Formulation of a Self-Consistent Model for Quantum Well *pin* Solar Cells

S. Ramey and R. Khoie
Department of Electrical and Computer Engineering
University of Nevada, Las Vegas
Las Vegas, NV 89154
ark@ee.unlv.edu, sramey@ee.unlv.edu

ABSTRACT

A self-consistent numerical simulation model for a *pin* single-cell solar cell is formulated. The solar cell device consists of a $p-AlGaAs$ region, an intrinsic $i-AlGaAs/GaAs$ region with several quantum wells, and a $n-AlGaAs$ region. Our simulator solves a field-dependent Schrödinger equation self-consistently with Poisson and Drift-Diffusion equations. The emphasis is given to the study of the capture of electrons by the quantum wells, the escape of electrons from the quantum wells, and the absorption and recombination within the quantum wells. We believe this would be the first such comprehensive model ever reported.

The field-dependent Schrödinger equation is solved using the transfer matrix method. The eigenfunctions and eigenenergies obtained are used to calculate the escape rate of electrons from the quantum wells, and the non-radiative recombination rates of electrons at the boundaries of the quantum wells. These rates together with the capture rates of electrons by the quantum wells are then used in a self-consistent numerical Poisson-Drift-Diffusion solver. The resulting field profiles are then used in the field-dependent Schrödinger solver, and the iteration process is repeated until convergence is reached.

In a $p-AlGaAs$ $i-AlGaAs/GaAs$ $n-AlGaAs$ cell with aluminum mole fraction of 0.3, with one 100 $A°$-wide 284 meV-deep quantum well, the eigenenergies with zero field are 36meV, 136meV, and 267meV, for the first, second and third subbands, respectively. With an electric field of 50 kV/cm, the eigenenergies are shifted to 58meV, 160meV, and 282meV, respectively. With these eigenenergies, the thermionic escape time of electrons from the $GaAs$ Γ-valley, varies from 220 pS to 90 pS for electric fields ranging from 10 to 50 kV/cm. These preliminary results are in good agreement with those reported by other researchers.

I. INTRODUCTION

The conversion efficiency of a single cell *pin* solar cell can be enhanced by

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incorporating one or more quantum wells in the intrinsic region of the device.(1) The incorporation of the quantum wells has two counteracting effects: the short-circuit current is increased because of the additional absorption of the low-energy photons in the lower bandgap quantum well; and the open-circuit voltage is decreased because of the increase in the recombination of the photoexcited carriers trapped in the quantum well. Experimental results have shown, nevertheless, that the additional photocurrent resulting from the extension of the absorption spectrum to lower energies can outweigh the accompanying drop in the open-circuit voltage, and devices with quantum wells incorporated in the i-region are indeed more efficient than the corresponding base-line bulk cell (2)-(3). The improvement in conversion efficiency is dependent on, among other parameters, the width of the quantum wells. Ragay el. al., (4) reported that both the open-circuit voltage and short circuit current increase with increasing well width.

Along with these experimental studies, a number of theoretical investigations have been performed. Corkish and Green (5) studied the effects of recombination of carriers in the quantum well and concluded that although the increased recombination reduces the open-circuit voltage, but limited enhancement in the conversion efficiency can be obtained with incorporation of the quantum well, albeit not as much as previously reported by Barnham and Duggan (1). Spectral response modeling of Paxman, et. al., (6) with emphasis on the absorption in the quantum wells showed good agreement with thier experimental results. Araujo, et. al. (7) used detailed balance theory and predicted that the conversion efficiency of the quantum well cell would not exceed that of the single cell base-line device. The results of photoresponse calculations by Renaud el., al., (8) revealed that introducing the quantum wells in the intrinsic region can lead to improved photocurrent without much degradation of the open-circuit voltage. Most recently, Anderson (9) presented an ideal model for the quantum well solar cell device, incorporating the recombination and generation in the quantum wells. Anderson concluded that under AM0 illumination the maximum conversion efficiency of the pin solar cell device increases from the base-line value of 27.5% to 29.8% with the well depth of 200 meV, but decreases to 27.3% when the quantum well is 400 meV deep.

The need for a comprehensive model is rather obvious, now that there seems to be an unsolved debate as to the ultimate advantage of incorporating quantum wells in the intrinsic region of a pin solar cell. In this paper we present formulation of one such model. In this model we have included the effects of several phenomena known to be of siginificant importance in the absorption of irradiation, and the transport of the photoexcited carriers. These phenomena include: 1) capture of electrons by the wells, 2) escape of electrons from the wells, 3) absorption of light in the wells, and 4) recombination of carriers in the wells. Our model is developed for a *pin* single-cell solar cell consisting of a $p - AlGaAs$ region, an intrinsic $i - AlGaAs/GaAs$ region with several quantum wells, and a $n - AlGaAs$ region. Our simulator solves a field-dependent Schrödinger equation self-consistently with Poisson and Drift-Diffusion equations. The field-dependent Schrödinger equation is solved using the transfer

matrix method.(10) The eigenfunctions and eigenenergies obtained are used to calculate the escape rate (11)-(12) of electrons from the quantum wells, and the non-radiative recombination rates of electrons at the boundaries of the quantum wells. These rates together with the capture rates (13)-(14) of electrons by the quantum wells are then used in a self-consistent numerical Poisson-Drift-Diffusion solver. The resulting field profiles are then used in the field-dependent Schrödinger solver, and the iteration process is repeated until convergence is reached.

II. SELF-CONSISTENT MODEL

A. The *pin* Solar Cell

The solar cell device consists of a $p-AlGaAs$ region, an intrinsic $i-AlGaAs/GaAs$ region with several quantum wells, and a $n-AlGaAs$ region. The energy band diagram of the device with four quantum wells in the intrinsic region is shown in Fig. (1). In our simulations we vary the following design parameters: the thickness of the regions, the doping levels of the n and p regions, the mole fraction of Al in $AlGaAs/GaAs$ quantum wells (the depth of the wells), the thickness of the quantum wells, and the number of quantum wells. The input parameters to our simulation programs include irradiation spectra, the transport parameters, band structure, and optical and absorption characteristics of the materials. The search for $i-v$ characteristics of the device begins with assigning an applied voltage and solving the system of differential equations for the terminal current densities. The simulation model also predicts the internal distributions of carriers densities, current densities, and electrostatic potentials. Several intermediate results will also be produced which includes the eigenenergies and eigenfunctions of electrons in the wells, capture and escape rates, and recombination lifetimes in the quantum wells.

B. Bulk Transport

The steady-state transport of electrons and holes in the *pin* structure are described by two current continuity equations written for the bulk regions as:

$$\frac{\partial n_b}{\partial t} = G - U + R_e^n - R_c^n + \frac{1}{q}\frac{dJ_n}{dx} = 0 \tag{1}$$

$$\frac{\partial p_b}{\partial t} = G - U + R_e^p - R_c^p - \frac{1}{q}\frac{dJ_p}{dx} = 0 \tag{2}$$

In these equations n_b and p_b are bulk electron, and hole densities, respectively, whereas J_n and J_p are electron, and hole current densities, respectively. The terms R_e^n and R_e^p are the rates of escape of electrons and holes from the bulk, and R_c^n and R_c^p are the capture rates of electrons and holes by the bulk. The escape and capture rates of carriers for the bulk system are indeed (assumed to be) identical to capture and escape rates of carriers for the quantum well

system. In other words, escape from the bulk is capture by the quantum wells, and capture by the bulk is escape from the quantum wells. That is why escape rates have positive contributions (as in generation) whereas capture rates have negative (as in recombination). These rates are related to the escape and capture times as: $R_e^n = \frac{n_w}{\tau_e^n}$, $R_e^p = \frac{p_w}{\tau_e^p}$, $R_c^n = \frac{n_w}{\tau_c^n}$, and $R_c^p = \frac{p_w}{\tau_c^p}$. where τ_e^n and τ_e^p are the electron and hole escape times, respectively, and τ_c^n and τ_c^p are electron and hole capture times, respectively. Details of the calculations of these escape and capture times are described in the following Section. The recombination in the bulk is assumed to be radiative recombination given by: $U = B(n_b p_b - n_{b0} p_{b0})$, where B is the radiative recombination constant. G is bulk generation rate and is given by: .

$$G = \int_0^{\lambda_c} \alpha(\lambda).N_{ph}.\left[exp(-\int_0^x \alpha(\lambda)dx)\right] d\lambda \tag{3}$$

where λ_c is set to correspond to the bandgap of the material.

The current density equations are written as:

$$J_n = qn_b\mu_n E + qD_n\frac{dn_b}{dx} \tag{4}$$

$$J_p = qp_b\mu_p E - qD_p\frac{dp_b}{dx} \tag{5}$$

Assuming low to moderate doping levels, and under 1 sun illumination we use the Einstein relationship for carrier mobilities and diffusion constants as given by: $D_{n,p} = \frac{kT}{q}\mu_{n,p}$. The above equations are solved together with Poisson equation:

$$\frac{dV^2}{dx^2} = \frac{q}{\epsilon}\left[N_A - N_D + n_b + n_w - p_b - p_w\right]. \tag{6}$$

The values of n_w and p_w are set to zero for the bulk systems. N_D and N_A are donors and acceptors doping levels.

C. Quantum Well Transport

Calculation of the absorption spectra in the quantum wells as well as the escape rate of carriers from the quantum well require the eigenfunctions and eigenenergies of the carriers in the quantum wells, which are obtained from a field-dependent Schrödinger equation given by:

$$\left[\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m^*(x)}\frac{d}{dx} + V(x)\right]\psi(x) = E_i\psi(x) \tag{7}$$

where $\psi(x)$ is the envelope function, E_i are the eigenenergies, and $V(x)$ is the potential profile. Non-constant effective mass $m^*(x)$ are assumed. The Schrödinger equation is solved using Transfer Matrix method (10) in which wave functions of the type:

$$\psi(x) = A_j e^{p_j(x-x_j)} + B_j e^{-p_j(x-x_j)} \tag{8}$$

are searched by finding constants A and B through matching the wave functions and their derivatives at the boundaries.

The current continuity equations for the quantum well system are written as rate equations in which net balance of four rates give rise to the current. These rate equations are given by:

$$\frac{dn_w}{dt} = \frac{n_b}{\tau_c^n} - \frac{n_w}{\tau_e^n} + G_w - U_w + \frac{1}{q}\frac{dJ_n}{dx} = 0 \tag{9}$$

$$\frac{dp_w}{dt} = \frac{p_b}{\tau_c^p} - \frac{p_w}{\tau_e^p} + G_w - U_w - \frac{1}{q}\frac{dJ_p}{dx} = 0 \tag{10}$$

In the above equations τ_c^n and τ_e^n are electron capture and escape rates, whereas τ_c^p and τ_e^p are hole capture and escape rates. The recombination term U_w is a modified Shockley-Read-Hall recombination rate given by :

$$U = \frac{\sigma_n \sigma_p v_{th} N_t [pn - p_0 n_0]}{\sigma_n [n + n_t] + \sigma_p [p + p_t]} \tag{11}$$

where the capture cross sections, σ_n and σ_p are modified based on $\psi_i(x)$ for the first three subbands in the quantum wells.(15)-(16) The generation term G_w is calculated from Equation (3) with the bulk absorption coefficient replaced with that of the quantum well. The absorption coefficients of the quantum wells are calculated by a model presented by Stevens, et. al.(17):

$$\alpha(\hbar\omega, \varepsilon) = M_{cv}^2(\varepsilon).q_{exciton}.L(\hbar\omega, E_{cv}^{1,1} - E_b) \tag{12}$$
$$+ \int_{E_{cv}^{1,1}}^{\infty} M_{cv}^2(\varepsilon).N q_{con} K(E', E_{cv}^{1,1}) L(\hbar\omega, E') dE'$$

where E_b is exciton binding energy, $q_{exciton}$ and q_{con} are exciton and continuum oscillator strengths, respectively and $E_{cv}^{1,1}$ is the $n = 1$ transition energy. The term $M_{cv}^2(\varepsilon)$ is the electron-hole wavefunction overlap integral and is calculated from the wavefunctions obtained from the Schrödinger solver. For more details of the quantum well absorption model, see Stevens, et. al.(17)

The escape rates of carriers are calculated using the model reported by Moss, et. al. (11):

$$\frac{1}{\tau_e} = \frac{1}{\bar{N}d}\sqrt{\frac{kT}{2\pi m_\Gamma^*}}\left\{1 + \alpha_L exp\left[(\Delta E_b^L)u(-\Delta E_b^L)/kT\right]\right\} exp(-\Delta E_b/kT) \tag{13}$$

where $u(x)$ is the Heaviside step function, L and Γ refer to specific valley, and d is the well width. For more details on Eq. (13) see Moss, et. al. (11) Capture rates are extrapolated from theoretical data reported by Blom, et. al. (14).

III. PRELIMINARY RESULTS

The system of equations described in Section II are solved using a finite difference numerical scheme. For a $p-AlGaAs$ $i-AlGaAs/GaAs$ $n-AlGaAs$ cell with aluminum mole fraction of 0.3, with one 100 $A°$-wide 284 meV-deep quantum well, the eigenenergies with zero field are 36meV, 136meV, and 267meV, for the first, second and third subbands, respectively. The corresponding wavefunctions are shown in Fig. 2. With an electric field of 50 kV/cm, the eigenenergies are shifted to 58meV, 160meV, and 282meV, respectively, and the amplitudes of the eigenfunctions are amplified as illustrated in Fig. 3. Using these eigenenergies, the thermionic escape time of electrons from the $GaAs$ Γ-valley, as a function of electric field, is calculated and plotted in Fig. 4. The capture rates of electrons, extraplolated from the data reported by Blom, et. al.(14), are reproduced in Fig. (5) as a function of energy difference $(E_c - E_i)$. The varaiations of $(E_c - E_i)$ with well width are shown in Fig (6).

We are reporting the development of a self-consistent Poisson-Schrödinger Drift-Diffusion solver for a *pin* quantum well solar cell. The effects of escape and capture of electrons and holes in the quantum wells are being studied. The degradation of open-circuit voltage due to increased recombination is being investigated by studying the recombination of carriers in quantum wells. Simulations are being performed to generate the $i - v$ characteristics of the cells under illumination.

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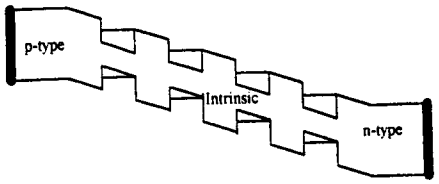

Figure 1: Energy band diagram of the solar cell with four quantum wells.

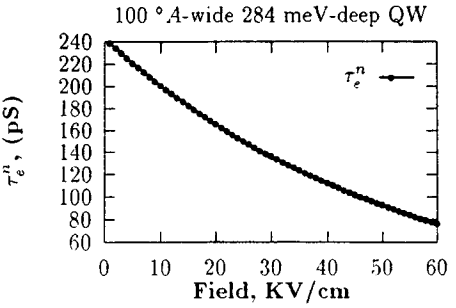

Figure 4: The thermionic escape time of electrons from the $GaAs$ Γ-valley to $AlGaAs$ Γ-valley as a function of electric field.

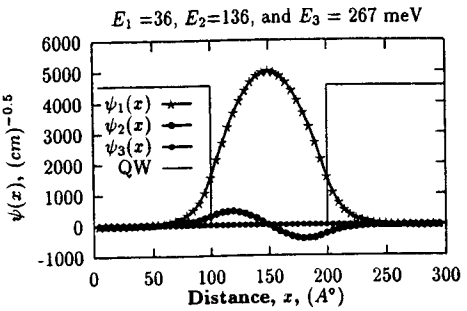

Figure 2: Eigenfunctions of a 100 $A°$-wide 284 meV-deep quantum well with no field.

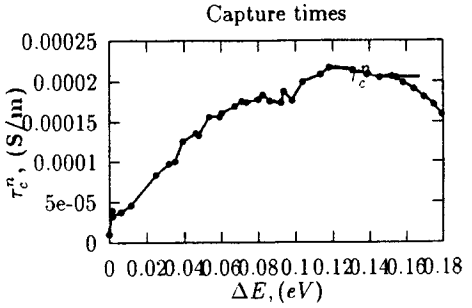

Figure 5: The capture time of electrons by the quantum well as a function of $E_c - E_i$.

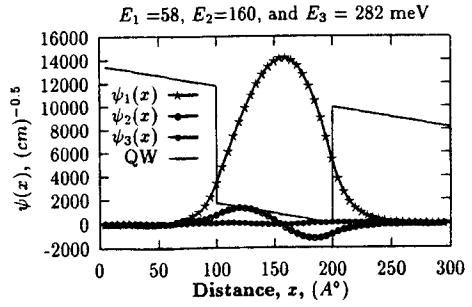

Figure 3: Eigenfunctions of a 100 $A°$-wide 284 meV-deep quantum well with 50 KV/cm field.

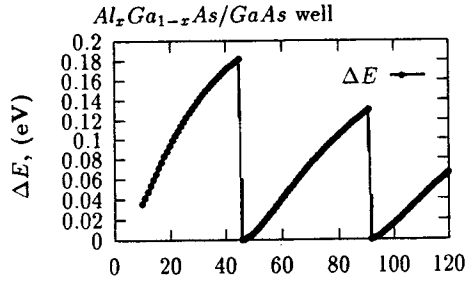

Figure 6: The energy difference $E_c - E_i$ as a function of well width.