Solar Energy Materials & Solar Cells 159 (2017) 633–639

Contents lists available at ScienceDirect

Solar Energy Materials & Solar Cells

journal homepage: www.elsevier.com/locate/solmat

Contribution of a single quantum dots layer in intermediate band solar cells: A capacitance analysis

Hela Boustanji [a,*], Sihem Jaziri [a,b], Jean-Louis Lazzari [c]

[a] Laboratoire de Physique de la Matière Condensée, Faculté des Sciences de Tunis, El Manar, 2092 Tunis, Tunisia
[b] Laboratoire de Physique des Matériaux, Faculté des Sciences de Bizerte, 7021 Zarzouna, Tunisia
[c] Aix-Marseille Université, CNRS, CINaM UMR 7325, Case 913, Campus de Luminy, 13288 Marseille cedex 09, France

ARTICLE INFO

Article history:
Received 29 July 2015
Received in revised form
8 January 2016
Accepted 29 March 2016
Available online 14 April 2016

Keywords:
GaSb/GaAs type II quantum dots
Schottky diode
Capacitance–voltage
Charge accumulation
Intermediate band solar cells

ABSTRACT

Theoretical model and numerical analysis of charge accumulation within a single GaSb quantum dots layer embedded in GaAs-based *Schottky* diode is performed. We hereby give an analytical calculation of the capacitance–voltage (*C*–*V*) characteristic of GaAs-based *Schottky* barrier structure incorporating GaSb self-assembled quantum dots layer. The *Schottky* barrier is derived in different bias voltage region based on solving analytically *Poisson's* equation, including the effects of the dots size dispersion and the *Fermi* statistics of the holes in the quantum dots. The numerical simulation of capacitance–voltage curves exhibits a plateau that is caused by the high carrier concentration and the saturation of the quantum dots levels upon the applied voltage. These results are in good agreement with experiments done by Hwang et al.

1. Introduction

The Intermediate Band Solar Cells (IBSC) is a photovoltaic concept which has been proposed in order to overcome the Schockley–Queisser limit [1]. Quantum dots (QDs) IBSC attract significant interest because the quantum dot solar cells (QDSCs) have the ability to absorb incident solar energy from any direction. The efficiencies is near 10% which have been achieved with these devices [2,3]. But the efficiency of colloidal QDSCs have advanced from 1% in 2005 to 8.5% in 2013 [3].The intermediate band (IB) is the concept of putting the energy levels, approximately in the middle of a band gap in order to increase the maximum photocurrent using the two-step photon absorption process. The main idea is the exploitation of zero-dimensional levels formed by QDs for the generation of additional photocurrent. The confined electronic states of InAs/GaAs type I QDs were initially used to produce IB like- states located within the depletion layer of a single p–n junction [4–6]. The IB solar cell concept with type II GaSb/GaAs QDs absorber [7] located outside the p–n junction has recently attracted extensive attention for its high theoretical efficiency of 63% [8]. Several works and efforts have been published to enhance the understanding of IBSC, including the effect of coupled semiconductor QD array on absorption coefficient [9], Auger generation [10–12] radiative and non-radiative processes in QD array [10,12], the emission and capture processes into QDs during drifting in the active region are determined by the technique deep-level transient spectroscopy (DLTS) [13], the inter-subband transition in low-dimensional semiconductors dot-in-well (DWELL)which depends on the power of two lasers [14,15].

Two approaches are involved to improve the efficiency and the performance of the solar cell. First QDs growth quality is generally optimized in terms [16] size, density, strain condition, elemental interdiffusion and density of defects. But intermediate levels introduced by type I QDs increase the radiative recombination process between electron and hole which is harmful to the solar cell efficiency. Moreover it is important for a solar cell to have high generation of free charge carriers and as low recombination mechanisms as possible. A complex interplay between charge accumulation and intrinsic traps has been early evidence by Krispin et al. by capacitance spectroscopy for InAs/GaAs QDs layer [17,18]. These recombination processes are enhanced when the absorber is placed within the built-in-field of a p–n junction. Thus charge accumulation, recombination and extraction effects within the first QDs layer in the absorbing stack are of importance to apprehend the performance of IB GaAs based solar cells, as the open circuit voltage, short current density, fill factor, and conversion efficiency all vary with the position of InAs/GaAs QD layer [19].

The collection and separation of carriers from the QDs is essential in order to enhance the efficiency. There are three important processes for extraction carriers from QD by thermal activation, tunneling carrier escape, and a two-step process of absorbing sub-gap photons of different photons energies. The

---

[*] Corresponding author. Tel.: +216 28286117.
E-mail address: helaboustangi87@yahoo.fr (H. Boustanji).

http://dx.doi.org/10.1016/j.solmat.2016.03.038

tunneling rate depends on the energy of the level and the triangular potential barrier due to the electric field [20,21]. Simulation results [22–24] have been reported for quantum dot arrays embedded in the intrinsic region of typical p-i-n structure. These results show the number of dot layers and the effect of spacer thickness are two important parameters which affect the conversion efficiency of the solar cell. The IB was formed if the spacer layer thickness was reduced which has been evidenced by Movla et al. [22] and by Shoji et al. [16]. This result have also presented by Dondapati et al. in the case of CdSe semiconductor films containing self-assembled nanocrystals (NCs) [25]. Reducing the distance between the NCs, the electronic coupling increases and the photocurrent in the pn junction is enhanced [25]. Elborg et al. [23] shows the decreases of the two-step photocurrent generation is caused when the bias increased the carrier tunneling escape and the recombination rate increased. For this, the recombination rate of carriers should be controlled in order to be in the optimization of the solar cell [22].

Type II QDs are attractive since they confine only electrons or holes, keeping the other outside. GaSb/GaAs QD is one such system in which only holes are confined in dots. Using of type II with long carrier lifetimes resulting from the spatial separation of carriers provides additional advantage for charge separation in solar cell absorber. The recombination lifetime between carriers has been much longer than that of type I because it is mainly determined by the overlap between electron and hole wave functions. In return, the absorption coefficient should be lower than that for type-I QDs for which an extended *Urbach* tail below-bandgap absorption improves the photo-generated current [26]. Indeed, due to numerous IB-like states in QDs, absorption via multiple photon transitions is improved and photocurrent generation is enhanced. Owing to the large confinement potential in GaSb/GaAs type-II QD, the thermal extraction process of hole is reduced. But hole extraction depends on the energy distribution of electronic levels, e.g. on the size and size dispersion of the QDs [13] as well as on potential grading due to Sb/As interdiffusion at GaSb/GaAs interface [27], in addition with other inelastic scattering with hot photoelectrons [28]. All these mechanisms motivate the study of filling and infilling of energy levels, in particular to understand the potential screening by the first GaSb/GaAs QDs layer for those cells with separated absorption and p/n junction collection [8,28].

2. Material and method

In this work we study theoretically the capacitance–voltage (*C*–*V*) characteristics of a *Schottky* diode structure referred to a sample containing a layer of GaSb/GaAs QDs [13]. The GaSb QDs were grown via the *Stranski–Krastanov* growth mode, where details of the growth are discuss in the Ref. [29]. For an overview of GaSb/GaAs QDs formation, see [26] and references therein. Our attention is focused on a GaAs-based *Schottky* barrier structure with a single layer of self-assembled GaSb/GaAs QDs located at a distance L_{conf} from the metal contact, as depicted schematically in Fig. 1.

To determine the capacitance of the *Schottky* diode we have to calculate the potential and the stored charge. The charge located in the GaSb QDs depends on the voltage, temperature and density of states (DOS). We assumed that the QDs are thin enough to consider the stored charge as a surface charge density. The total charge in the QDs structure is given:

$$Q = eS(p_{conf} - N_A w) \tag{1}$$

where e is the elementary charge, S is the surface area of the *Schottky* contact, P_{conf} is the charge density accumulated in QDs, N_A is the constant charge density of ionized impurity, and w is the depletion region.

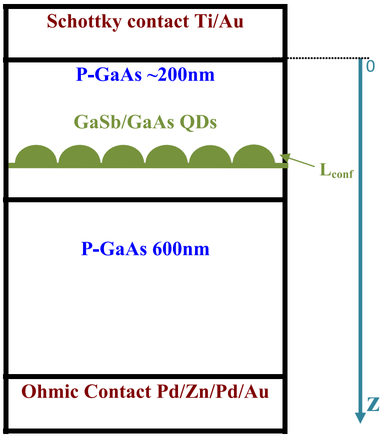

Fig. 1. Details of the QDs layer structure used for capacitance characterization. A similar reference structure is studied separately without QDs layer (GaAs control). L_{conf} is the distance from the *Schottky* contact to the layer with GaSb/GaAs QDs [4].

The valence band of such a structure (see Fig. 2) containing a GaAs-based *Schottky* barrier incorporating GaSb QDs could be determined by solving the *Poisson* equation [30,31]:

$$\frac{d^2}{d^2z}\varphi(z) = \frac{e}{\varepsilon}N_A^- - \frac{e}{\varepsilon}p_{conf}\delta(z - L_{conf}) \tag{2}$$

where $\varphi(z)$ the potential distribution in the structure along the z direction, ε is the dielectric constant equals the product of relative dielectric constant of GaAs ($\varepsilon_r = 12.5$) and the dielectric constant of the vacuum ε_0. The charge density in the right-hand side of the *Poisson* equation consists of two components, namely $N_A^-(z) = \frac{N_A(z)}{1 + 4\exp\frac{(E_A - E_F)}{KT}}$ is the constant charge density of ionized impurity at room temperature and is taken to be $1.37\,10^{17}\ \text{cm}^{-3}$ [13]. We recall p_{conf} is the charge density accumulated in QDs given by the integral of the product of the DOS and the energy distribution:

$$p_{conf} = 2N_{QD}\int_{-\infty}^{+\infty} g_i D(E) f_p(E) dE \tag{3}$$

where N_{QD} is the areal dot density which estimated from atomic force microscopy studies on uncapped samples to be 5.3×10^{10} cm^{-2} [29], g_i is a parameter that accounts for the degeneracy of the level and $f_p(E)$ is the Fermi–Dirac occupation probability for the hole in QD. The problem consists now in determining the *Fermi* level. Only the occupied states were considered in our calculations. We assumed that the *Fermi* level in the dots was the same as in the highly doped substrate [32]. E_F Is the common *Fermi* level for the whole structure corresponding to a given applied bias V:

$$f_p(E) = \frac{1}{1 + \exp\left(\frac{E_F - E}{KT}\right)} = \frac{1}{1 + \exp\left(\frac{e\varphi_{conf} - E}{KT}\right)} \tag{4}$$

where φ_{conf} is the potential at the position L_{conf} calculated in next section by Eq. (7).

The density of state $D(E)$ in QDs can be written in a delta function form in the ideal case of no dispersion of QD size. The effect of the QDs size dispersion can be taken into account by Gaussian broadening of the DOS, according to:

$$D(E) = \sum_{i=1}^{Nlevels} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(E - E_{di})^2}{2\sigma^2}} \tag{5}$$

with a Gaussian standard deviation σ of around 100 meV.

We here define $E_{di} = -e\varphi_{conf} + E_{dot,i}$ as the hole energy level of the QD. The QD shape is modeled by hemispherical lens with a dot height $h = 2.3$ nm and a 17 nm base radius floating on 2ML GaSb