Thermionic Current Losses due to Quantum Trapping in III-V Superlattice Solar Cells

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Abstract: - Thermionically escaping electrons comprise traveling quantum mechanical waves liable to trapping and backscattering due to nearest neighbor quantum wells in a multi-layer photovoltaic device. Such losses due to scattering and trapping are taken into consideration in this communication, where transmitted waves are calculated after scattering and trapping take place. In such lossy multiquantum well "lines", computations show that thermionic-carrier current density values may drop by a factor close to 66 % due to overall scattering (i.e. trapping and backscattering combined) namely, for 6nm width (GaAs-AlGaAs) undoped quantum well at room temperature, current densities are expected to drop from 0.4 mA/cm^2 (with recombination losses but with no scattering) down to a range of 0.136 mA/cm^2 (with both recombination losses and overall scattering).

Keywords: Transport, quantum well, thermionic currents, photovoltaic nanostructures, quantum PV

1. Introduction

Photo-generation in multiple quantum well nanostructures is heavily burdened by two groups of loss mechanisms: recombination losses and overall carrier scattering. These processes are expected to seriously affect the transport properties of photovoltaic nanostructures, especially in designs that include multi-layers in the intrinsic regions of p-i-n geometries. In this communication, interest is focused in Photogenerated carriers that have already escaped from quantum wells, by *thermionic emission*, and which are affected by quantum size effects. In other words, thermally escaping excess electrons, once in the energy continuum above the edge of the quantum well, are expected to be drifting along the growth direction along with trapping and reflection due to nearest-neighboring quantum wells. For a single quantum well, trapping, reflection and transmission are evaluated from first principles, and transmission results are applied to thermal current densities.

2. Theory

Two types of quantum well design adoption are generally of interest: (a) quantum wells are far from each other (wide gap material or AlGaAs layers are much wider compared to narrow gap layer widths) ensuring zero tunneling current contribution and (b) thin AlGaAs layers that succeed in forming tunneling currents. In either case, photo-excited carriers may find themselves in the quantum wells, where they face two options: either recombine or contribute to current. Depending on the geometry design mentioned above, these carriers might either escape thermionically to the continuum of the conduction band or tunnel through thin potential barriers to be collected at the end of the device. In absence of any type of tunneling, thermionic carriers can be found analytically or numerically, by calculating non-negligible current densities (*mA/cm^2/per quantum well*), by considering low n-doping (hence excluding impurity scattering) of the

GaAs layers. Thus, a favorable device design could be that of a *p/i (mqw)/n* solar cell. The device structure in mind is a p/i/n GaAs-AlGaAs solar cell with the intrinsic region comprised of a sequence of quantum wells and potential barriers made out of low and wide gap GaAs and AlGaAs layers respectively. Miniband solutions exist in these finite quantum wells, so that they may serve as traps of photo-generated carriers arising from the valence band after optical excitation. Illumination causes direct generation of electron-hole pairs (EHP's), thus contributing to carrier-concentration in each well. Such population increases in the quantum wells are likely to escape from the wells into the conduction band continuum leading to prospective collected currents. Excess carriers δn (in cm^{-3}) and related thermal current densities per quantum well, during illumination, have been calculated elsewhere [1] showing direct correlation between incident photon flux and escaping electrons. In the process, Auger and radiation recombination mechanisms are taken into account [2, 3, and 4]. Diffusing photo-carriers are found, by solving the diffusion equation (analytically or numerically) in one dimension (along x). Main parameters of the diffusion process are the diffusion capability of the carriers, their diffusion length and of course the interplay between generated and recombined carriers, as expressed by means of generation and recombination rates in the two loss-processes named above.

$$G(\lambda) = (2\pi)^4 c \int_\lambda \frac{d\lambda}{\lambda^4 (e^{hc/\lambda k T_S} - 1)} \qquad (1)$$

Modeling of carriers traveling in the vicinity of a quantum well includes an incident electronic plane wave of strength 100%, which is expected to be affected by the potential "disturbance" in the carrier's immediate vicinity. This may be represented by a back-traveling plane wave b, while as expected, transmission and trapping are represented by standing waves (inside the quantum well) and by traveling plane waves of strength c, as shown below, for a quantum well of width a:

$$\Psi(x) = \begin{cases} e^{ikx} + be^{-ikx}; x < 0 \\ ge^{iqx} + fe^{-iqx}; 0 \le x \le a \\ ce^{ikx}; x > a \end{cases} \qquad (2)$$

With k (m^{-1}), q (m^{-1}):

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad q = \sqrt{\frac{2m(E+U)}{\hbar^2}} \qquad (3)$$

Where E is the energy of the particle, and U is the depth of the quantum well. Continuity at interface x=0 and x = a dictates:

$$\begin{bmatrix} b \\ g \\ f \\ c \end{bmatrix} = \begin{bmatrix} 1 & -1 & -1 & 0 \\ -k & -q & q & 0 \\ 0 & \lambda_q & \lambda_{-q} & -\lambda_k \\ 0 & q\lambda_q & -q\lambda_{-q} & -k\lambda_k \end{bmatrix} \begin{bmatrix} -1 \\ -k \\ 0 \\ 0 \end{bmatrix} \qquad (4)$$

In the matrix representation, four parameters (b, (g, f), c) are expressed in terms of quantum well geometry, through the elements of the 4x4 matrix. The physical meaning of the four basic parameters is the following: b-represents reflected wave and c essentially measures the intensity of the transported wave, once past the interfering quantum well. For an incident wave (coefficient equal to 100%), the matrix representation above includes: (a) trapping parameters (*g*, *f*) due to quantum well structures (b) the backscattering factor *b* and (c) the transmission factor *c*. Solving for the elements of the first matrix above, one finds the following: for backscattering, the following complex coefficient is found:

$$b = \frac{k^2 - q^2}{\Delta} \lambda_k (\lambda_{-q} - \lambda_q) \qquad (5)$$

Trapping is found to be described by the (g, f) complex coefficients:

$$g = \frac{2k(k+q)}{\Delta}\lambda_k \lambda_{-q} \qquad (6)$$

$$f = \frac{2k(q-k)}{\Delta}\lambda_k \lambda_q$$
(10)

Finally transmission is to be found from:

$$c = \frac{4kq}{\Delta} \qquad (7)$$

Where the complex denominator is:

$$\Delta = (k+q)^2 \lambda_k \lambda_{-q} + \lambda_k \lambda_q [(k-q)^2 - 2q^2] \qquad (8)$$

With
$$\begin{Bmatrix} \lambda_k = e^{ika} \\ \lambda_{-k} = e^{-ika} \\ \lambda_q = e^{iqa} \\ \lambda_{-q} = e^{-iqa} \end{Bmatrix} \qquad (9)$$

By Letting δ_1 = Re (Δ), δ_2 = Re (Δ):

The transmission coefficient is:

$$c = \frac{4\,kq}{\delta_1 + i\delta_2} \qquad (10)$$

With

$$|\Delta|^2 = \delta_1^2 + \delta_2^2 = (k+q)^4 + [(k-q)^2 - 2q^2]^2 \cos(2qa)$$
(11)

Hence:

$$|c|^2 = \frac{16(kq)^2}{(k+q)^4[1 + B(q,k,a)]} \qquad (12)$$

Where

$$B(q,k,a) = \begin{bmatrix} (\frac{k-q}{k+q})^2 - \\ 2(\frac{q}{k+q})^2 \end{bmatrix}^2 \cos(2qa) \qquad (13)$$

3. Computations and results

Parameters and geometry used for computation of $|c|^2$ values have been selected as follows: (a) 4 to 6.5 nm quantum wells are considered (b) for such geometry, k and q values are of the order of 0.187 nm^{-1} and 0.533 nm^{-1} respectively (c) the unit-less B (q, k, a) factor as in (13) above, is found to be of the order of 0.74. Thus, $|c|^2$ is found to be of the order of 33.9%, indicating about 34% transmission of the initial wave. This means that 66% of the initial uninhibited thermal currents are lost due to the existence of a single quantum well alone. At 30^{o}C, with doping levels as low as 10^{10}-10^{11} cm^{-3} (intrinsic medium in the intrinsic region of a superlattice solar cell), and with excess carrier concentration at levels of the order of 10^{15} cm^{-2}, quantum wells of 6 nm yield (without quantum well overall scattering) thermal current densities near 0.4 mA/cm^2, while actual contribution drops down to 0.136 mA/cm^2. At -10^{0}C (0.3 mA/cm^2 uninhibited) final contribution becomes 0.102 mA/cm^2.

4 Thermionic currents

The above brief analysis dealt with trapped carriers in individual quantum wells, in other wise superlattice grown solar cells. As is the case for such structures [4], carriers are generated in quantum wells, when illuminated via solar photons. Photo-generation increases the concentration of quantum mechanically trapped electrons in the wells, where they are liable to either thermal escape and/or recombination [see 6, 7, 9]. In quantum photovoltaics (quantum PV from now on), quantum wells are in essence quantum traps that eventually offer advantages to devices like solar cells. On one hand, excess carriers get photogenerated (in addition to those of the host layer), and on the other the optical window widens energy wise: two or more media involved in the device offer the possibility of higher solar photon absorption, because of wide gap media involved. The latter becomes the major advantage of multilayered devices, where excess current due to excess carriers are developed. Summarizing, in this section we are presenting a connection between thermal currents (out of the wells) and trapped carriers. Thermionic currents are evaluated via a general form as follows:

$$j = qL\iint dxdEg(E)\,f(E)\delta n(x)v(E) \quad (14)$$

Where the integration involves quantum well special extent x, excess carriers in quantum wells, density of states (DOS) g in the quantum well, and the carrier velocity v as a function of the carrier energy in the quantum well, and where by L we mean the periodicity of extent of an individual quantum well. The factor δn(x) represents net carrier concentration in a quantum well, after recombination losses. Note that dominant recombination loss for quantum wells of thickness near 5-6 nm is the cumulative Auger effect, as dominating over bulk, radiative and or phonon recombination [8, 12, 14, and 15]. Under this in mind, we can re-write [19, 11]:

$$j = \frac{qm^{*}L}{\pi\hbar^{2}}\iint dxdEf(E)n_{ph}(x)v(E) \quad (15)$$

In (15), m* is the carrier's effective mass, the term $n_{ph}(x)$ is the total photo-generation in a quantum well as found after major carrier losses have been taken into account. This term is explicitly found to be [17]:

$$n_{ph} = n(x)\left(\frac{\alpha\Phi_{ph}}{C}\right)^{1/3} + n_{o}(x) \quad (16)$$

Where n(x) is some function of x (no units), $n_o(x)$ is the dark carrier concentration (when illumination is terminated), α is the absorption coefficient of the medium involved, F is the solar photon flux and C is the cumulative Auger effect in a quantum well. Note that in (16) the energy variation is considered from the lowest energy eigen-value in the quantum well to (essentially) infinity. In Fig. 1 below, the geometry of the device is depicted: (a) two quantum wells are shown with one eigen-energy in each (b) the distance between conduction and valence band of 1 eV represents the optical gap introduced by the structure and ensures infrared absorption in 1.24 μm (c) the medium (narrow gap) is taken to be Ge (germanium) (d) wide gap medium is shown to be GaAs (gallium arsenide, 1.42 eV band gap) (e) shown are thermionic currents J_1 and J_2, indicating that only 34% of thermal escape currents survive due to nearest neighboring scattering.

5 Conclusions

Modern solar cells are fundamentally different from their bulk counterparts, in that they exploit quantum size effects, due to their small size. Quantum phenomena in these devices appear as photo-generated carriers in discrete energy quantum levels in quantum wells, where losses and thermal escape are two competing factors. In this communication we present, for the first time, a connection between useful net thermionic currents and current losses due to quantum trapping. Direct calculation, of net photocarriers and subsequent thermionic currents out of single quantum wells, embedded in the intrinsic region of p/i/n GaAs-AlGaAs solar cells, is possible. Computations have shown that 6nm GaAs layers interfaced with thick AlGaAs layers in the intrinsic region are expected to contribute current densities close to 0.14mA/cm^2, and at illumination levels of 10^{17} incident photons per unit area. Also, 2.7mA/cm^2 (per quantum well) current density is predicted at 30^{o}C (for 10nm well width and 10^{12} cm^{-3} GaAs doping. Although doping in the intrinsic region is kept at low levels (so that impurity scattering is minimized), it is not clear (as yet) if multiplicity of quantum wells in the illuminated intrinsic region of *p/n(mqw)/n* solar cells, will improve overall collected current densities. As it has been shown, quantum size effects are serious inhibiting factors in final current collection: escaping carriers are highly likely to be scattered in two ways: by reflection and by trapping. Reflection and trapping due to a nearest quantum well is inevitable for incident electrons. In this communication, 66% overall losses of current is reported, losses which are directly correlated to the quantum nature of the nano-structures themselves.

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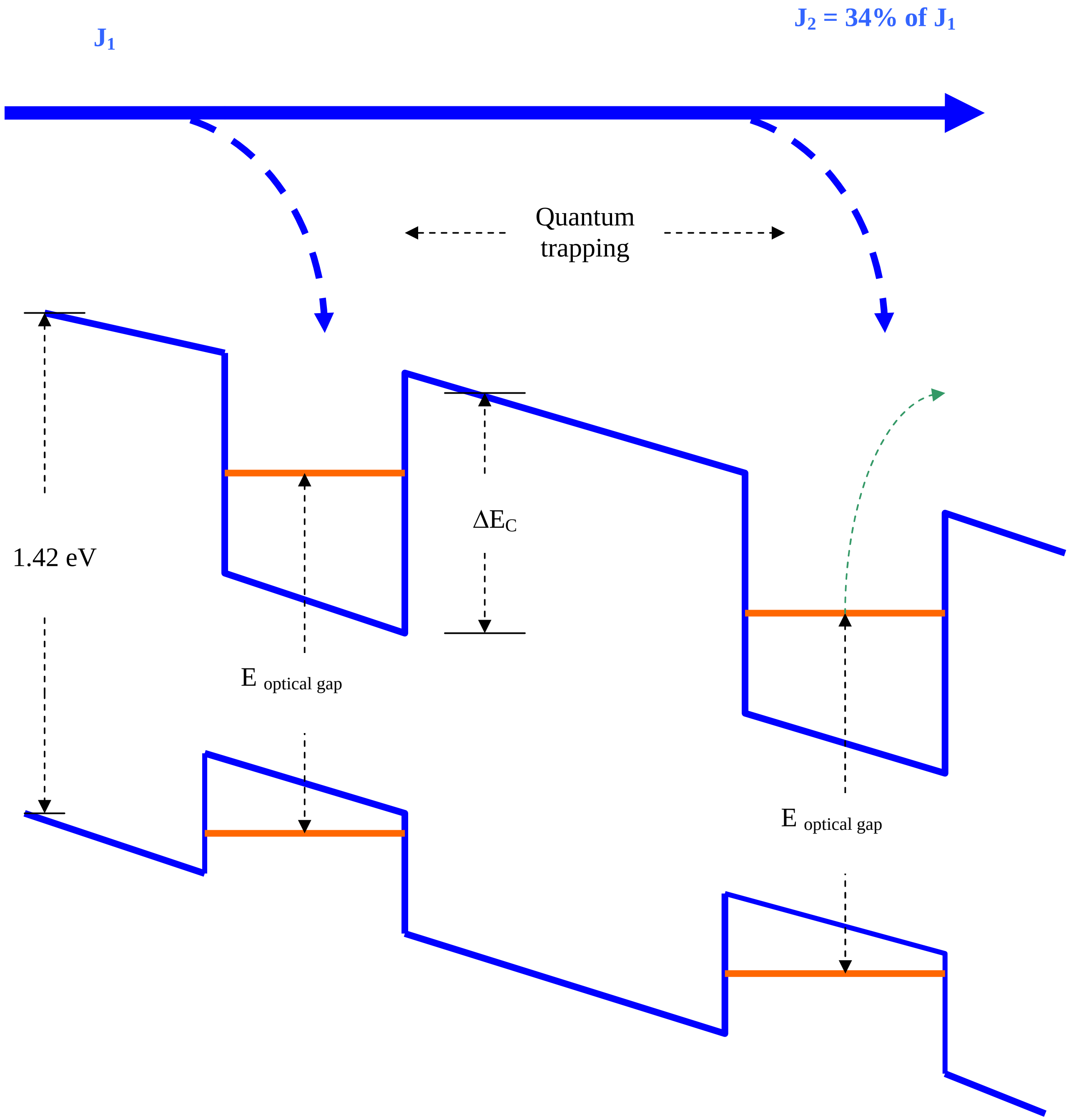

Figure 1: A portion of the mid-region: escaping carriers from quantum wells: Shown are (a) Optical gap E_{opt} (b) Wide gap host (GaAs) and (c) Eigen-energies in the quantum wells. Width selection allows for single solution in the quantum wells.