A Refined Ideal Model for AlGaAs/GaAs Quantum Well Solar Cells

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Quantum well solar cells are heterostructure devices promising significant efficiency enhancements over conventional cells. An existing model for quantum well solar cell current-voltage characteristics has been refined. This refined model, unlike its predecessor, is in good agreement with previous experimental results for AlGaAs/GaAs. The model predicts some efficiency enhancements for quantum well solar cells if non-radiative recombination is dominant—when in the detailed balance limit there would be none—even in such a poor quantum well solar cell material as AlGaAs/GaAs.

INTRODUCTION

Originally proposed by Barnham and Duggan (1990), quantum well solar cells (QWSCs) were touted as a means of enhancing solar cell efficiency over that of conventional cells. A QWSC consists of a p-i-n junction constructed from high band-gap semiconductor with thin layers of lower band-gap semiconductor grown epitaxially in the intrinsic region. The intention is that the open-circuit voltage be still controlled by the bulk barrier material, called the ‘barriers’, while the sections of lower band-gap material, called the ‘wells’, absorb additional photons, increasing the short-circuit current and thus the efficiency. The well layers are so thin that quantum mechanics becomes necessary for an accurate description: hence ‘quantum well’ solar cells.

There exist several models attempting to predict the behaviour of QWSCs. For recent reviews see Anderson (2002) and Barnham et al. (2002). Of particular relevance to this article are the models of Anderson (1995) and Rimada (2000), the latter of whom has also published in collaboration with Hernández (Rimada & Hernández, 2001a,b). The main details of Rimada’s model appear in Rimada (2000).

Anderson (1995) treated the QWSC by adding to the ideal diode equation for a p-n junction additional terms to account for the generation and recombination of carriers in the intrinsic region, though under some heavily idealized assumptions. Rimada extended Anderson’s model by removing the complete absorption assumption and accounting for well/barrier interface recombination. To calculate the absorption coefficients, however, application of the model to a particular QWSC material was necessary. He chose AlGaAs/AlGaAs. (Although Anderson selected material data for InP-based QWSCs, his results were reasonably valid for all QWSCs.) Rimada and Hernández’s main results were a critical dependence of efficiency on quantum well depth and finding that efficiency enhancements for practical AlGaAs/AlGaAs QWSCs over any equivalent homostructure AlGaAs cell are achievable.

This article will present results from further development of this progression of models. Details will be available in Lade & Zahedi (2003).

THE MODEL OF RIMADA

The present authors have no objection to Rimada’s current-voltage relation,

\[ J(V) = J_0 (1 + r_k \beta \left( \exp \left( \frac{qV}{kT} \right) - 1 \right) + r_w \alpha + r_i \left( \exp \left( \frac{qV}{2kT} \right) - 1 \right) - qF, \]  

which includes Rimada’s adjustment for interface recombination. (For symbol definitions, see Rimada...
Our concern is with the method used to calculate the absorbed photon flux $\Phi$.

Consider a QWSC with $NW$ wells, each of length $LW$ and with bulk band-gap $EW$, in an intrinsic region of length $W$ with 'barrier' band-gap $EB$. Rimada calculates the flux absorbed in the barriers in the presence of a spectral photon flux $N_{ph}(\lambda)$ as

$$ F_B = \int_{E_B}^{\infty} N_{ph}(E) \cdot \exp[\alpha_B(E) \cdot W] \cdot dE $$

and the flux absorbed per well as

$$ F_W = \sum \Delta \cdot \exp[\alpha_W(\lambda_n) \cdot LW] \cdot \Delta \lambda_n, $$

where the summation is performed over all permitted transitions $\lambda_n$, with linewidths $\lambda_n$. Here $\alpha_B(E) > 0$ and $\alpha_W(\lambda) > 0$ are the barrier and well absorption coefficients respectively and the integral and summation have been written as over energy and wavelength respectively purely for convenience. The total flux absorbed is then calculated as

$$ F = F_B + NW \cdot F_W. $$

The barrier absorption spectrum is taken from the literature. The well absorption spectrum is calculated from a formula. Only those transitions corresponding to conservation of quantum number are, to a good approximation, allowed (Bastard, 1988). The well energy levels are calculated using a variation of the standard implicit formula for one-dimensional, single (equivalently, for multiple wells, the limit of wide barriers), finite quantum wells.

THE REFINED MODEL

According to equation (3), the well absorption spectrum consists of a series of peaks of linewidth $\lambda_n$ at energies corresponding to the well transition energies. This is because "the light is absorbed ... through discrete levels of energy" (Rimada & Hernández, 2001a: 720). According to Bastard (1988), however, the absorption spectrum is stepped. The carriers are only confined in one direction; energy in excess of the transition energy can therefore be used for electron motion perpendicular to the growth direction. We use Bastard’s expression in the refined model to calculate the well absorption coefficients.

More serious, however, is that the exponential factor in equations (2) and (3) will evaluate to greater than unity and therefore the model will have more photons absorbed than are incident on the cell. Inserting typical absorption coefficients (Aspnes et al., 1986) into equation (2) gives extremely large results. To achieve reasonable results, we suggest that Rimada used absorption coefficients generally smaller than appropriate, so that the exponential factor was approximately unity and complete absorption was effectively assumed.

A more appropriate expression is

$$ F = \int_{E_W}^{\infty} N_{ph}(E) \cdot \left[1 - \exp(-\alpha_B(E) \cdot W - NW \cdot \alpha_W(E) \cdot LW\right] \cdot dE. $$

Note that the well absorption spectrum is now continuous rather than discrete. Rimada’s model with these alterations comprises the refined model.

Of particular interest is a graph produced by Rimada and Hernández (2001a; Fig. 5, vs = 30 cm/s case), which has been reproduced almost exactly in simulations by the present authors in Figure 1. (That the results can be reproduced accurately suggests a correct interpretation of the model.) It shows efficiency increasing almost linearly with the number of wells. The efficiency passes 40% before Rimada and Hernández terminate the graph at 35 wells, due to tunnelling becoming significant.

The predictions of the refined model under the same material data are also shown in Figure 1. It predicts vastly different efficiencies, with no efficiency enhancement at all for the QWSC over the cell without wells, at least for this configuration and with these material properties. This result, although poor for the QWSC, appears more realistic than Rimada’s linear increase in efficiency with number of wells apparently, up to tunnelling, without limit.
Figure 1. AlGaAs/AlGaAs efficiency as a function of number of wells as predicted by Rimada's and the refined model, under the same material data. The upper curve reproduces the results of Rimada and Hernández (2001a; Fig. 5, vs = 30 cm/s case). Wells of length 1 nm with $E_B = 1.88$ eV and $E_W = 1.75$ eV were used.

The main cause of the differences, in this case, is Rimada's use of equation (4), which clearly gives a linear relationship between short-circuit current (equal to $qF$) and the number of wells. If the flux absorbed in each well were small, the linear approximation of equation (4) would be valid. The large increases in short-circuit current generated in the simulations as the number of wells is increased, however, which lead to the large efficiency increases in Figure 1, show that the flux absorbed in each well as calculated by Rimada was not sufficiently small for this approximation.

EXPERIMENTAL COMPARISON

Before comparing with experimental results, for the sake of accuracy a review was undertaken of all the required material data (Lade & Zahedi, 2003). During this review, the study was narrowed to consider only AlGaAs/GaAs QWSCs since, according to Timmons (1992), the interface recombination velocities at AlGaAs/AlGaAs interfaces are several orders of magnitudes worse than at AlGaAs/GaAs. This comes without significant loss of relevance, since most studies of AlGaAs/AlGaAs QWSCs use only the AlGaAs/GaAs case. The least well-known properties were the bulk non-radiative lifetimes (between 0.1 and 1 ns for the barriers and 10 times longer for the wells were used) and the interface recombination velocity $v_s$ (like Rimada, between 30 and 300 cm/s). Also introduced were a quantum-mechanical method for calculating the well density-of-states, instead of assuming a three-dimensional distribution, and a method for evaluating the radiative recombination current using detailed balance theory (Araújo & Martí, 1994), instead of phenomenologically applying a fixed radiative recombination coefficient.

We now compare the experimental results for the cells of Aperathitis et al. (2000) with the predictions of Rimada's model and the refined model. We use the results for three of their cells, under AM1.5 illumination: one GaAs cell (GS62) and two Al$_{0.36}$Ga$_{0.64}$As/GaAs QWSCs, one with 40 wells of length 5.4 nm (GS64) and the second with 23 wells also of length 5.4 nm (GS65). Further details of the cells' construction and structure are available in their article. Though GS64 has more wells than the number at which Rimada & Hernández terminated their simulations in Figure 1, the barriers here are sufficiently long so that Rimada’s expression for minimum barrier length (Rimada, 2000) is not violated.

The efficiency predictions of Rimada’s model and the refined model together with the experimental results are shown graphically in Figure 2. Rimada’s original data was used in the implementation of his
model. The revised data introduced above were used for the refined model, with, for simplicity, the median value of 0.5 ns for the barrier non-radiative lifetime (and 5 ns for the wells). Varying these lifetimes would numerically affect the predicted open-circuit voltages and efficiencies, but would leave the qualitative trends largely unaffected.

Though numerically slightly higher—most probably due to neglect of front-surface reflectivity—the refined model’s efficiencies qualitatively agree with the experimental results: a decrease in efficiency between the homostructure GS62 cell and cell GS64, then a slight decrease again to GS65. Rimada’s model, meanwhile, predicts a large increase in efficiency from cell GS62 to GS64, and with GS65’s efficiency also significantly greater than GS62’s. This model’s large short-circuit current, 83.7 mA/cm² for the cell GS64 compared to the refined model’s 14.3 mA/cm² and the experimental 10.2 mA/cm², is predominantly responsible for this, and is what the alterations of section 3 aim to change.

The refined model’s efficiencies, returning to Rimada’s data, change by less than 2%. The differences between the predictions of Rimada’s and the refined model therefore stem primarily from the alterations of section 3 (like the large differences also observed in Figure 1), not the change of material data at the start of this section.

![Figure 2. Experimental and predicted efficiencies for the cells of Aperathitis et al. (2000). The unfilled extensions show the effects of decreasing \( v_s \) from 300 to 30 cm/s.](image)

**GENERAL RESULTS**

In simulations, efficiency enhancements for some AlGaAs/GaAs QWSCs over the GaAs cell under non-radiative regimes were calculated by the refined model (Lade & Zahedi, 2003). This is in spite of the fact that in the detailed balance (that is, ideal) recombination limit with constant quasi-Fermi level separation, as both we and Rimada have assumed, no such enhancements are possible (Araújo & Martí, 1994). This is because the GaAs band-gap is already greater than optimum for AM1.5 illumination (Lade & Zahedi, 2003). That practical QWSC efficiency enhancements are nevertheless available even under the restrictions of detailed balance theory and the poor material quality of AlGaAs/GaAs is encouraging for the future prospects of QWSCs.
CONCLUSIONS

The model of Rimada (in collaboration with Hernández) extended that of Anderson by removing the complete absorption assumption and accounting for well/barrier interface recombination. The present authors continued and refined this progression, primarily by revising the equations used to calculate the absorbed flux. The predictions of the refined model appeared both more realistic and more consistent with experimental results, with the main cause of the differences the changes to the equations for absorbed flux.

Efficiency enhancements of some AlGaAs/GaAs QWSCs over the GaAs homostructure cell have been observed, even though no such enhancements are available in the detailed balance limit.

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REFERENCES

Rimada, J.C. (2000), Modelación de celdas solares p-i-n de AlₓGa₁₋ₓAs con pozos cuánticos en la región intrínseca, MSc thesis, Universidad de la Habana.