# Losses due to Quantum Size Effects in Thermionic Currents in III-V MQW Solar Cells

ARGYRIOS C. VARONIDES & ROBERT A. SPALLETTA
Department of Physics and Electrical Engineering, University of Scranton,
A Jesuit University, Scranton, PA 18510, USA

*Abstract:* - Quantum wells in solar cells are important probes for the study of free carrier behavior. Photo-generated carriers in quantum wells contribute to transport and hence current only via thermionic escape, and once they are in the conduction band continuum, they can be treated as propagated plane waves subject to constraints of the crystal lattice. It is pointed out that neighboring quantum wells act as scattering centers causing back-scattering and trapping (standing waves). On the other hand, 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 only 16 to 25% of thermionically escaping carriers get through, and the rest remain trapped in quantum wells and/or reflect back to neighboring unit cells. For 6nm-width (GaAs-AlGaAs) un-doped quantum wells, illuminated at room temperature, current densities are expected to drop from 0.4 mA/cm$^2$/qu. well (with recombination losses but with no scattering) down to a range between 0.064 to 0.100 mA/cm$^2$/qu. well (with both recombination losses and overall scattering included in this study).

*Key-Words*: Transport, quantum well, thermionic currents, photovoltaic nanostructures

## 1 Introduction

Multiple layer solar cells are well known for their immediate advantages over their bulk counterparts. Devices that convert light into electricity are of paramount importance, and ways to increase conversion efficacy gains naturally become the epicenter of intense research. Multilayered solar cells have proven themselves as the primary devices for current and (efficiency enhancement) for quite some time now. They are based on the following design: a bulk p-n junction is extended into a p-i-n structure where the mid region is an un-doped long layer of AlGaAs (host material). The p- and n- regions are intentionally thin to suppress relaxation of carriers (minimize losses). The intrinsic region is then grown via a succession of wide and narrow gap layers. This means that layers of the host material are interfaced with layers of a narrow gap material (GaAs). The result is an energy landscape with two conduction bands comprising quantum wells the height of which is the exact difference of the conduction bands.

In addition to being probes where quantum size effects affect the transport of generated carriers, multilayered solar cells offer advantages over traditional silicon bulk counterparts. The mere existence of quantum size effects offers excess carriers in more places than ones provided by bulk counterparts. Advantages of multilayered structures are (a) wider optical gap values that go beyond the band gap values of the host material, and hence gains in shorter wavelength absorption (b) effective mass separation (between electrons and holes) and hence reduction of losses due to recombination (c) p-i-n design adaptation, where long depletion region is provided via the intrinsic region: free carriers in the intrinsic region accelerate due to electrostatic fields and collection efficiencies increase (d) quantum wells act as carrier traps under dark and illumination. The issue of what happens to free carriers once in the conduction band is the main theme (although nowhere in this communication it is to be claimed that the problem of carrier transport is to be solved completely, rather a proposal for future more comprehensive approach is rather made) in this communication. Hetero-PV (hetero-epitaxial photovoltaic devices) structures provide electricity once they are under illumination with white light (solar photons). The currents collected may become minimal or substantial depending on a number of factors, such as loss mechanisms due to impurities or phonon scattering in the crystal structure or loss at layers interfaces. For hetero-PV devices, thermionic escape from the quantum wells becomes of vital importance, when illumination occurs. Photo-generation in multiple quantum well nanostructures [1, 2, 3] 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 on photo-generated carriers that have already escaped from quantum wells, by thermionic emission [4, 5] 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 with appreciable trapping and reflection probabilities due to nearest-neighboring quantum wells. For a single quantum well, the transmission probability is evaluated from first principles, and 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 when compared to narrow gap layer widths) ensuring zero tunneling current contribution and (b) thin-barrier 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 derived analytically or computed numerically, by calculating non-negligible current densities (*mA/cm$^2$/per quantum well*), by considering low or no doping at all (hence excluding impurity scattering in the otherwise un-doped intrinsic region of a p-i-n structure) of the GaAs layers. The device structure considered here 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 photogenerated carriers arising from the valence band after optical excitation. Illumination causes direct generation of electron-hole pairs (EHP's), thus contributing to carrier-concentration increases in each well. Such excess carriers are likely to escape from the wells into the conduction band continuum leading to prospective collected currents. Excess carriers $\delta n$ (in cm$^{-3}$) and related thermal current densities per quantum well, during illumination, have been calculated elsewhere [6] showing direct correlation between incident photon flux and escaping electrons. In the process, only Auger and radiation recombination mechanisms are taken into account, since direct-gap materials do not show any other dominating recombination mechanisms [7, 8, 9]. Diffusion of photo-carriers may be dealt with 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. The diffusion equation reads as follows:

$$\delta n''(x) - \frac{\delta n(x)}{L_n^2} + G(\lambda)\frac{[\alpha(\lambda)(1-R)]/L_n^{\;2}}{b\delta n(x) + c\delta n^2(x)} e^{-\alpha(\lambda)x} = 0 \qquad (1)$$

Where δn(x) is the net excess carrier concentration in a quantum well, $L_n$ is the photo-carrier diffusion length, b, c are the radiation and Auger capture coefficients, G is the flux rate (cm$^{-2}$ s$^{-1}$) [10]:

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

$\alpha(\lambda)$ is the absorption coefficient, *R* is the reflectivity of the device, and x represents distance along the growth direction [11, 12, 13, 14, and 15]. Thermally escaping carriers can be *seen* as plane waves traveling in the conduction band. This means that analysis of carrier transport may be based on plane waves traveling in the crystal. Thus, modeling of carriers traveling, near a quantum well, includes an incident electronic plane wave of strength 100%, which affects the potential "disturbance" in the carrier's immediate vicinity. This may be represented by a back-traveling "reflected" plane wave r, while as expected, transmission and trapping are represented by *standing* waves [(g, f) inside the quantum well] and by transmitted plane waves represent via a transmission coefficient t, as shown below, for a quantum well of width L. The corresponding wave function for a case of electrons approaching a quantum well (of width *L*) from the left is usually expressed as follows:

$$\begin{aligned}&\Psi_{left}(x) = e^{ikx} + re^{-ikx}; \quad \text{for } x<0\\ &\Psi_{in}(x) = ge^{iqx} + fe^{-iqx}; \quad \text{for } 0<x<L\\ &\Psi_{right}(x) = te^{ikx}; \text{ for } x>L\end{aligned} \tag{3}$$

With, *k*($m^{-1}$), *q*($m^{-1}$) the energy mini-band-dependent wave numbers for the three regions involved, namely, region to the left of a quantum well at the *x=0* interface, middle region from *0 to L*, and region to the right of a quantum well at the interface *x=L*.

Continuity of the wavefunction and its first derivative at the three interfaces, leads to the following system of four unknowns:

$$\begin{bmatrix} r\\ g\\ f\\ t\end{bmatrix}\begin{pmatrix} 1 & -1 & -1 & 0\\ -k & -q & q & 0\\ 0 & e^{iqx} & e^{-iqx} & -e^{ikx}\\ 0 & qe^{iqx} & -qe^{-iqx} & -ke^{ikx}\end{pmatrix} = \begin{bmatrix} -1\\ -k\\ 0\\ 0\end{bmatrix} \tag{4}$$

In this matrix representation, the four parameters [r, (g, f), t] depend on quantum well geometry and can be directly solved. The physical meaning of the four basic parameters is the following: *r* represents reflected wave and *t* essentially measures the intensity of the transported wave, once electron waves are past the *interfering* quantum well. For an incident wave (strength coefficient equal to one or *100%*), the matrix representation above includes: (a) *trapping* parameters (*g, f*) due to quantum well structures (b) the backscattered or reflected field *r* and (c) the transmission factor *t.*

Solving for the transmission probability leads to the following expression:

$$|t|^2 = \frac{1}{1 + 2\cos^2(qL) + \frac{1}{2}\left(\frac{k}{q} + \frac{q}{k}\right)^2} \tag{5}$$

As seen from (5), the transmission probability oscillates from a minimum to a maximum value

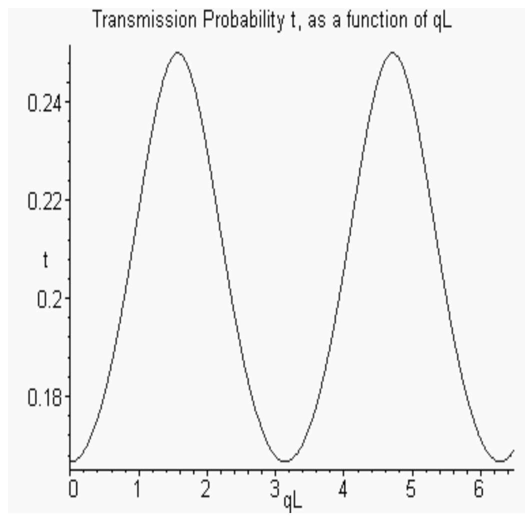


Fig.2. Oscillations of the transmission probability, as a function of the qL product. Maximum values do not exceed 25% and minimum values are above 16%.

along with the *qL* factor. It is to be noted though that the energy of the excess carriers depends on the width of each quantum well, and thus the *k* and *q* factors also depend on the width. Variations of the *qL* product do cause oscillations of the transmission probability but at the cost of changing the wave-numbers as well. For quantum wells of the order of 5 to 6 nm, the third factor in the denominator of (5) is of the order of 2.5 with tiny variations around this value, so that it is safe to seek a plot of transmission probabilities as a function of the *qL* product, as in Fig. 2.

## 3 Computations and results

Parameters and geometry used for computation of $|t|^2$ values are selected as follows: (a) 5 to 6 nm quantum wells (b) for such geometry, k and q values are of the order of 0.187 $nm^{-1}$ and 0.533 $nm^{-1}$ respectively, corresponding to energy minibands near 20meV/quantum well. The carrier mass is taken to be as the equivalent of 0.067 of the electronic rest mass, the band offset at 0.300 meV, for a 30% Al alloy heterostructure. Thus, the transmission $|t|^2$ fluctuates between 16 and 25% respectively, meaning that 75% to 84% of the initial uninhibited thermal current is to be lost due to the existence of a neighboring quantum well. At 30°C, with virtually no doping, and with excess carrier concentration at levels of the order of $10^{12}$ $cm^{-2}$, quantum wells of 6 nm reduce thermal current densities from 0.4 $mA/cm^2$ to less than 0.100 $mA/cm^2$ per quantum well. At $-10^0$C (0.3 $mA/cm^2$ uninhibited) final contributions become less than 0.075 $mA/cm^2$.

# 4 Conclusion

Photo-generation of electrons in solar cells is responsible for useful current collection. Multilayered solar cells offer grounds for quantum size effects. In this context, plane wave models can be used for the behavior of carriers in quantum well structures. Direct calculation, of net photocarriers and subsequent thermionic currents out of single quantum wells, which are 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 near 0.100 $mA/cm^2$, and at illumination levels of $10^{17}$ incident photons per unit area. 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. Quantum size effects are seriously inhibiting current production: escaping carriers are likely to be scattered in two ways: by reflection and by trapping.

# 5 References


[1] AC Varonides, Physica E 14 (2002), 142.

[2] M. Takeshima, J. Appl. Phys. Lett. 29 (1985) 3846.

[3] Y. Tian, et al., IEEE Trans. Electron Dev. 46 (4) (1999) 656.

[4] D.K. Schroeder, in: Semiconductor Materials and Characterization, Wiley, New York, 1992.

[5] A.S. Brown et al., Physica E 14 (2002), 121.

[6] K.W.J. Barnham et al., Physica E 14 (2002), 27.

[7] K. Hess, Advanced Theory of Semiconductors, IEEE Press, New York, 1998.

[8] P.K. Pathria, Statistical Mechanics, Pergamon Press, Oxford, 1978.

[9] S.M. Sze, Physics of Semiconductors, John Wiley and Sons, New York 1981.

[10] M.I. Dyakonof, V.Y. Kachorovski, Phys. Rev. B 49 (1994) 17130.

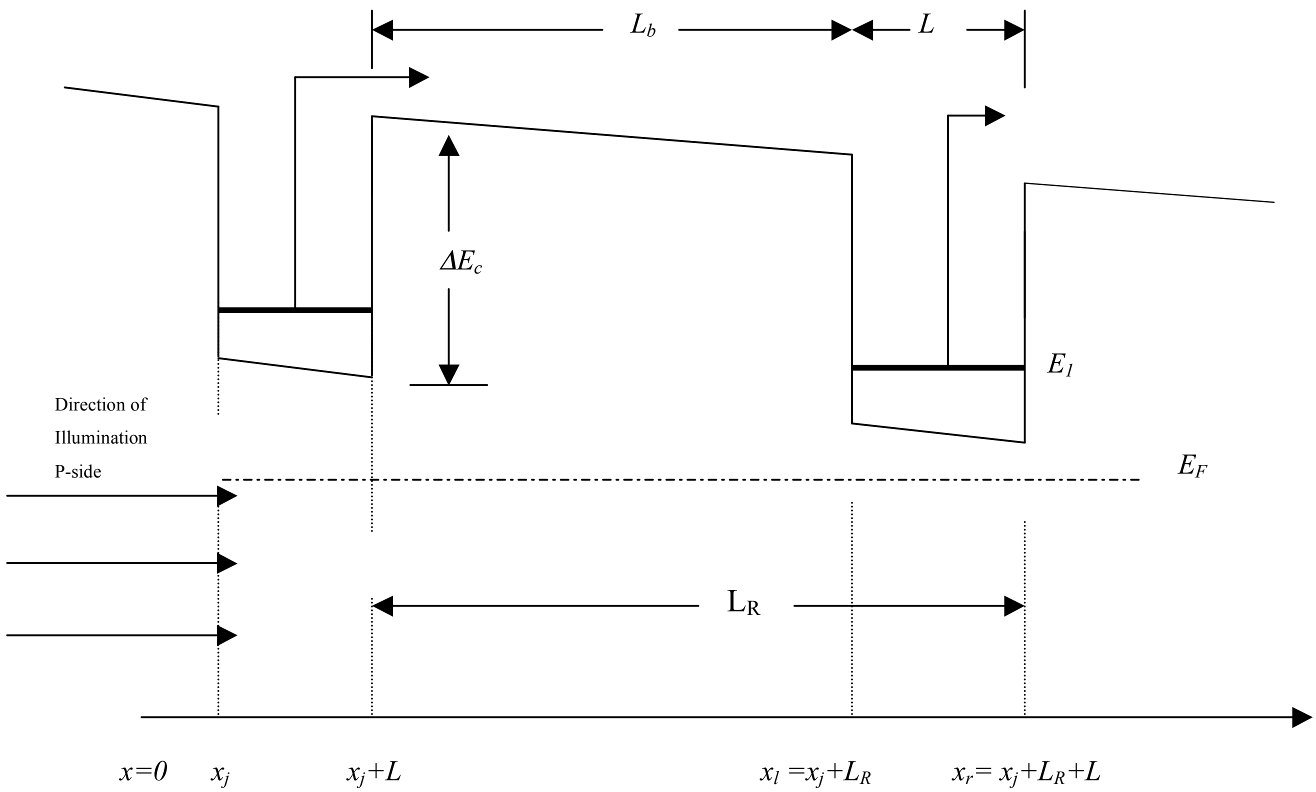


Fig.1. Geometry or energy-band diagram adopted for the p-i-n structure: (a) pre-selected qw's widths ensure only one energy miniband in the undoped qw's (b) $\Delta E_c$ is the band gap discontinuity and the repeat distance is $L_R=L+L_b$ (c) arrows from the qw's indicate electrons thermionically escaping from $E_1$ to the continuum of the conduction band (d) the Fermi level $E_F$ is shown against the bands (e) illumination is assumed from the p-side of the device (far left).