

Conductivity of Quantum-Dot Crystal Simulation Using Physics Based Models

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Abstract—In this paper we present physics based analysis of Quantum Dot Arrays (QDA) conductivity. Photovoltaic devices based on QDA have a potential for delivering the ultra-high efficiency photovoltaic (PV) cells for energy generation in space and terrestrial applications. Model and results are analyzed and discussed.

Keywords- Quantum Dot, Photovoltaic, Physics Based, TCAD.

Quantum Dot Arrays (QDA) have a potential for delivering the ultra-high efficiency photovoltaic (PV) cells for energy generation in space and terrestrial applications [1], Fig. 1(a), PV cell efficiency versus QD size and interdot distance. QD array conductivity is an important property and it is proposed to use for integration the QD quantum system model into traditional 3D TCAD software we develop (3D NanoTCAD simulator at CFDR). This paper presents a model we have proposed for such a QD array structure, which we have implemented into our NanoTCAD device simulator. While we have a large selection of quantum and kinetic models developed, and validated [2], this currently presented model has a number of advantages: it is relatively simple, accurate and fast, and deliver the conductivity, which compares well with available data [3,4]. The proposed approach considers a 3D regimented array of quantum dots using an envelope function approximation [2]. The regimentation results in an artificial crystal where the atoms are represented as quantum dots. This structure is referred to as a quantum dot crystal (QDC). In order to determine the conductivity and mobility of a cubical QDC, the energy dispersion, group velocity, Fermi energy, and conductivity must be calculated. The energy dispersion is calculated by solving the Schrödinger equation of a cubical quantum dot with finite potential barriers. The solution to the Schrödinger equation has a form similar to the Kronig-Penny model [2]. The energy dispersion of a cubical QDC can be determined along specific quasi-crystallographic directions. Our approach is based on accurate calculation of energy dispersion and density of states in QDC, following the models in [3,4] and their extensions we have performed. An example of calculated density of state is shown in the insert of Fig 1. One of GUI interfaces with the NanoTCAD software developed is shown in Fig 2.

I. MODEL DEVELOPMENT

The energy dispersion of a cubical QDC can be determined along specific quasi-crystallographic directions. Figure 1 shows the dispersion relation for a QDC along the [100] quasi-crystallographic direction for an InAs/GaAs system. A quantum dot size of $L=10\text{nm}$ and barrier thickness of $H=5\text{nm}$ was simulated. The effective masses and conduction band offset for the simulated system are as follows: $m_{\text{InAs}}^* = m_{\text{w}}^* =$

$0.04m_0$, $m_{\text{GaAs}}^* = m_{\text{B}}^* = 0.0665m_0$, $E_{\text{C_offset}} = 0.45\text{eV}$, where m_0 is the electron rest mass. The carrier wave vector is labeled as q and is subscripted with the particular quasi-crystallographic direction. Each energy band is characterized by the three quantum numbers: n_x , n_y , and n_z . The superscript of each miniband denotes the degeneracy of that particular miniband. Spin degeneracy is not counted in the energy dispersion calculation. It is taken into consideration for the density of states (DOS) calculation.

The density of states is the number of carrier states allowed per unit volume per unit energy interval. Mathematically, it is given by the following,

$$DOS(E) = \frac{2}{(2\pi)^3} \int_v \delta(E - E_n(\bar{q})) d\bar{q} \quad (1)$$

where the integration is carried over the whole Brillouin zone [2]. As stated above, the factor of 2 accounts for the spin degeneracy of an electron. Figure 2 shows the DOS for the 111 miniband. The data obtained for the DOS of each miniband is stored and used to calculate the position of the Fermi level of the QDC. The Fermi level is determined from the neutrality equation

$$N_D^+ + p = N_A^- + n \quad (2)$$

where N_A^- , N_D^+ , n and p denotes the concentration of the ionized acceptors, donors, free electrons and holes, respectively. For an n-type QDC, the neutrality equation can be rewritten in the following form

$$\frac{N_D}{2 \exp\left(-\frac{E_D - E_F}{k_B T}\right) + 1} + \sum_l \int_{E_{\text{min}}^{(l)}}^{E_{\text{max}}^{(l)}} \frac{G_h^{(l)}(E)}{\exp\left(-\frac{E - E_F}{k_B T}\right) + 1} dE = \sum_n \int_{E_{\text{min}}^{(n)}}^{E_{\text{max}}^{(n)}} \frac{G_e^{(n)}(E)}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1} dE \quad (3)$$

where the summation over n is carried out over all mini-bands in the conduction band and the summation over l is carried out over all mini-bands in the valence band [2]. The energies E_{min} and E_{max} are the edges of the corresponding mini-bands. This equation is numerically solved for E_F using the calculated DOS for the lower energy minibands (111, 112, 122), appropriate energy ranges and chosen values for the dopant energy (E_D) and doping level. Only the 111, 112 and 122 mini-bands are used in the calculation because the DOS for the higher energy mini-bands are orders of magnitude lower than that of the said mini-bands and do not affect the Fermi energy calculation whether they are considered or not. For a doping concentration of $1e16 \text{ cm}^{-3}$, E_D of 0.3 eV and temperature of 300K a Fermi level of 0.140 eV was obtained. The reference energy is the bottom of the energy barrier (see DOS insert in Fig.1).

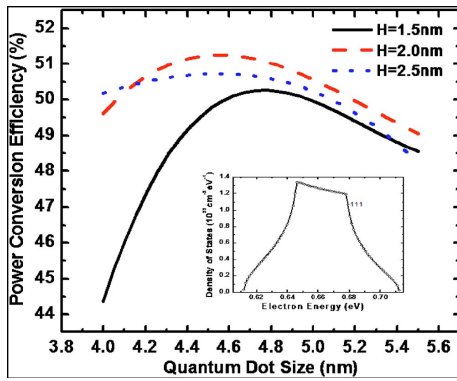


Fig. 1. 51% Efficient QDPV cell [1].

In order to calculate the conductivity and thus the mobility a QDC the contributions from each mini-band in the conduction band of the structure must be considered. Mathematically, this is written

$$\sigma = \sum_n \sigma^{(n)} \quad (4)$$

where the tensor components are given by Eq. (5):

$$\sigma_{ij}^{(n)} = \frac{e^2 \tau_0}{4\pi^3 k_B T} \int_{QBZ} v_i^{(n)}(\mathbf{q}) v_j^{(n)}(\mathbf{q}) \frac{\exp\left[\frac{E^{(n)}(\mathbf{q}) - E_F}{k_B T}\right]}{\left\{ \exp\left[\frac{E^{(n)}(\mathbf{q}) - E_F}{k_B T}\right] + 1 \right\}^2} d\mathbf{q} \quad (5)$$

Here, e is the elementary electron charge, k_B is Boltzman's constant, T is the temperature, $v^{(n)}$ is the group velocity vector, E_F is Fermi's energy of an electron, and \mathbf{q} is the electron wave vector. The n index signifies a particular mini-band. The integration is carried out over the entire Quasi Brillouin Zone (QBZ). The relaxation time (τ_0) is assumed to be constant and equal to a value characteristic for the given materials. In our case, $\tau_0 = 10^{-12}$ sec. It is apparent that electron dispersion and the position of the Fermi level determine the conductivity. In addition, the group velocity is dependent on the mini-band structure and electron dispersion in the QDC. In general, it is given for the n -th subband by Eq. (6):

$$v_i^{(n)}(\mathbf{q}) = \frac{1}{\hbar} \frac{\partial E^{(n)}(\mathbf{q})}{\partial q_i} \quad (6)$$

where $E^{(n)}$ are the energies for each n -th mini-band. In order to determine the conductivity of a QDC, the group velocity must be calculated first. Since the group velocity is also dependent on the wave vector, we must choose a appropriate quasi crystallographic direction for the calculation. Given the symmetry of the cubical QDC, the conductivity has the relation $\sigma_{xx} = \sigma_{yy} = \sigma_{zz}$. Thus, whether the [100], [010], or [001] direction is chosen, group velocity and conductivity will yield identical results. For simplicity, the [100] direction has been chosen for the subsequent calculations. Using the above results for group velocity along with the results obtained for electron dispersion and Fermi position, the conductivity of the QDC was calculated. Using the values that were mentioned above, a total conductivity of 489.32 S/m was obtained for a QDC of $L=10\text{nm}$ and $H=5\text{nm}$. This value was then used to

calculate the mobility of the QDC. For electrons, the mobility is given by

$$\mu = \frac{\sigma}{eN} \quad (7)$$

where e is the elementary charge, σ is the total conductivity and N is the carrier concentration given by Eq. (8).

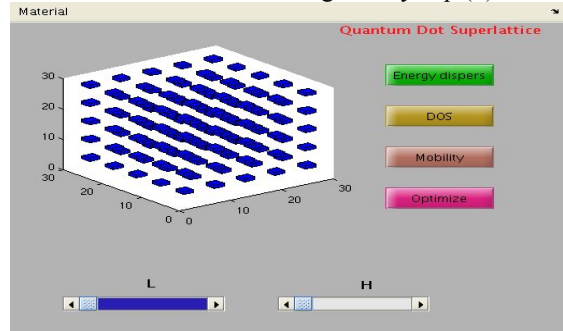


Fig. 2. 3D CFDR NanoTCAD device simulator GUI.

$$N = \sum_n \int_{E_{min}^{(n)}}^{E_{max}^{(n)}} \frac{G_e^{(n)}(E)}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1} dE \quad (8)$$

Substituting the appropriate values into Eq. (7) and solving, a mobility of 772.73 cm^2/Vs is obtained for a QDC of $L=10\text{nm}$ and $H=5\text{nm}$. This process was repeated for holes. A hole mobility of 0.3213 cm^2/Vs was obtained. The process can be expanded to find the conductivity for different concentrations of the $\text{Ga}_x\text{In}_{1-x}\text{As}/\text{GaAs}$ system for varying levels of doping. Fig. 3 shows the results of such a simulation.

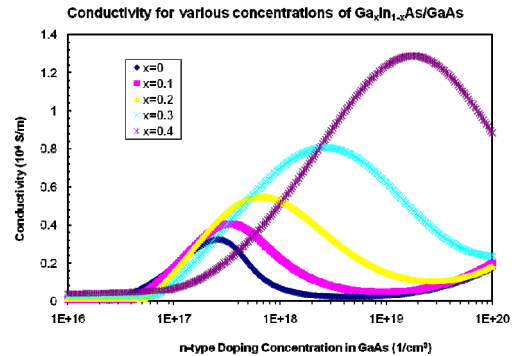


Fig. 3 Calculated QDA conductivity of $\text{GaInAs}/\text{GaAs}$ dot/host system as a function of doping level.

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