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The effect of band offsets in quantum dots

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ABSTRACT

The insertion of quantum dots in a host material produces band offsets which are greatly dependent on the field of strains brought about by this insertion. Based on the Empiric KP Hamiltonian model, the energy spectrum of the quantum dot/host system is easily calculated and a relationship between the conduction and valence band offsets is determined by the energy at which the lowest peak of the sub-bandgap quantum efficiency of an intermediate band solar cell is situated; therefore knowledge of the valence band offset leads to knowledge of both offsets. The calculated sub-bandgap quantum efficiency due to the quantum dot is rather insensitive to the value of the valence band offset. However, the calculated quantum efficiency of the wetting layer, modeled as a quantum well, is sensitive to the valence band offset and a fitting with the measured value is possible resulting in a determination of both offsets in the finished solar cell with its final field of strains. The method is applied to an intermediate-band solar cell prototype made with InAs quantum dots in GaAs.

1. Introduction

The intermediate-band (IB) solar cell [1] (SC) contains several levels or bands permitted to the electrons in the forbidden bandgap of a semiconductor. These permitted values may be used for the transfer of electrons from the valence band to the conduction band by absorbing low-energy photons. The triple-level system arising in this case, may emulate a triple-junction solar cell. Shockley and Queisser, in an elegant paper, calculated the detailed efficiency limit of a single-junction solar cell to be 41% [2]. For an IBSC, the efficiency value determined in a similar manner is 63% [1]. There are several different ways of manufacturing IBSCs [3], whose operation is described further in [4].

In semiconductor materials, the intermediate band may be formed by quantum dots [5] (QDs). A type I QD produces offsets in the host material bands leading to a well in the conduction band (CB), and a pedestal in the valence band (VB). They both produce confined states (the pedestal is attractive for the negative-mass holes) with energy levels which are within the band gap of the host material; those derived from the CB offset form the IB. Unfortunately, efficiency higher than a control cell without QDs has seldom been produced, and when so, only marginally [6]. The main reason is that the absorption of low energy (sub-bandgap) photons by the QDs is too weak. This stresses the importance of a good characterization and modeling of the photon absorption process.

A very important aspect in QD characterization in a semiconductor device is the determination of the potential offsets in the CB and in the VB, which is the depth of the CB well and the height of the VB pedestal. In this paper we will present a method to determine these offsets. The method will be applied to the determination of the offsets produced by InAs QDs in a GaAs host.

InAs QDs can be obtained by growing an InAs layer on the GaAs substrate. Because of the large mismatch in the lattice constant, the structure will grow according to the Stransky–Krastanov mechanism, which means the formation of a thin film first, and after that, islands grow thus forming the QDs. However, a fine continuous layer remains which is referred to as the wetting layer (WL). This InAs thin film, in this case, can be regarded as a quantum well. It produces a photo-generation, stronger to that of the QDs, close to the bandgap.

1.1. The energy spectrum

After the formation of the QDs, their characterization through experiments is a very important task. Photoluminescence (PL) is perhaps the most commonly used technique. It can be performed on a finished device or in samples *ad hoc*. An interesting PL signature of the confined states is presented in reference [7], the PL plots are reproduced in Fig. 1. According to the authors the peaks represent the position of the confined electron levels below the

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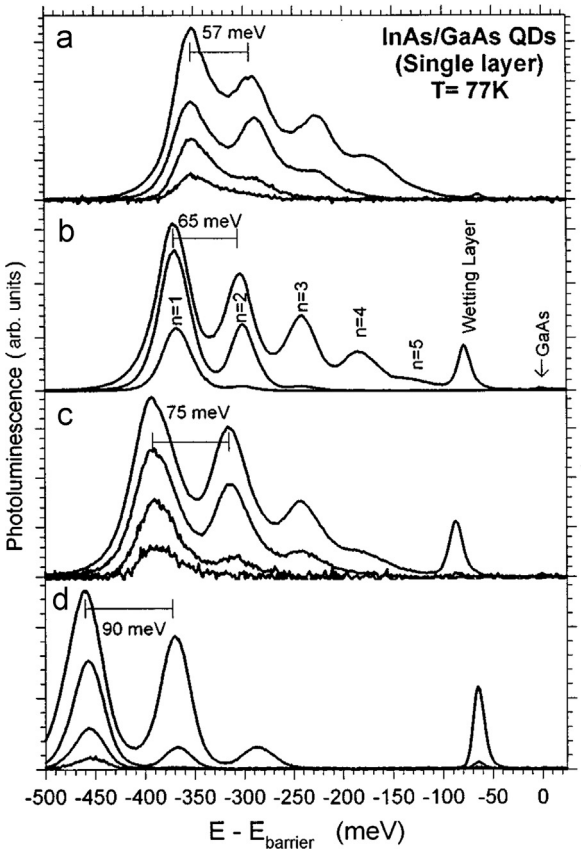

Fig. 1. Tuning of the intersublevel energy spacing with the substrate temperature during the growth of InAs/GaAs QD's. Larger QD's with smaller intersublevel energy spacings are obtained at higher temperatures: (a) Shows T_{growth}=535 °C, (b) T_{growth}=515 °C, (c) T_{growth}=500 °C, and (d) T_{growth}~480 °C, giving an adjustable intersublevel energy spacing of between 57 and 90 meV. The state-filling spectroscopy is obtained with photoluminescence at 77 K, with the highest excitation of a few kW/cm^2 above the barrier energy.

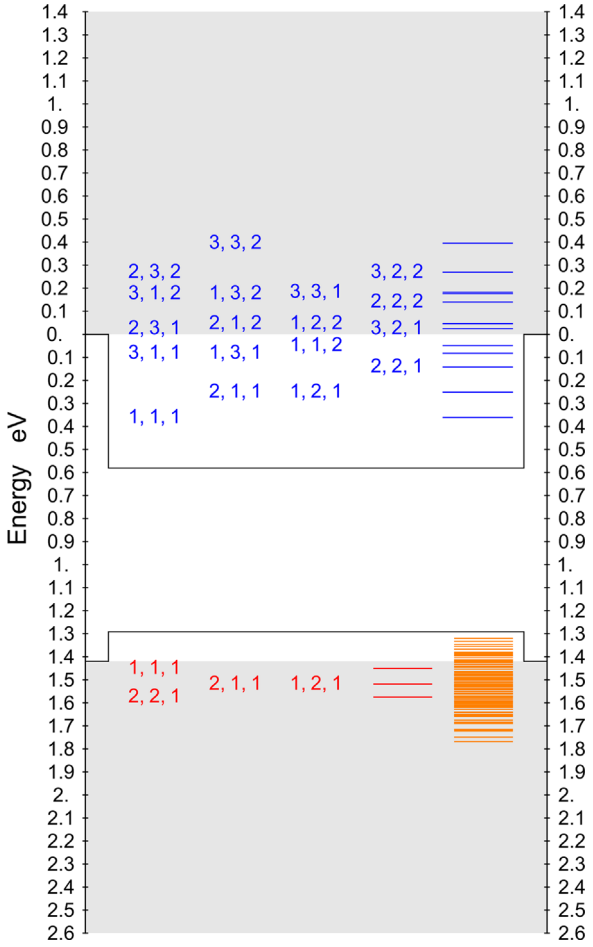

Fig. 2. Energy levels in InAs QD in GaAs calculated with the parameters of Table 1.

Table 1
Parameters used for the calculation of the energy spectrum of the QD of Fig. 2

Parameter	Value	Source
Host bandgap, Eg (eV)	1.42	[14]
InAs relative *cb* effective mass relative to mass *in vacuo*, m_{cb}	0.0294	[15]
InAs relative *lh* effective mass relative to mass *in vacuo*, m_{lh}	0.027	[15]
InAs relative *hh* effective mass relative to mass *in vacuo*, m_{hh}	0.333	[15]
InAs/GaAs CB well offset (eV)	0.58	[16] and this paper
InAs/GaAs VB pedestal offset (eV)	0.22	[16] and this paper
QD height (nm)	6	TEM
QD base side (nm)	14.9	[16]

host CB edge. In each panel the different curves reflect a variation in the laser excitation that pumps electrons from the VB to the CB. The PL is produced by luminescent emission from the levels of the electrons confined by CB offset potential to the VB states. More levels (the excited states) are revealed by increasing the excitation. In panel (b) the levels are labeled. The different panels refer to different samples that have been built according to the description in the caption. For more details see reference [7].

Modeling is another of the tasks which are necessary for understanding the behavior of the QD structures. IBSCs have been modeled frequently. Modeling can be derived from *ab initio* calculations [8] or from k · p methods among others. This analysis is based on a model of the QD based on the Empiric KP Hamiltonian [9,10] (EKPH). In contrast to the *ab initio* calculations this model, although less accurate, can be used with modest calculation equipment (a laptop) and is relatively fast; details may be found in reference [11], a method summary is described in reference [12].

The method requires us to solve four effective-mass Schrödinger equations: for the conduction band (*cb*) states and the heavy hole (*hh*), light hole (*lh*) and split-off (so) bands in the valence band (VB). One of the reasons for the rapidity of the method is that it assumes that the QDs are squat parallelepipeds with well/pedestals (the band offsets) of constant depth/height. This allows the states to be written as $|hh121\rangle$ for instance, the three digits being the quantum numbers – n_x, n_y, n_z – corresponding to three very simple one-dimensional Schrödinger equations if the potential is considered separable [13]; the quantum numbers may be conserved even if this approximation is refined, as we have done. The conduction band (CB, with capital letters) and the VB include not only states bound to the QD, such as $|hh121\rangle$ or $|cb111\rangle$, but also extended states characterized by (slightly modified) Bloch functions. In the EKPH method the calculation of the energy spectrum is almost instantaneous. It is presented in Fig. 2 for the set of parameters enlisted in Table 1.

The energy levels are calculated with an upgraded [13] separable approximation (to the first order, very close to the exact value). The labeling is simplified, omitting the band, because the position reflects the band they belong to (and also for reasons of space).

The IB, in this plot, is formed of the states near the host CB which are within the host bandgap. They are *cb* states, detached