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

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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 field-dependent Schrödinger equation is solved using the transfer matrix method. The eigenfunctions and eigenenergies obtained are used to calculate the escape rate of carriers from the quantum wells, the capture rates of carriers by the wells, the absorption spectra in the wells, and the non-radiative recombination rates of carriers in the quantum wells. These rates are then used in a self-consistent finite-difference numerical Poisson-drift-diffusion solver. We believe this is the first such comprehensive model ever reported.

Keywords: Quantum well, solar cell, Schrödinger, escape, capture, recombination

1. INTRODUCTION

The conversion efficiency of a single cell *pin* solar cell can be enhanced by incorporating 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 [2–3].

Along with these experimental studies, a number of theoretical investigations have been performed. Corkish and Green [4] studied the effects of recombination of carriers in the quantum well and concluded that although the increased recombination reduces the open-circuit voltage, limited

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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]. Araujo *et al.* [5] used detailed balance theory and predicted that the conversion efficiency of the quantum well cell would not exceed that of the base-line device. The results of photoresponse calculations by Renaud *et al.* [6] revealed that introducing the quantum wells can lead to improved photocurrent without much degradation of the open-circuit voltage. Most recently, Anderson [7] presented an ideal model for the quantum well solar cell device, incorporating the recombination and generation in the quantum wells. Anderson concluded that the improvement in efficiency is achieved only when the depth of the quantum well is less than about 200 meV.

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 which we self-consistently include the effects of:

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.

The standard drift-diffusion equations are modified to account for generation and recombination in the quantum wells and the transfer of electrons and holes between the bulk and quantum well systems.

2. SELF-CONSISTENT MODEL

The steady-state transport of carriers in the *pin* structure is described by current continuity equation written for the bulk regions as:

$$\frac{\partial n_b}{\partial t} = G_b - U_b + \frac{n_w}{\tau_e^n} - \frac{n_b}{\tau_c^n} + \frac{1}{q}\frac{dJ_n}{dx} = 0, \quad (1)$$

where n_b and n_w are electron densities in the bulk and quantum wells, respectively. J_n is electron current density. The two additional terms to the standard bulk current continuity equation incorporate the effect of carrier transfer into and out of the quantum wells. The terms n_w/τ_e^n and n_b/τ_c^n are the electrons escape and capture rates, respectively. These rates are also used in the continuity equations for the quantum wells, as given by:

$$\frac{\partial n_w}{\partial t} = \frac{n_b}{\tau_c^n} - \frac{n_w}{\tau_e^n} + G_w - U_w = 0. \quad (2)$$

In the above equations τ_e^n and τ_c^n are the electrons escape and capture times, respectively. The escape times of carriers are calculated using the model reported by Moss *et al.* [8] and capture times are extrapolated from theoretical and experimental data reported by Blom *et al.* [9]. Similar equations are written for holes. The boundary conditions for continuity equations are derived from surface recombination velocity model.

In the above continuity equations, the recombination in the bulk is modeled with radiative and non-radiative mechanisms. The term G_b is bulk generation rate and is given by:

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

where λ_c is set to correspond to the bandgap of the material. The recombination in the quantum well U_w is a modified Shockley-Read-Hall recombination rate given by:

$$U_w = \frac{\sigma_n \sigma_p v_{th} N_t [pn - p_0 n_0]}{\sigma_n [n + n_t] + \sigma_p [p + p_t]} \quad (4)$$

where the trap density, N_t, is derived from the density of the interface states. The generation term G_w is calculated from Eq. (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 reported by Stevens *et al.* [10].

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

$$\left[\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m^*(x)}\frac{d}{dx}+V(x)\right]\psi(x)=E_i\psi(x) \qquad (5)$$

where $\psi(x)$ is the envelope function, E_i are the eigenenergies and $V(x)$ is the potential profile. Non-constant effective mass $m^*(x)$ is assumed. The Schrödinger equation is solved using the transfer matrix method [11]. The above equations, together with Poisson and drift-diffusion equations are solved using a finite difference scheme.

3. RESULTS

The energy band diagram of the *pin* solar cell device with four quantum wells in the intrinsic region is shown in Figure 1. We simulated five *pin* devices all with a acceptor doping level of 10^{18}/cc

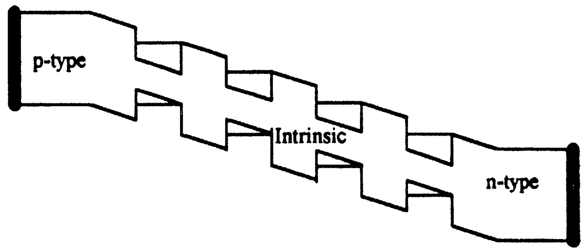

FIGURE 1 Energy band diagram of the solar cell with four quantum wells.

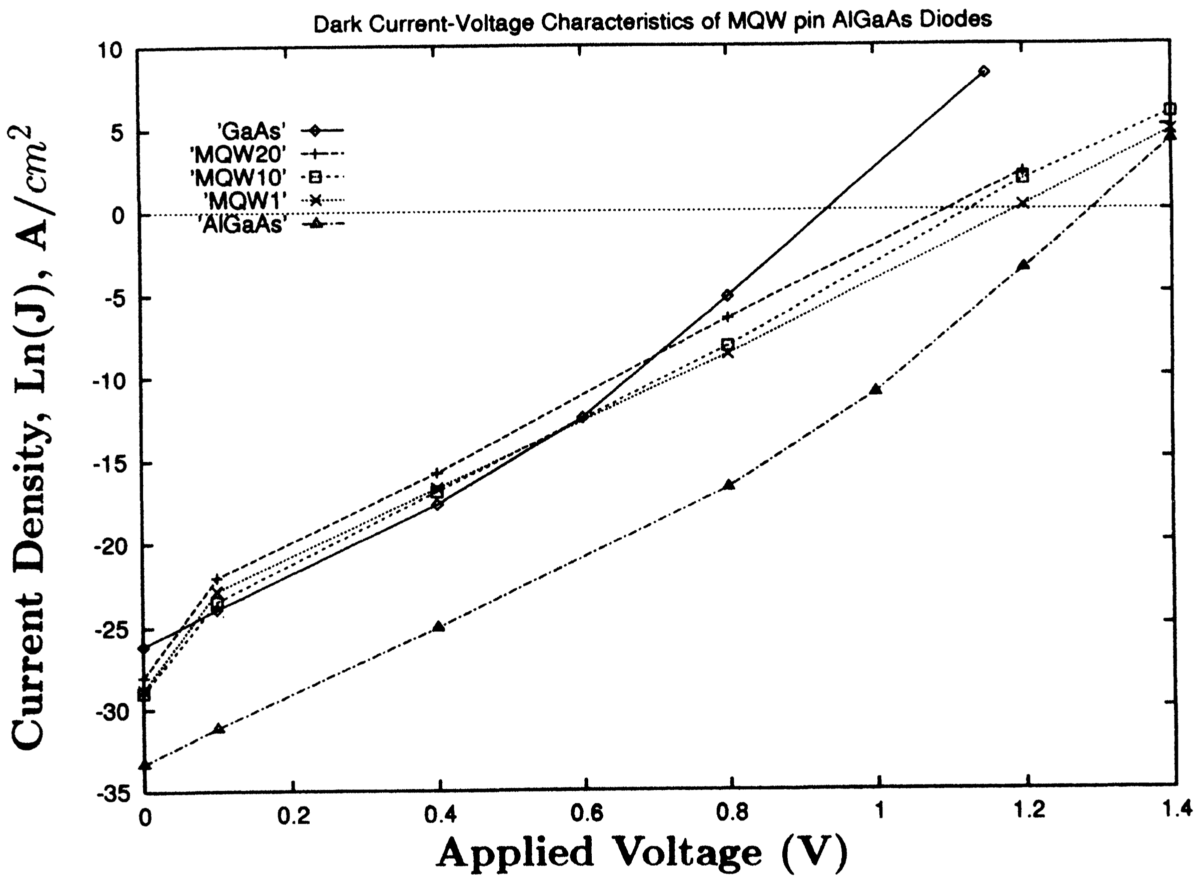

FIGURE 2 Dark characteristics of MQW *pin* solar cells.

and donor doping level of 4×10^{17}/cc in the 0.2 μm *p*-region and 0.3 μm *n*-region, respectively. The intrinsic region of all five devices is 0.5 μm. The first device is a base-line GaAs, the second device is a base-line AlGaAs device and the remaining three devices are AlGaAs devices with 1, 10 and 20 quantum wells, respectively. The mole fraction of Al is 0.3 in all AlGaAs devices and all quantum wells are 100 Å wide.

We simulated the dark characteristics of all five cells and the results are shown in Figure 2. Because the model incorporates both radiative and non-radiative recombination for the bulk material, the slope of the dark current is qv/nkT, with the ideality factor n ranging from one for exclusively radiative recombination to two for exclusively non-radiative. In the *pin* devices without quantum wells, n approaches one at high forward bias where radiative recombination becomes more important. At low biases the non-radiative recombination dominates and n is 1.9 for the AlGaAs device at 0.1 volts applied.

The recombination in the quantum wells is modeled as non-radiative interface recombination using a modified Shockley-Read-Hall expression. With the introduction of quantum wells into the *pin* device, this non-radiative recombination dominates at all biases and the ideality factor equals about 1.7 for all the quantum well devices. The observed crossover of the $i-v$ curves of the quantum well devices and the GaAs device has also been reported by Ragay *et al.* [3].

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