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Electronic transport in QD based structures: from basic parameters to opto-electronic device simulations

S. Illera, J. D. Prades, A. Cirera and A. Cornet

MIND/IN²UB Departament d'Electrònica, Universitat de Barcelona, C/Martí i Franquès 1, E-08028 Barcelona, Spain

E-mail: `sillera@el.ub.edu`

Abstract. We present a theoretical model that explains the optoelectronic response of nano-devices based on large quantum dot (QD) arrays. The model is grounded on rate equations in the self-consistent field regime and it accurately describes the most important part of the system: the tunnel junctions. We demonstrate that the ratio between the optical terms and the transport rates determines the final device response. Furthermore, we showed that to obtain a net photocurrent the QD has to be asymmetrically coupled to the leads.

1. Introduction

Silicon quantum dots (Si QD), embedded in insulator matrices such as SiO_2, have opened a new branch of possibilities in the electronics due to the novel electronic properties based on the quantum confinement. Discrete energy states appear inside the wide band gap of the insulator matrix, making possible tunable band gap devices. Concerning opto-electronic devices, the possibility to modify the energy band gap as a function of the QD radius can be exploited in order to build light absorbers for photovoltaic applications.

In order to generate a net photocurrent, the photo-generated electron has to be extracted before recombining. Thus, the charge transport from the location of photo-generation to the leads becomes a crucial point that governs the response of the system. These transport mechanisms depend on the tunneling processes being strongly dependent on the insulator material and also on the geometrical arrangement of the QDs.

2. Theoretical model

A compact model to explain ballistic electrical transport in the self-consistent field regime in these kind of systems was reported by the authors previously [1, 2]. The transport formalism was compared to Non Equilibrium Green's Function Formalism (NEGFF) obtaining similar results [3] and it also showed the possibility to combine it with Density Functional Theory (DFT) [4]. The general framework describes the electrical transport between N QDs embedded in a dielectric matrix coupled to two electrodes (L lead and R lead) as a network of multi-tunnel-junctions under external bias voltage polarization. It is based on the Transfer Hamiltonian formalism [5] to describe the currents between the different parts of the system. Assuming that the QDs are independent, the non-equilibrium distribution functions can be obtained solving a

set of non-coherent rate equations [6]. Moreover, the effect of the trapped charge in the QDs has been included solving the transport equations and the Poisson equation self-consistently, within the self-consistent field regime, explaining a first order the Coulomb blockade effects [7]. From the previous developed formalism, large systems based on QD arrangements can be simulated in a great detail taking into account the particular properties of the QDs.

In the spirit of the rate equation type model, we assume that the optical and transport processes are independent [8]. Thus, the rate equations have been modified in order to reflect the stimulated generation/recombination carrier processes. For each energy level, they read as

$$\frac{dn_j^i}{dt} = \underbrace{\frac{2\pi q}{\hbar}|T_{Lj}|^2 \rho_L \rho_j^i (f_{Lj} - n_j^i)}_{\text{Left lead contribution}} + \underbrace{\frac{2\pi q}{\hbar}|T_{Rj}|^2 \rho_R \rho_j^i (f_{Rj} - n_j^i)}_{\text{Right lead contributions}}$$

$$+ \underbrace{\sum_{k,i'\neq i} \frac{2\pi q}{\hbar}|T_{jk}^{ii'}|^2 \rho_j^i \rho_k^{i'} (n_k^{i'} - n_j^i)}_{\text{Neighboring QDs contribution}} + \underbrace{\sum_k q R_{kj} \frac{\rho_k^i}{\rho_j^i} n_k^i (1 - n_j^i) - \sum_k q R_{jk} n_j^i (1 - n_k^i)}_{\text{Light terms}}, \quad (1)$$

where the superscript i and i' refer to the ith and i'^{th} QDs, respectively. j and k refer to the jth and k^{th} energy level of the corresponding QD. n_j^i is the non-equilibrium distribution function of the jth level in the ith QD. ρ_L and ρ_R are the density of states (DOS) of the leads evaluated at the energy of the energy level j, and ρ_j^i is the degeneracy of the jth energy level of the ith QD. The QD DOS includes the local potential in each QD as the solution of the Poisson equation (see Ref. [1]). f_{Lj} and f_{Rj} are the distribution functions of the leads (left and right, respectively) described by the Fermi Dirac distribution function taking into account that the external bias voltage (V) modifies the electrochemical potentials $\mu_L - \mu_R = -qV$.

$|T_{Lj}|$ and $|T_{Rj}|$ are the transmission coefficients between the QD and the leads whereas, $|T_{jk}^{ii'}|$ is the transmission coefficient among the ith and i'^{th} QDs. For the description of the tunneling processes through the oxide, we have used the WKB approximation [9] as we have described previously in Ref. [2].

The QD is treated as a finite spherical potential well within the effective mass approximation [10]. The height of the potential well is the difference between the conduction/valence band energy level of the dielectric matrix and the ones that form the QD. The width of the well is $2R$, where R is the QD radius. The carriers effective masses are assumed to have different values in the QD and in the dielectric matrix.

Concerning the optical transition rates R_{jk}, they were calculated using the Fermi's Golden Rule in the dipole approximation within the strong confinement regime [11, 12]. This is the usual treatment of the light interaction and a formal derivation can be found in many text books [13, 14].

Solving Eq. 1 in the steady state condition, the QD non-equilibrium distribution function for each energy can be obtained. Therefore, the charge stored in the ith QD is $N_i = \sum_j 2\rho_j^i n_j^i$, where we take into account the spin factor 2. Once the charge has been calculated, the Poisson equation is solved and the self-consistent solution of the local potential and the charge is imposed [1]. From the non-equilibrium distribution functions, the current through the device can be obtained as $I = \sum_i^N \sum_j \frac{2q^2}{\hbar}|T_{Lj}^i|\rho_L \rho_j^i (f_{Lj} - n_j^i)$ where the current sums over all the N QDs (i) and the corresponding energy levels of each QD (j).

3. Si QDs optical simulations: the role of the QD arrangement

Here, we are going to focus on the specific case of silicon QDs (Si QDs) embedded in a SiO_2 matrix (Si/SiO_2 QDs). The inputs needed to describe this system are: the carrier effective

masses, the confinement potentials, the Si bulk band gap and the dielectric constants. The value of the parameters can be found elsewhere [2].
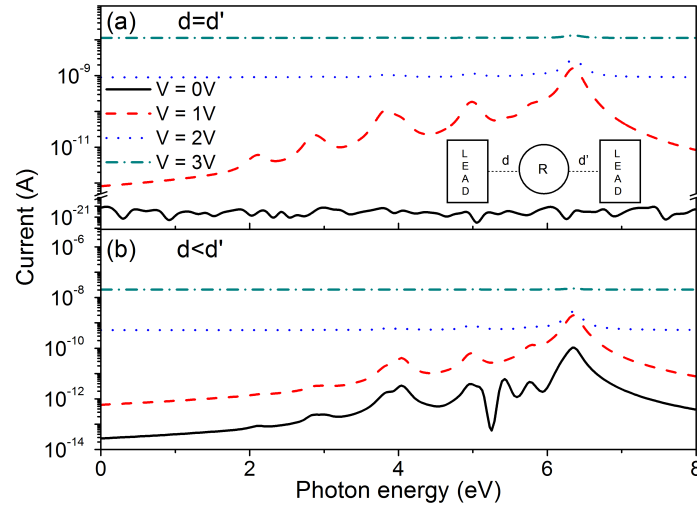

Figure 1. Photocurrent as a function of the energy of the incident light with an external applied bias voltage for (a), the symmetric case ($d = d' = 1.78nm$) and (b), asymmetric case ($d = 1.47nm$ and $d' = 2.09nm$). The scheme of the single Qd of $R = 1.05nm$ placed between the two electrodes is shown in the inset.
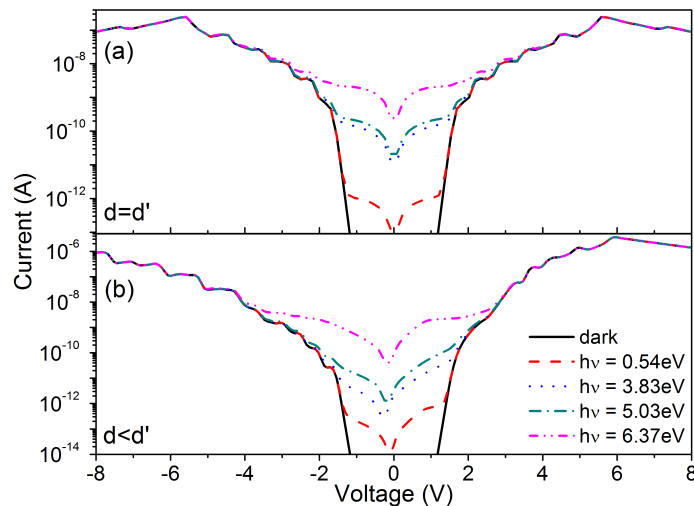

Figure 2. Total I(V) curve (in absolute value) for the symmetric (a) and asymmetric (b) cases in dark and under different illumination conditions.

The system under study is a single Si QD embedded in SiO_2 under illumination connected to two electrodes with a constant external bias voltage applied. We present two scenarios: the QD symmetrically connected $d = d'$ to the leads and in asymmetric configuration $d \neq d'$.

The obtained photocurrent as a function of the energy of the incident photons for different external bias voltages for the symmetric and asymmetric cases are shown in Fig. 1(a-b), respectively. For the V=0 case, in the symmetrically coupled system (a), the current is zero since the incoming hole currents for each side equal the outgoing electron currents. This analysis

is inferred from the sum of all current terms; for the electron energy levels $I_{opt} - I_{Le} - I_{Re} = 0$ and for the hole levels $I_{Lh} + I_{Rh} - I_{opt} = 0$; where I_{opt} is the optical flux created among the electron/hole energy levels. I_{Le} and I_{Re} are the electron fluxes whereas I_{Lh} and I_{Rh} are the hole fluxes from the left and right leads, respectively. For the symmetrical coupling to both leads, $I_{Le} = I_{Re}$ and $I_{Lh} = I_{Rh}$. Therefore, $I_{Le} = I_{Lh}$ and the total current is zero since the hole currents compensate the electron ones. For the asymmetrical case (b), $I_{Le} \neq I_{Lh}$ and a net photocurrent is generated in the V=0 case.

When an external bias voltage is applied, the transmissions coefficient between the QD and the two leads change. Thus, the system becomes asymmetric and a net current appears. The current peaks are related to the maximum transition probabilities for an incident photon reflecting the absorption spectra. When the voltage increases, the current tends to be independent of the incident photon energy.

In Fig. 2(a-b), the obtained current voltage curves I(V) under external illumination as a function of the incident photon energies are shown for the symmetric and asymmetric cases. For the illuminated case, the main differences appear for small voltages when the optical terms dominates in Eq. 1 and the electrical response of the system differs from the dark case. Recovering the dark trend for higher voltages, when the current terms in Eq. 1 dominate again. Thus, the electrical response of the system is a competition between the two processes: the pure light current term and the external bias voltage term.

4. Conclusions

In conclusion, we present a theoretical framework based on non-coherent rate equations combined with the Transfer Hamiltonian approach to explain the transport properties of the next generation of optoelectronic devices based on the QDs properties. From a simple example based on a single Si QD embedded in SiO_2, we have demonstrated that the QD tunneling couplings to the leads play an important role in the final photoresponse of the system, being zero the net photocurrent when the QD is symmetrically coupled to he leads. The photocurrent response recover the shape of the absorption spectra. Concerning the I(V) curves in dark and illumination conditions, we have shown that the main differences appear due to the ratio between the optical and electrical terms.

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