The intrinsic losses of quantum dot intermediate band solar cells

Zahra Arefinia[1], *Member, IEEE* and Asghar Asgari [1,2]

[1] *Research Institute for Applied Physics and Astronomy, University of Tabriz, Tabriz, 51666-14766, Iran*, arefinia@tabrizu.ac.ir; arefinia@ieee.org

[2] School of Electrical, Electronic and Computer Engineering; University of Western Australia, Crawley, Australia

***Abstract*- Thermalisation and below-bandgap loss mechanisms of intermediate band solar cells (IBSCs) comprised of $InAs_{(1-x)}N_x$ quantum dots (QDs) embedded within intrinsic layer of $AlP_{0.5}Sb_{0.5}$ p-i-n solar cell is calculated. a Finite element method is used for solving Schrödinger equation to calculate possible energy band configurations of $AlP_{0.5}Sb_{0.5}$: barrier/ $InAs_{(1-x)}N_x$: square pyramid–shaped QDs with different nitrogen concentration. It is found that there is a minimum total loss of ~27% for nitrogen concentration less than 0.01 of $InAs_{(1-x)}N_x$ QD- IBSCs.**

I. Introduction

The most feasible implementations of the intermediate band solar cell (IBSC) are quantum dot (QD) solar cells with several layers of QDs embedded within the intrinsic region of p-i-n semiconductor structures. InAs QDs in a GaAs matrix has been most commonly utilized for the fabrication of QD-IBSCs [1, 2]. But, the efficiency of fabricated InAs/GaAs IBSCs is lower than the one of the GaAs reference cell without QDs [3]. Because, the band gap of QDs and host material is not optimal and several IB presents within the GaAs band gap [4]. Therefore, we have tried to find optimal QDs and barrier materials to prevent the appearance of confined states in the valence band (VB) for minimum loss. Thus, IBSCs have been studied in which the intermediate band (*IB*) is constituted by the ground state of $InAs_{(1-x)}N_x$ QDs in a $AlP_{0.5}Sb_{0.5}$ matrix. The bandgap of this system should be optimized with the amount of nitrogen atoms to allow the basic principles of IB operation to be proven. Then, the reducing of intrinsic losses due to the IB and the relative magnitude of each loss mechanism can be investigated.

Therefore, in this paper, the effect of nitrogen concentration on the dominant loss processes, thermalization and below band gap, of $InAs_{(1-x)}N_x/AlP_{0.5}Sb_{0.5}$ QD-IBSCs is investigated by numerical simulations. It is found that the total loss can be reduced by appropriate nitrogen concentration.

II. QD-IBSC Structure

Fig. 1 shows a cross–sectional view of QD-IBSC which is $AlP_{0.5}Sb_{0.5}$ p-i-n structure with a stack of $InAs_{(1-x)}N_x$ QDs layers embedded within the intrinsic region. The unit cell of QDs used for our calculations is also indicated Fig. 1. We assume square pyramids –shaped QDs of $InAs_xN_{(1-x)}$ with base lengths of a_1=a_2=4 nm in the x and y directions, respectively, and the height of h=5nm in the z direction. The cube unit cell of inter-dot spacings with the lengths of L_1=L_2= L_3=9nm in the x, y, and z directions, respectively, filled by the matrix material of $AlP_{0.5}Sb_{0.5}$.

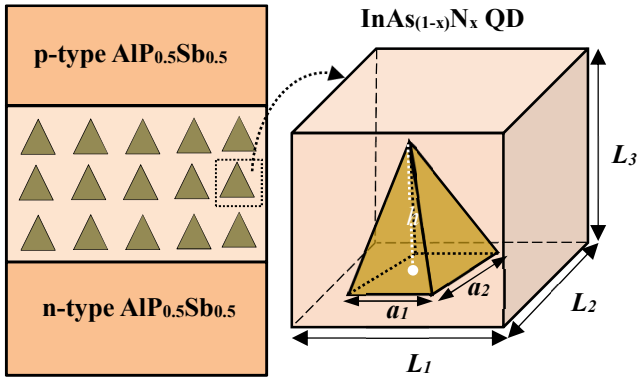

Fig. 1: Cross–sectional view of QD-IBSC The unit cell of square pyramids –shaped QDs is shown in the right side.

II. Simulation Approach

The unit cell of Fig. 1 is discretized into elements and nodes based on Delaunay triangulation technique and then the location of nodes is iteratively improved [5]. Then, finite-element method (FEM) [6] is applied to solve three-dimensional Schrödinger equation for the conduction band (*CB*). With obtaining the electron energy levels and subsequently the E_{g1} bandgap between the *IB* and the *CB* and E_{g2} bandgap between the valence band (*VB*) and the *IB* (see Fig. (2)), we can calculate intrinsic loss processes [7, 8]. The photons with energies higher than the highest bandgap of $E_{g1}$and E_{g2} are absorbed creating electron-hole pairs. The thermalisation loss (L_{th}) is calculated by subtracting the number of absorbed photons multiplied by the E_{g2} bandgap energy from the total energy of the photons absorbed as:

$$L_{th} = \frac{1}{p_{in}} \cdot \left(\frac{2\pi}{c^2 h^3}\right) \cdot \int_{E_{g2}}^{\infty} \frac{E^3 - E_{g_2} \cdot E^2}{\exp\left(\frac{E-\mu}{kT_s}\right) - 1} dE \qquad (9)$$

where p_{in} is the input power, E is energy, c is the speed of light, h is Planck's constant, k is Boltzmann's constant, T_s is the sun temperature and μ is the chemical potential.

The photons with energy less than the lowest bandgap of E_{g1} and E_{g2} do not have enough energy to generate an electron-hole pair and are not therefore absorbed. The below-

bandgap loss ($L_{belowEg}$) is depending on the position of the *IB* through E_{g1}, as below:

$$L_{belowEg} = \frac{1}{p_{in}} \cdot \frac{2\pi}{c^2 h^3} \int_0^{E_{g1}} \frac{E^3}{\exp\left(\frac{E-\mu}{kT_s}\right) - 1} dE \qquad (9)$$

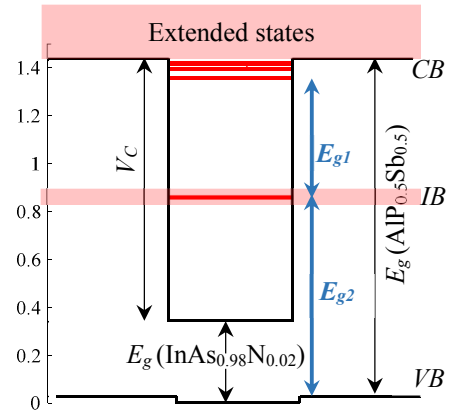

Fig. 2: Schematic view of $AlP_{0.5}Sb_{0.5}$: barrier/ $InAs_{0.98}N_{0.02}$: QD. V_C is the conduction band offset. The electron energy levels of conduction band well is shown with red lines. The overlapping of ground state in the conduction band well forms *IB*. The difference between the ground state and first excited state is E_{g1} and the difference between the *VB* and the *IB* is E_{g2}.

III. Results and Discussion

As depicted in Fig. 3, with increasing nitrogen content, L_{th} increases. Because, with increasing nitrogen concentration, as seen in Fig. 4, E_{g2} decreases and the absorption rang of QD-IBSC increases and the energy range in which strong interaction between excited carriers and lattice phonons occurs and carriers cool to the bandgap edge, increases.

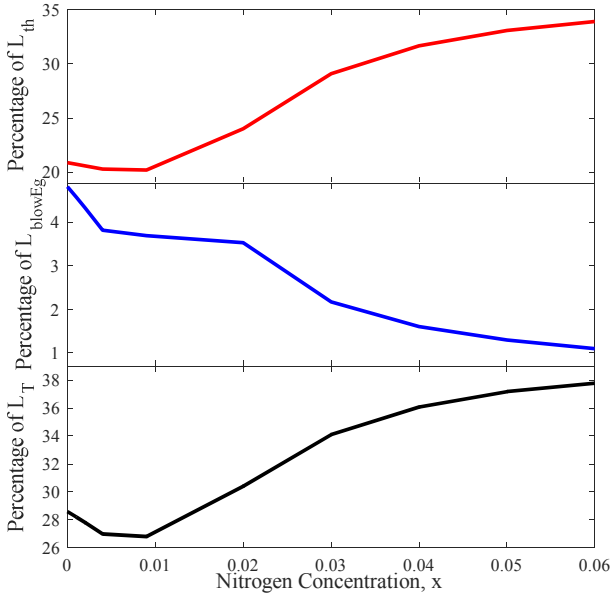

Fig. 3: L_{th}, $L_{belowEg}$ and L_T of $AlP_{0.5}Sb_{0.5}$: barrier/ $InAs_{(1-x)}N_x$ QD-IBSCs as functions of nitrogen concentration.

$L_{belowEg}$ of QD-IBSC as a function of nitrogen concentration is shown in Fig 3. It is found that $L_{belowEg}$ decreases with increasing nitrogen concentration due to the decrement of E_{g1} as shown in Fig. 4. As a result, QD-IBSCs become transparent to a narrower range of wavelengths. QDs with higher nitrogen concentration have higher electron effective mass (see Fig. 4) and create smaller V_C. Then, the difference between ground state and *CB* (if there is one energy level in the well) or the difference between ground state and first excited state (if there is more than one energy level in the well, as Fig. 2) which is E_{g1} becomes smaller. Fig. 3 also shows the total loss (L_T) which is the sum of L_{th} and $L_{belowEg}$. It is seen a minimum L_T of ~27% for $InAs_{0.991}N_{0.009}$ QD.

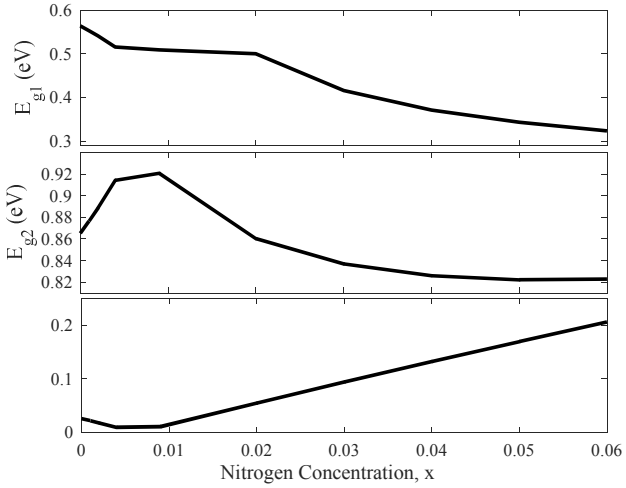

Fig. 4: The value of E_{g1}, E_{g2} and electron effective mass of $InAs_{(1-x)}N_x$ as functions of nitrogen concentration for $AlP_{0.5}Sb_{0.5}$: barrier/ $InAs_{(1-x)}N_x$ QD-IBSC.

References

[1] N. A. Kalyuzhnyy, S. A. Mintairov, R. A. Salii, A. M. Nadtochiy, A. S. Payusov, P. N. Brunkov, *et al.*, "Increasing the quantum efficiency of InAs/GaAs QD arrays for solar cells grown by MOVPE without using strain-balance technology," *Progress in Photovoltaics: Research and Applications,* vol. 24, pp. 1261-1271, 2016.

[2] A. D. Utrilla, D. F. Reyes, J. M. Llorens, I. Artacho, T. Ben, D. González, *et al.*, "Thin GaAsSb capping layers for improved performance of InAs/GaAs quantum dot solar cells," *Solar Energy Materials and Solar Cells,* vol. 159, pp. 282-289, 2017.

[3] S. Hubbard, C. Cress, C. Bailey, R. Raffaelle, S. Bailey, and D. Wilt, "Effect of strain compensation on quantum dot enhanced GaAs solar cells," *Applied Physics Letters,* vol. 92, p. 123512, 2008.

[4] A. Luque, P. G. Linares, E. Antolín, E. Cánovas, C. D. Farmer, C. R. Stanley, *et al.*, "Multiple levels in intermediate band solar cells," *Applied Physics Letters,* vol. 96, p. 013501, 2010.

[5] P. Persson and G. Strang, "A Simple Mesh Generator in MATLAB," *SIAM Review,* vol. 46, pp. 329-345, 2004/01/01 2004.

[6] S. S. Rao, *The Finite Element Method in Engineering*: Elsevier Butterworth Heinemann, 2005.

[7] S. A. Mann, S. Z. Oener, A. Cavalli, J. E. M. Haverkort, E. P. A. M. Bakkers, and E. C. Garnett, "Quantifying losses and thermodynamic limits in nanophotonic solar cells," *Nat Nano,* vol. 11, pp. 1071-1075, 12//print 2016.

[8] L. C. Hirst and N. J. Ekins‐Daukes, "Fundamental losses in solar cells," *Progress in Photovoltaics: Research and Applications,* vol. 19, pp. 286-293, 2011.