Physica B 408 (2013) 98–103

Contents lists available at SciVerse ScienceDirect

Physica B

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

Strain effects on resonant parameters in asymmetric $In_{1-x}Ga_xAs$ quantum dot molecules

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ARTICLE INFO

Article history:
Received 10 September 2012
Received in revised form
29 September 2012
Accepted 1 October 2012
Available online 7 October 2012

Keywords:
Quantum dot molecule
Strain
Resonant parameters

ABSTRACT

We investigate theoretically the strain effects on resonant properties in asymmetric $In_xGa_{1-x}As$ vertically stacked coupled quantum dots. The strain can modify the resonant electric field and the energy splitting between the bonding and antibonding molecular states of electrons (holes) in quantum dot molecules. The strain reduces resonant electric fields for both electron and hole resonance. However, it is found that molecular bonding is enhanced (suppressed) for electron (hole) resonance when considering the strain. The reversal of electron and hole bonding characters is attributed to different strain components acting on their respective energy bands. Such strain difference also leads to different composition dependence of resonant electric fields for each electron or hole resonance.

1. Introduction

Quantum dot molecules (QDM) formed by two coupled quantum dots (QD) exhibit bonding and antibonding molecular-like properties [1–4]. The energy splitting between the bonding and antibonding states is given by the tunnel coupling strength, i.e., the overlap between the hybridized orbitals in the interdot barrier. Currently, much interest has been focused on tuning electron and hole tunneling in a controllable way, motivated by their possible applications in spintronics, optoelectronics, and quantum information technologies [5,6].

In vertically coupled QDs, the splitting between the bonding and antibonding levels (Δ_{BAB}) can be tailored by changing the barrier length [5,7–9]. A more flexible method to tune the tunnel coupling is the use of longitudinal electric fields, since Stark shifts induced by external electric fields shift electron wave functions between two QDs [5,6,10–12]. It is now possible to apply electric fields upon asymmetric QDMs in order to form coherent molecular states [13–15]. Coherence is found clearly as "anticrossings" in the two lowest levels versus electric fields where the minimum Δ_{BAB} is obtained under a critical resonant electrical field (F_c). Experimentally, the anticrossings appear in the exciton photoluminescence spectrum where electron (hole) resonant tunneling occurs [13,14,16,17]. The resonance associates with the shift of electron or hole from one dot to the other. Meanwhile, the optical transitions from *intradot* (e,h in the same dot) to *interdot* (e,h in the isolated dot) excitons take place [15–17]. The two resonant parameters Δ_{BAB} and F_c are respectively correlated with the strength of molecular bonding and the ability of exciton dissociation. Experiments and theories show that both QD structure and magnetic fields can influence these two physical parameters [13,16–18].

Strain due to the lattice mismatch at the interfaces between two semiconductors is the driving force for the growth of self-assembled QDs [19–21]. Simultaneously, electronic structures and optical properties of the dots are also affected by the strain, and thus, strain control is regarded as an important means to modify emission wavelengths of QDs [20,22,23]. A large number of theoretical works have been devoted to such strained QD systems using single-band effective-mass approximations [1,24], multiband *kp* model [25–27] and pseudopotentials [28,29]. For QDMs, Jaskólski et al. study strain effects on the electric structure of strongly coupled self-assembled InAs/GaAs quantum dots using tight-binding approach [30]. They confirm the effect of strain-induced localization of the ground hole state in the lower dot. However, experimentally, it is difficult to address the influence of the strain on bonding characters of QDMs due to the variations of alloy distribution and complex three-dimensional structure in individual QDs from dot to dot. These uncertainties will mainly lead to shifts of resonant parameters. To solve the problem, the tunneling energies obtained from the experiments are used to fit the curves of photoluminescence (PL) spectrum versus electric fields in Refs. [9,14]. In these cases, influences of both strain and structure have been ignored and included in the parameter of

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http://dx.doi.org/10.1016/j.physb.2012.10.001

tunneling energy. Thus, the impact of strain on the anticrossing properties of QDMs under external electric fields is not systematically investigated, in particular, its influence on the resonant parameters (F_c and Δ_{BAB}) for different QDM structures accompanied by electron or hole resonance. Correspondingly, it is highly desirable for simulating QDMs to gain a better understanding of the strain effects on the properties of molecular bonding, and is also significant for designing molecular structures using strain-engineering technology.

Here we use the effective-mass model to systematically investigate the strain effects on coupling feature of resonant tunneling in two asymmetric QDM systems designed for electron and hole resonance. This paper is organized as follows. In Section 2 we present the structure models and theoretical methods used in this work. The strain effects on the resonant tunneling properties of electron and hole are shown in Sections 3.1 and 3.2, respectively. Finally, the conclusion is summarized in Section 4.

2. Model and calculation

Fig. 1(a) and (b) shows the vertically stacked $In_{1-x}Ga_xAs/GaAs$ asymmetric QDM structures studied in this paper. Each truncated pyramid with {0 1 1} side facet is characterized by the quantum dot height h, the dot width w and the dot separation distance d. To realize the anticrossing of two lowest energy levels, we design the asymmetric structure with $h1 > h2$ ($h1 < h2$) for electron (hole) resonance. Asymmetry control in self-assembled InAs QDs can be realized easily with the "indium flush" growth method in molecular beam epitaxy technology [13,14]. The band edge diagrams of Fig. 1(a) illustrate how the QDM asymmetry determines the electron tunneling. The bottom QD is thicker, it has a smaller ground energy, so a positive electric field across the QDM easily brings the individual QD electron levels into resonance, while the hole levels are detuned. When the order of the QDs is reversed, the positive electric field brings the QD hole levels into resonance (Fig. 1(b)).

To maximize the effects of strain, we consider the single-band effective-mass model to calculate the electronic properties of QDMs. The Hamiltonian of the system in external electric field is written as

$$H_{e,h} = \frac{p_{e,h}^2}{2m_{e,h}} + V_{e,h} + H_s + ez \bullet F \quad (1)$$

where $H_{e,h}$ and $V_{e,h}$ are, respectively, the single electron (hole) Hamiltonian and confinement potentials, and H_s is the strain-dependent one. The electric field F is assumed to point along the vertical [0 0 1] growth direction. The electron–hole Coulomb and exchange interactions are neglected in this work.

Since we are interested in the strain effects and therefore consider constant composition for each sample, changing the amount of Ga x actually alters both the confinement potentials and the strain distribution in and around the coupled dots. Hence, the dependence of tunnel coupling on the composition can reflect the influence of strain on the resonant state of QDMs. Furthermore, as shown from Eq. (1), the advantage of the model is that the strain effect can be separated from the structure and alloy parameters, since we can easily switch on/off the strain field and

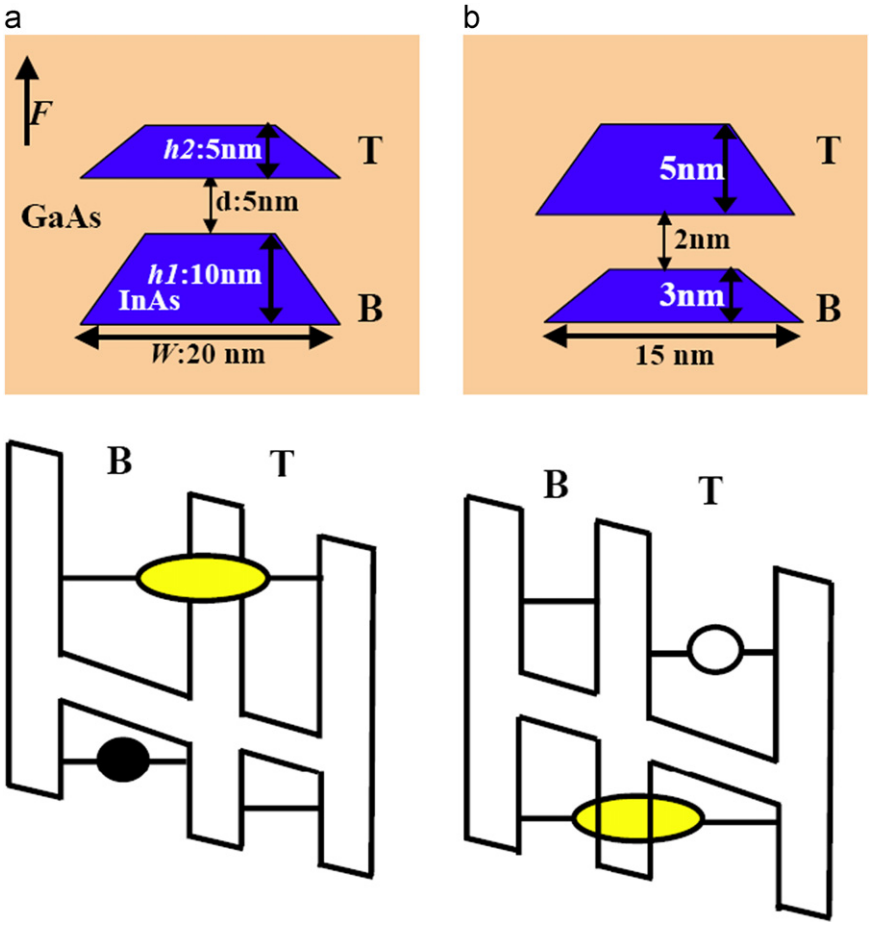

Fig. 1. Asymmetric QDM structures studied in this paper and band edge potentials for both types of QDM under forward electric field. (a) For electron resonance, $w=20$, $h1=10$, $h2=5$, and $d=5$ nm; (b) for hole resonance, $w=15$, $h1=3$, $h2=5$, and $d=2$ nm. Both QDMs result in electron and hole tunneling resonances, respectively.