Chapter 34
Quantum Confinement Modeling and Simulation for Quantum Well Solar Cells

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ABSTRACT

In this chapter, the authors present the modelling and simulation of the multi-layered quantum well solar cells as well as the simulated results of this model. The quantum confinement of a semiconductor induces new energy levels, located in the band gap, as well as resonant levels located in the conduction and valence bands. These levels allow supplementary absorption in the visible and near infrared range. The quantum efficiency of the supplementary absorption is calculated within the infinite rectangular quantum well approximation. As the absorption excites carriers in the gap of each layer, even a small absorption significantly increases the photocurrent (by photoassisted tunneling) and, therefore, the cell efficiency. The results of the simulation are presented for the internal quantum efficiency of the transitions between the resonant levels of GaAs, as well as the internal quantum efficiency of the transitions between the confinement levels for GaAs and $Al_xGa_{1-x}As$. *New directions for the research of quantum well solar cells are indicated.*

1. INTRODUCTION

The "*quantum well*" photovoltaic cells were first proposed in 1990 (Barnham & Duggan, 1990), based on the idea that the use of the quantum wells could improve the photovoltaic cells by extending their spectral response, as well as by increasing the photocurrent. One year later, this idea was experimentally proved by using a $GaAs/Al_xGa_{1-x}As$ multi-layered structure (Barnham, et al., 1991). From this moment on, the use of the Multi-Layered Photovoltaic (MLPV) cells became one of the most used approaches for a high efficiency PV cell. Generally, such cells are *p-i-n* type diodes, with the intrinsic region formed by a multilayered

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structure (Paxman, et al., 1993; Anderson, 1995; Connolly, 1997; Raisky, et al., 1999; Green, 2000; Barnham, et al., 2002; Anderson, 2002; Abbott, 2003; Sato, et al., 2005; Jani, et al., 2005; Norman, et al., 2005; Myong, 2007; Hong, et al., 2007). Most of these cells have layers of tens or even hundreds of nanometer thickness, so that the quantum effects are reduced; nevertheless they are also called in some texts "quantum well" PV cells (see for instance Ref. 5). However, MLPV cells with real quantum sizes (Multi-Layered Quantum Well Photovoltaic—MLQWPV) are also studied (Myong, 2007; Hong, et al., 2007).

The E 2456-06 ASTM International Standard "Terminology for Nanotechnology" states that sizes between 0.1 and 1 μm are to be called "submicronic," while the prefix "*nano*" is to be used for sizes between 1 nm and 100 nm only. On the other hand, an analysis of the quantum effects proves that the quantum size appears under about 20 interatomic distances (e.g. about 5 nm), where the band structure is replaced by an energy level structure and the momentum conservation law is no longer valid (Heitmann, et al., 2004; Fara, et al., 2007).

The true quantum well photovoltaic cells use the special advantages of the low dimensional systems, where at least one size is at quantum scale. This leads to two important contributions.

The first contribution is a strong Quantum Confinement (QC) effect. Indeed, at this size, it was proved that the material nature role is secondary with respect to the QC (Iancu, et al., 1998; Iancu, et al., 2006).

The second contribution is the increased role of the surface/interface. The area/volume ratio is $1/d$, where d is the minimum size, so that, at quantum sizes, this ratio is greater than 2×10^8 m^{-1}. Then, the cells are classified with respect to their dimensionality in 2D, 1D, 0D and fractals. The MLPV (and the Multi-Layered Quantum Well Photovoltaic—MLQWPV) cells are 2D. In literature, they are divided in Multiple Quantum Wells (MQW) and Superlattice (SL) systems (Connolly, 1997; Myong, 2007), the difference being based on the barrier layer thickness (Myong, 2007). However, this interpretation is not correct. The SL structures replace the resonant levels from the conduction and valence bands of the "quantum wells" with resonant bands. This is not correlated with the barrier thickness, but with the total number of layers, for reasons similar with those that define the quantum size (Heitmann, et al., 2004; Fara, et al., 2007). In the following, only MQW structures will be considered.

We have to mention the recent results obtained regarding plasmonic solar cells which have important prospects for the future. They use nanoparticles to benefit from plasmonic effect in order to improve absorption and finally, the solar cell current response (Catchpole, 2008).

The aim of this chapter is to model MLQWPV cells in order to find out how to improve them. Section 2 deals with the QC effects. Section 3 calculates the quantum efficiency of a layer and discusses the optical improvements of the cells. Section 4 summarizes all the simulation results.

2. QUANTUM CONFINEMENT EFFECTS

As we have stated, the MLQWPV cells have a *p-i-n* structure, with a multi-layered *i* region (e.g. GaAs/$Al_xGa_{1-x}As$). It is well known that the band gap difference between the layers acts like a quantum well and induces the appearance of resonant levels in both the conduction and valence bands (MQW structure). These levels improve the absorption and therefore increase the cell efficiency. If the number of layers is big enough, the resonant levels are replaced with resonant bands (SL structure). An example of both structures, under an external bias V, is presented in Figure 1 (adapted from Jani, et al., 2005). E_w, t_w and E_b, t_b are the gaps and thicknesses of the quantum well and barrier layers, respectively. For MLQWPV cells, both t_w and t_b are of the order of $5 \div 10$ nm.