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Simulation of Quantum Dot p-i-n Junction Solar Cell using Modified Drift Diffusion Model

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Abstract

We model quantum dot p-i-n junction solar cell such by modifying the Drift Diffusion equation by bringing in the coupling of the quantum dot region to the rest of the device parametrized by the coupling co-efficient and the Transmission co-efficient. We simulate the device by varying the energy of the QD and report that our model is consistent with the experimental results. We report that with addition of single quantum dot, the Short Circuit Current increases and the Open Circuit Voltage decreases with increase in energy level of the quantum dot. However the Jsc and Voc increase with the interfacial parameters.

Keywords: solar cell; quantum dot; drift-diffusion equation; efficiency

INTRODUCTION

The production cost of the photovoltaic device technologies is directly affected by the energy conversion efficiency of the cell. The thermodynamic limit of photovoltaic energy conversion is 86% and the efficiency of the wafer solar cell is very less than this limit.[1]. Since last couple of decades in order to fashion novel solar cells i.e. to

increase the efficiency a need to develop a new technology has lead to the research of, structure control of matter, at the sub 100nm length scale.

The intermediate band solar cells which are designed by the semiconductor nanostructures have contributed significantly to this research[2]. Semiconductor Quantum Dots (QD) allow three dimensional confinement of the charge carriers as their size is below the Exciton Bohr radius. Thus, the confinement of charge carriers lead to finite number of energy levels within the QD. The size of the QD allows tuning of the energy levels within it and hence the position of the intermediate band created by the QD vary the efficiency of the cell[3].

We present a simulation tool for a QD p-i-n junction solar cell, where the energy level within the QD can be varied. The interfacial issues which occur within the nanostrucutured PhotoVoltaic device due to the introduction of a QD, whose material is different than the host cell, are also parameterized. The QD p-i-n junction solar cell is divided into two scale lengths, the bulk scale for the regions of the cell which do not contain the QD, and the nano scale for the region of the cell which contains the QD. The nanoscale region is simulated using the Transfer Hamiltonian Approach and the bulk scale region is simulated using the Drift-Diffusion model.

The QD is positioned in the intrinsic (i-)region of the cell, and we have considered only one QD within the i-region in the center of the cell. The p and the n region of the cell are the bulk semiconductor.

In our modified Drift-Diffusion Formalism, we present the current-voltage characteristics of QD $p-i-n$ junction solar cell and we take into account of the effects of quantum confinement, electric field, and conduction-valence band asymmetry in calculating the electron and hole density in the QD[4]. We do not take into account the generation within the QD, we only consider quantum confinement and transport of carrier by tunneling through the QD.

A. *Transport equation for bulk semiconductor*

The density of electrons, n and holes, p, within the bulk solar cell regions of intrinsic carrier density ni at temperature T are represented in terms of the quasi-Fermi levels, Efn and Efp.

$$n = N_c \exp\left(E_{fn} - E_c\right)/kT = n_i \exp\left(E_{fn} - E_i\right)/kT$$
$$p = N_p \exp\left(E_v - E_{fp}\right)/kT = n_i \exp\left(E_i - E_{fp}\right)/kT \quad (1)$$

where, E_c and N_c are the band energy and the effective density of states of the conduction band; E_v and N_v are the band energy and the effective density of states of the valence band.

E_i is the intrinsic potential energy, which is given as,

$$E_i = \frac{1}{2}\left(E_c + E_v\right) \tag{2}$$

The basic equations governing the transport through bulk semiconductor, are based on two simple principles: that the number of carriers of each type must be conserved; and that the electrostatic potential due to the carriers charges obey Poisson's equation[5]. For a semiconductor containing electrons and holes, conservation of electron number requires that

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla \cdot J_n + G_n - U_n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla \cdot J_p + G_p - U_p \tag{3}$$

where G_n, G_p is the volume rate of generation and U_n, U_p are the volume rate of recombination of electrons and holes respectively. In the presence of electric field and concentration gradient, the total current for electron and holes is

$$J_n = qD_n \frac{dn}{dx} + qn\mu_n E$$

$$J_p = -qD_p \frac{dp}{dx} + qn\mu_p E \tag{4}$$

Poisson's equation relates the change in carrier densities to the intrinsic potential φ, where

$$E_i = -q\phi \tag{5}$$

$$\frac{d^2\phi}{dx^2} = \frac{q}{\varepsilon_0}\left(n - p + N_a - N_d\right) \tag{6}$$

where q is the charge of the electron, and N_a and N_d are the local concentrations of dopant impurities which are assumed to be fully ionized.

The continuity equations for electrons and holes comprises of three unknowns, n(x), p(x) and $E_i(x)$. We solve them using finite difference method, and using ohmic boundary conditions we obtain the distribution of E_{fn}, E_{fp} and E_i both for the equilibrium and non-equilibrium case.

In our model, we take into account radiative, Auger and trap assisted or SRH recombination mechanisms. The net recombination rate is the sum of all mechanism.

$$U = U_{rad} + U_{Aug} + U_{SRH} \quad (7)$$

Radiative Recombination:

$$U_{rad} = B_{rad}\left(np - n_i^2\right) \quad (8)$$

where B_{rad} radiative recombination coefficient is carrier density independent and is a property of the material.

Auger recombination:

$$U_{Auger} = \left(np - 1\right)\left(nC_n + pC_p\right) \quad (9)$$

where C_n and C_p are the Auger coefficients for the n and p region, based on the type of the material.

For Shockley Read Hall recombination through a single trap state E_t, in the band gap

$$U_{SRH} = \frac{np - n_i^2}{\tau_n\left(p + p_t\right) + \tau_p\left(n + n_t\right)} \quad (10)$$

where, $\tau_n(\tau_p)$ are the lifetimes of electrons (holes) and $n_t(p_t)$ are the densities of electrons (holes) at equilibrium when the Fermi level lies at E_t.

B. *Transport through Quantum Dot*

The transport through the QD is studied using the Transfer Hamiltonian Approach. The interactions between the QD and the p and n regions are introduced by transmission coefficient and capacitive coupling coefficients[6]. The current and the carrier density within the QD depend upon the probability of tunneling through it. The effect of the change in the carrier distribution of the p and n region is computed using the Schrodinger Poisson Solver. The QD is assumed to have only a single level, which will evolve when the bias across the QD changes. As the carriers will flow throughthe QD,

the potential as well the number density of the QD will change. Assume no inelastic scattering in the QD and symmetric transmission coefficient.

The current[7] between the two parts of the system is given as:

$$\frac{dN_i}{dt} = \frac{4\pi q}{hbar}\left(\int T_{pi}\rho_p\rho_i\left(f_p - f_i\right) + \int T_{ni}\rho_n\rho_i\left(f_n - f_i\right)\right)dE \quad (11)$$

where, T_{pi}, T_{ni} are the transmission coefficients between the quantum dot and the p and n regions. f_p, f_n and f_i are the fermi distributions for the p, n regions and for the quantum dot. ρ_p, ρ_n and ρ_i are the density of states for p, n and the quantum dot. N_i is the carrier density of the quantum dot.

The total charge density within the QD is given as:

$$N_i = \int \rho_i\left(E\right) n_i\left(E\right) dE \quad (12)$$

We only consider a single state with energy level ǫ in the QD. To take coupling with p and n into account, we assign a Lorentzian shape DOS centered on ǫ and the half width value is proportional to the strength of the coupling [8].

The current through the QD will effect the electrostatic potential V_i within the QD, this is taken into account using the Poisson's equation.

$$\vec{\nabla}\cdot\left(\varepsilon_r \vec{\nabla} V_i\right) = -\frac{q\Delta N_i}{\Omega\varepsilon_0} \quad (13)$$

The general solution of the Poisson's equation in the QD, will depend upon the capacitive coupling with the p and n region and the increase in potential as a result of the injection of one electron into the QD [9].

$$U_i = \sum_{j\neq i}\frac{C_{ij}}{C_{tot,i}}\left(-qV_j\right) + U_0\Delta N_i \quad (14)$$

Hence, the local potential depends on the increasing charge density, but at the same time the charge depends on the DOS that is modified by the local potential. Hence the local potential and the charge density have to be solved self-consistently.

The evolution of energy level within the QD, is given as the sum of the potential due to lectrostatic effect and the equilibrium position of the energy level, given as.

$$E(n) = \varepsilon(n) + U_i \quad (15)$$

where, n = 0, 1, 2, 3.

The p − i − n solar cell is simulated using one dimensional drift-diffusion equation for the p and n region, where the QD is placed between the p and n region. Hence the potential difference that is acting on the QD is obtained from the Built-in-Voltage of the solar cell. And the QD is placed in the simulation at the centre, and the depletion region boundaries of the p and n region modify the local potential within the QD.

RESULTS AND DISCUSSION

It has been experimentally reported in [5] that the photocurent available from a p − i − n solar cell can be increased by the addition of QDs to the undoped region. At the same time, the open circuit voltage Voc reduces by introducing areas of lower band gap where recombination is enhanced. We report the change in the Short circuit current Isc and open circuit voltage Voc, with change in the energy level of the QD is consistent with the IV characteristic of the experimental results as reported by [1].

The ultimate efficiency limit when a QD having a single energy level is introduced in the Si solar cell is shown presented. For a QD of bandgap 0.8eV, within the i-region of the Si solar cell has the upper limit of 41%, as shown in Fig 1.

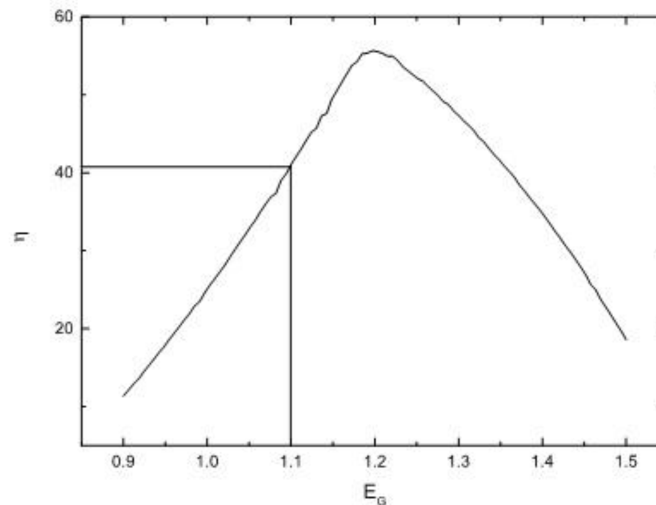

Figure 1. Plot of efficiency η to the band gap of the host material E_G . I The maximum efficiency of 40.1% is obtained for a Quantum Dot of band gap 0.8eV within the i-region of the Si solar cell.

The characteristics of the QD p-i-n junction solar cell have also been calculated with different values of Transmission Coefficient T, as shown in Fig. 2,3. The different

values of 'α_D' represent the capacitive coupling coefficient. The Fig. 2,3. show that as the value of T increases, we observe increase even in the Jsc and Voc parameters of the cell. The mathematical representation of the interface parameters T and 'α_D' decide the characteristics of the cell.

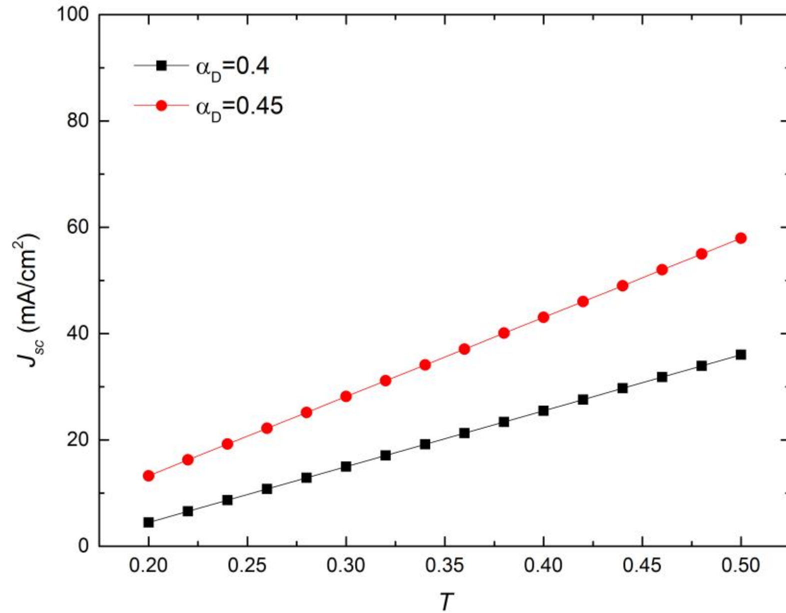

Figure 2. Plot of Short Circuit Current Jsc to Transmission coefficient T. Jsc increases with 'α_D'.

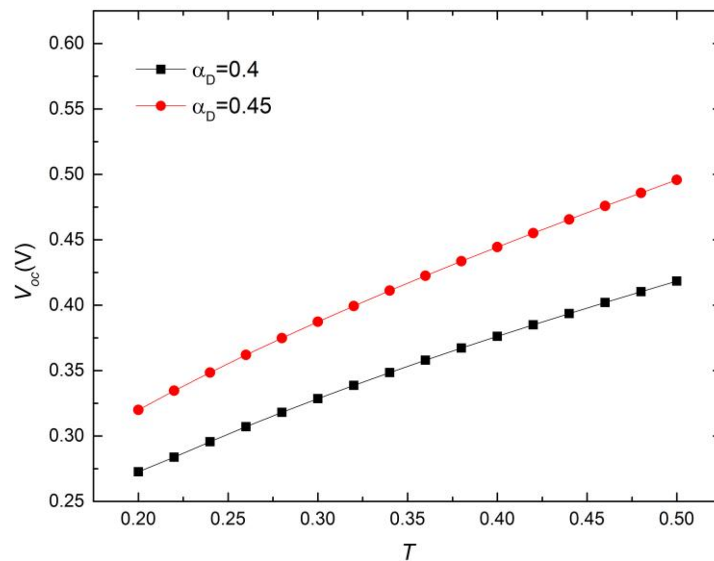

Figure 3. Plot of Open Circuit Voltage Voc to Transmission coefficient T, Voc increases with 'α_D'.

Our proposed theoretical model for QD solar provides a simple and transparent method for describing electrons transport, it can also be extended to include more number of QDs. This framework requires less computational complexity, compared to the Monte-Carlo Simulation, and the limitation of Drift-Diffusion equation, of not able to be implemented in the nano scale, has been overcome. Our model is a powerful and intuitive method for simulating Nanostructured devices.

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