performances as transparent electrodes and active layers which make them promising solutions for fast-response and energy efficient applications. Graphene-based heterojunction solar cells were first studied by Li et al. [1] where graphene served as a transparent electrode and the active layer for electron–hole separation.

On the other hand, the functionality of semiconductor quantum wires as an active layer holds realization of efficient solar cells. Vertically aligned quantum wires absorb more light than their bulk counterparts, because of scattering and trapping incident light. Thus silicon quantum wires (SiQWs) substrate improve probably the cell performance of graphene/silicon Schottky junction. The fabrication process of the graphene/SiQW Schottky junctions has advantages in terms of both cost and simplicity which makes it a promising candidate for future high performance solar cell applications [2]

Motivated by the experimental studies, in this paper, the effect of SiQWs diameter on the performance of SiQWs/G is investigated. As shown in Fig. 1, a graphene layer has been deposited on vertically aligned p-type SiQWs with length of L to make Schottky junctions. The SiQWs array consists of QWs with rectangular cross section with area $d_1 \times d_2$ and unit cell of $a_1 \times a_2$. The doping concentration of SiQWs is 3×10^{15} cm^{-3}.

II. Modeling Approach

The procedure of simulation is based on electrical device modeling coupled with optical modeling. [3, 4]. For electrical modeling, the semiconductor equations, consisting of Poisson, continuity, and drift-diffusion equations is solved simultaneously. [5] Since light trapping in SiQWs will not only improve optical absorption but also boost the surface recombination simultaneously [6, 7], it becomes a dominant concern in electrical modeling. At the same time, radiative, Shockley-Read-Hall and Auger recombinations is also included. For optical modeling, the optical absorption of SiQWs is evaluated by Fermi's golden rule through the solving of Schrödinger equation [8]. In addition, the transmissivity of light between air and SiQWs is calculated by optical conductivity of graphene computed using the tight-binding Hamiltonian[9].

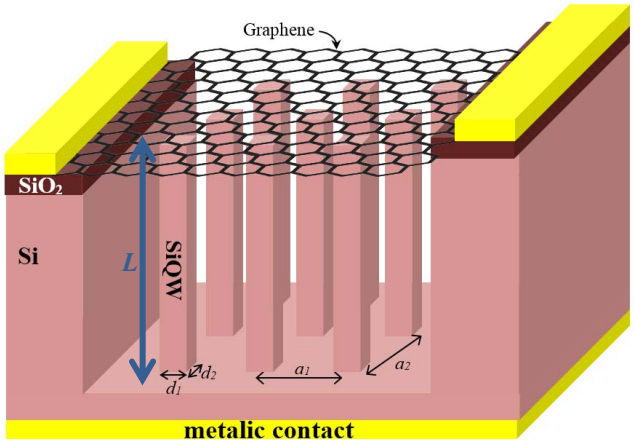

Fig. 1: Schematic view of the SiQWs/G solar cell.

III. Results and Discussion

For the simulations, we consider $d_1=d_2=d$ and $a_1=a_2=a$. J–V characteristics of a p-SiQWs/G and p-Si/G with monolayer graphene, a=7 *nm* and d=6 *nm* is simulated under AM 1.5G solar spectrum in Fig. 2. Remarkably improved performance is obtained for p-SiQWs/G than p-Si/G due to both larger J_{sc} and higher V_{oc}. To understand the reasons of improved performance of p-SiQWs/G, it can be pointed out that bulk Si has an indirect band gap, with the valence band maximum at the Γ point and the conduction minimum at about 85% along the Γ to X direction. Thus, photons cannot provide the momentum difference in this material and phonon absorption is necessary, making it a weaker second order process [10]. But, narrow width [110] and [100] SiQWs are direct band gap. This arises from folding of four degenerate indirect X conduction valleys of bulk Si into the Brillouin Zone center due to confinement in transverse directions [11, 12]. The direct band gap of SiQWs per se increases the optical efficiency. Furthermore, according to the Schottky-Mott model, the amount of Schottky barrier

can be obtained with the graphene work function, electron affinity and band gap of semiconductor. A schematic energy diagram of the bulk Si and SiQW is show in Fig. 3. It is found that SiQW has a larger band gap and smaller electron affinity than bulk Si. The increment of $(E_g)_{SiQW}$ is more than χ_{SiNW} reduction, therefore, the Schottky barrier height of p-SiNWs/G increases, leading to improved J_{sc} compared to p-Si/G. The higher V_{oc} of p-SiNWs/G can be attributed to the larger band gap of SiQWs than bulk Si because of the quantum size effect. The band gap shift of SiNWs with a=7 *nm* and d=6 *nm* is 147 *meV*. Another reason of increased V_{oc} in p-SiNWs/G compared to p-Si/G is due to the logarithmic dependence of V_{oc} on J_{sc}.

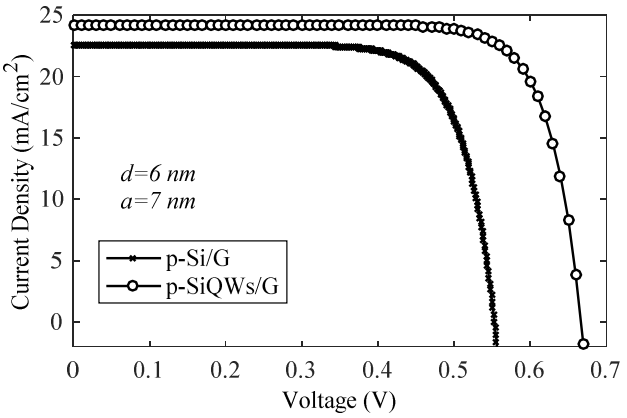

Fig. 2: photo-current density–voltage characteristics of p-type Si/G and SiQWs/G solar cells.

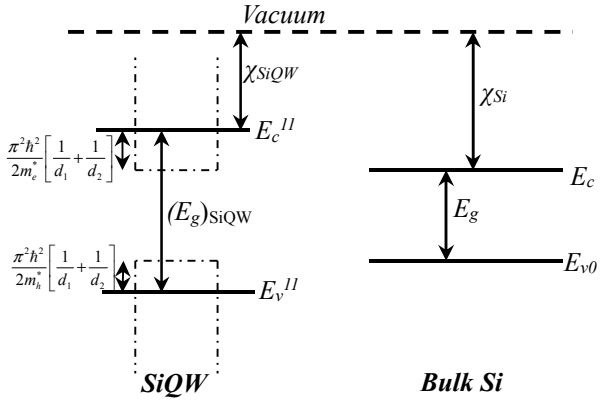

Fig. 3. A band diagram of a SiQW and bulk Si. χ_{Si}, E_g, E_{c0} and E_{v0} correspond to the electron affinity, band gap, conduction and valence band edge of Si, respectively. χ_{SiNW}, $(E_g)_{SiNW}$, E_c^{11} and E_v^{11} correspond to the electron affinity, band gap, first conduction and valence subband edge of SiQW, respectively.

Fig. 4 shows the effect of SiQWs width, d, in a constant unit cell on the p-SiQWs/G solar cell performance. However, the increased surface-to-volume ratio of SiQWs with larger d decreases the charge carrier collection due to the surface recombination increment, but the larger surface area of SiQWs with larger d provides better light absorption and efficient charge separation. Therefore, the increasing of d, increases J_{sc} owing to the SiQWs absorption coefficient increment. Also, it can be seen from Fig. 4, V_{oc} decreases with d increasing due to the decreasing of SiQWs band gap. Because SiQWs with larger d have lower ground state energy and as a result smaller band gap. The maximum efficiency (η) of p-SiNWs/G for small d=2 nm results from direct ban gap transition and band gap increasing, and for large d=9 nm results from SiQWs absorption coefficient increment.

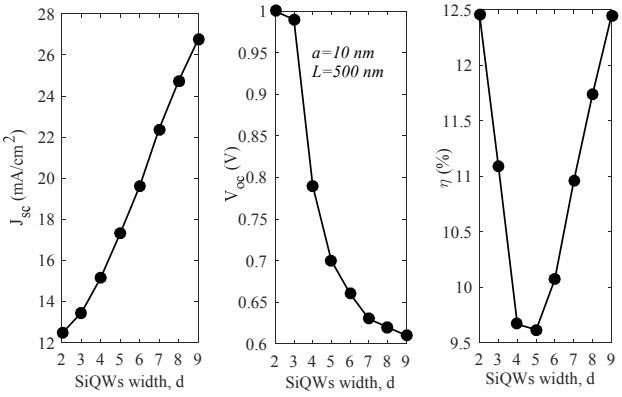

Fig. 3: J_{sc}, V_{oc} and η of p-SiQWs/G solar cells as functions of SiQWs width.

ACKNOWLEDGMENT

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