Modeling of Si-QD Solar Cell in MATLAB

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In this paper, the modeling and analysis of single bi-layer Si-QD solar cell is addressed. The modeling of solar cell is done in MATLAB. The photo currents are calculated for various Si-QD diameters like 2.5, 3, 3.5 and 4 nm and SiO_2 barrier layer thicknesses like 2.5, 2 and 1.5 nm. It has been observed that with the Si-QD diameter, the photo-current increases. On the other hand, photo-current varies conversely with barrier layer thickness due low carrier tunneling probability through barrier.

Keywords: Quantum Dot, Si-QD, Barrier layer, Quantum Confinement Effect (QCE), Photo-current.

1. NTRODUCTION

The introduction of quantum dots application in photovoltaic devices has drawn the attention of many researchers. Reducing the cost incurred by silicon (Si) wafer is the major advantage. At the same time developing high efficiency solar cells using single material limited by its band-gap is a difficult task. Reducing the number of steps involved in the fabrication of solar cells is also essential for cost cutting. All these challenges have motivated researchers for 3rd generation solar cells. Researchers use nano-particles or quantum dots of different materials for enhancing light absorption, charge generation, and the efficiency of solar cells. In order to reduce the overall cost of high efficiency solar cells, researchers fabricate quantum structure of dimension less than 10 nm. The Si nano-crystals or Si quantum dots (Si-QD) of diameter less than 10 nm show quantum confinement effect (QCE). The QCE allows engineering band-gap of a material with QDs by controlling QDs size [3]. Indeed, the quantum confinement effect manifests itself by significant modification of electronic band structure of Si nanocrystals when their size is reduced to below the exciton Bohr radius (~4.9 nm) of bulk Si crystals. In particular, quantum confinement effect provokes the increasing of the effective bandgap of Si nanocrystals. Moreover, for indirect bandgap semiconductors, like Si, geometrical confinement of carriers increases the overlap of electron and hole wave functions in momentum space and thus enhances the oscillator strength and as a consequence increases its absorption coefficient. From this effect, one can expect Si nanocrystals to behave as direct bandgap semiconductors. Though, the momentum conservation rule is only partially broken and Si nanocrystal strongly preserves the indirect bandgap nature of bulk Si crystals Si nanostructures are thus the perfect candidates for higher bandgap materials in all-Si tandem cell approach.

Carrier tunneling probability through dielectric, known as barrier layer increases as its thickness reduces [1]. Based on this concept very thin SiC, SiNx or SiO2 layer in superlattice (SL) can be used in the Si-QD cell. In the present modeling and simulation work, the super lattice with QDs having bandgap in the range of 1.5-2.0 eV has been introduced as intrinsic layer (*i*-layer) for absorbing high energy photons [2]. QDs in a-Si layers sandwiched between dielectric layers in a super lattice structure increases its bandgap energy, which in turn should increase V_{OC} [3].
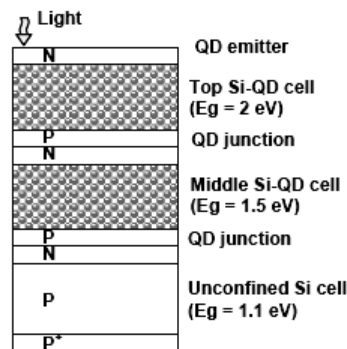

Fig. 1 – Schematic of all- Si Tandem solar cell

Ab initio calculations using density functional theory (DFT) indicate that the increasing of the optical bandgap of Si nanocrystals (or in other words quantum dots (QDs)) is expected to vary from 1.4 to 2.4 eV for a nanocrystal size of 8-2.5 nm. However, further DFT calculations have found that in addition to quantum confinement effect in small QDs, the matrix has a strong influence of the resulting energy levels.

Some researchers [4, 5] have used RF magnetron sputtering to deposit alternating layers of SiO_2 and SRO (Si rich oxide formed by co-sputtering Si and SiO_2) of thicknesses down to 2 nm. Deposition of multilayers, consisting typically of 20-50 bi-layers, is followed by anneal in N_2 ambient from 1050 to 1150 °C, typically for 1 h. During annealing, the excess silicon in the SRO layer precipitates to form Si nanocrystals between the stoichiometric oxide layers, as shown in Fig. 2.

The thin multilayer structure ensures that the Si QDs are constrained in diameter by the layer thickness and a reasonably uniform size dispersion is achieved with variation within about 10 %.

Transport properties are expected to depend on the matrix in which the silicon quantum dots are embedded. As shown in [6], different matrices produce different transport barriers between the Si dot and the matrix, with tunneling probability heavily dependent on the
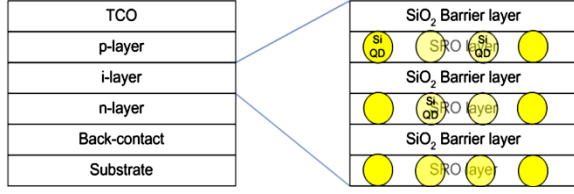
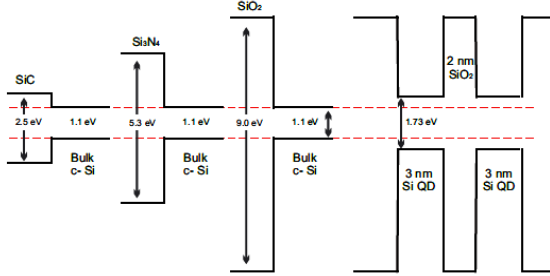**Fig. 2** – Schematic of Si-QD solar cell superlattice in *i*-layer

Fig. 3 – Bulk band alignment between crystalline silicon and its carbide, nitride and oxide, the band gap increases for quantum confined Si dots of 3 nm diameter to 1.73 eV

height of this barrier. Si_3N_4 and SiC give lower barriers than SiO_2 allowing larger dot spacing for a given tunneling current.

2. ALGORITHM

The steps involved in modeling of Si-QD solar cell in MATLAB are as shown below:

• The number of photons corresponding to wavelength, λ from 280 nm to 1200 nm is read from excel file [9];

• As shown in Fig. 4 the average Si QD diameter increases as the O/Si ratio is decreased from 1.3 to 0.86. The Si QDs are approximately 4 nm in the $SiO_{0.86}/SiO_2$, 3 nm in $SiO_{1.0}/SiO_2$ and 2.5 nm in $SiO_{1.3}/SiO_2$. The measured optical absorption of these samples is shown in Fig. 5.
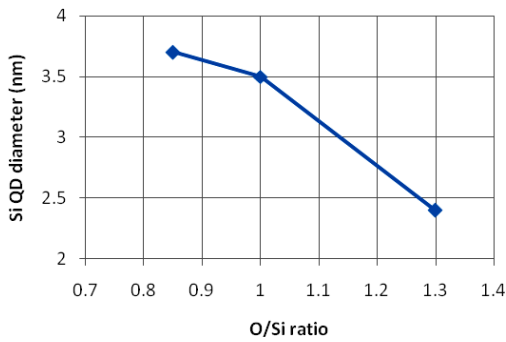

Fig. 5 – Si QD diameter as a function of O/Si ratio in annealed SiO_x/SiO_2 multilayer films [5, 6]

• For given range of λ, absorption co-efficient, α is read. The value of α for different dot sizes like 2.5, 3, 4 nm [4] have already been computed beforehand and stored in separate excel worksheet.

• Find absorptance and from it find number of photons absorbed in silicon QD layer.

As barrier layer of SiO_2 is sandwiched between two consecutive layers of Si-QD, carrier tunneling is to be considered to find effective number of carriers tunneled through barrier layer. Hence, tunneling probability is computed for given $(E_0 - E)$, i.e. from 2 eV, 1.75 eV, 1.65 eV and 1.5 eV to 3.2 eV for QD sizes of 2.5, 3, 3.5 and 4 nm respectively. Some researcher [11] has came up with a simple generalised analytic model describing the size-effective bandgap (EQD) for the lowest energy states for 3D confinement:

$$E_{QD} = E_{bulk} - \frac{3.6q_e^2}{\varepsilon d} + \frac{2\hbar^2\pi^2}{d^2\mu} + smaller\,terms \qquad (1)$$

Where, E_{bulk} is the bulk bandgap, ε is the silicon dielectric constant taken to be 11.7, μ is the reduced mass of the electron-hole pair, and d is the nanocrystal diameter.
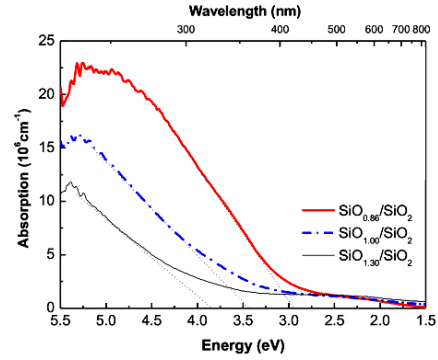

Fig. 6 – Room temperature absorption co-efficient of annealed SiO_x/SiO_2 multilayer [4], [6]

The probability that a carrier will tunnel through a dielectric can be expressed as follows:

$$T_t \approx 16 \times \exp\left(-2 \times \sqrt{\frac{2m^*(E_0 - E)}{\hbar^2} \times W}\right) \qquad (2)$$

where, T_t = Tunneling probability, m^* = effective mass of electron, E_0 = Barrier height, E = Energy of carrier, $\hbar$ = Planck's constant and W = barrier thickness[4].

From expression (1) it is understood that reducing barrier width or dielectric thickness increases tunneling probability. The difference term between conduction band edges of SiO_2 layer and Si-QD $(E_0 - E)$ can be calculated by using expression given below:

$$E_0 - E \approx \frac{E_{g,SiO_2} - E_{g,Si-QD}}{2} \qquad (3)$$

where, E_{g,SiO_2} = Conduction band edge of Silicon Oxide and $E_{g,Si-QD}$ = Conduction band edge of Silicon quantum dot [7]. For example by substituting the values $E_{g,SiO_2} = 9$ eV and $E_{g,Si-QD} = E_{opt,Si-QD} = 2.6$ eV in expression (3), we get $E_0 - E \approx 3.2$ eV. As the bandgap of *i*-layer increases, the cell's V_{OC} is expected to increase significantly [8-11]:

• For the carriers that posses energy higher than barrier height of 3.2 eV in case of SiO_2, carriers will not tunnel through barrier but simply passes through the barrier and generates electron-hole pair (EHP).

- Photo current for single layer of Si-QD and barrier layer is found by integrating carriers available at the surface of the cell.
- J_0 is assumed to be 9.6×10^{-9} mA/cm^2
- V_{OC} is found from the standard expression given below:

$$V_{OC} = \frac{nkT}{q} \ln\left(\frac{J_{sc}}{J_0} + 1\right) \qquad (4)$$

3. RESULTS AND DISCUSSION

As shown in Table 1 modeling of Si-QD solar cell is done for single bilayer of SiO$_2$ and SRO. In order to analyse the dependency of dot diameter on the photo-current, various dot sizes are chosen like 2.5, 3, 3.5 and 4 nm with different barrier layer thicknesses like 1.5, 2, 2.5 nm. It is clear from the results that the short-circuit current J_{sc} for 2.5 nm dot diameter ($E_{QD} = 2$ eV) is 0.3859 mA/cm^2 for 2.5 nm barrier layer thickness, whereas, for 4 nm dot diameter J_{sc} has been increased to 1.247 mA/cm^2 for 1.5 nm barrier layer thickness. Open circuit voltage V_{OC} is varying with dot size and inversely with barrier layer thickness.

Table 1 – Description of the special paragraph styles

Thickness SiO$_2$		2.5 nm		2 nm		1.5 nm	
Dot Size (nm)	E_{QD} (eV)	J_{sc} (mA/cm^2)	V_{oc} (Volt)	J_{sc} (mA/cm^2)	V_{oc} (Volt)	J_{sc} (mA/cm^2)	V_{OC} (Volt)
2.5	2	0.3859	0.4525	0.4071	0.4539	0.456	0.4568
3	1.75	0.6266	0.465	0.6579	0.4663	0.7294	0.4689
3.5	1.65	0.8817	0.4738	0.9268	0.4751	1.0288	0.4778
4	1.5	1.055	0.4785	1.1138	0.4799	1.247	0.4828

4. CONCLUSIONS

In this work the single layer Si-QD solar cell has been modeled and simulated for wavelength 280 nm to 1200 nm. The model has been simulated for various dot sizes like 2.5, 3, 3.5 and 4 nm and various barrier layer thicknesses like 2.5, 2 and 1.5 nm. From the results, it has been concluded that as the dot size increases the QCE decreases and the optical band-gap approached towards bulk Si material *i.e.* 1.124 eV from 2 eV, 1.75, 1.65 and 1.5 eV for Si-QD sizes of 2.5, 3, 3.5 and 4 nm respectively. The J_{sc} is found to increase from 0.3859 mA/cm^2 to 1.055 mA/cm^2 for 2.5 nm dot size to 4 nm for barrier layer thickness of 2.5 nm. On the other hand, the J_{sc} also increases with reduction in barrier layer thickness, i.e. from 1.055 mA/cm^2 for 2.5 nm thick barrier layer to 1.247 mA/cm^2 for 1.5 thick barrier layer.

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