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Asymmetric Stark shift in an impurity doped dome-shaped quantum dot with wetting layer

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ABSTRACT

The effects of vertical electric field and donor impurity on the electronic properties of the dome-shaped InAs/GaAs quantum dot coupled to its wetting layer were investigated. The dependence of the electron density, energy and Stark shift of the S-, P- and WL-states on the applied electric field was studied with and without impurity. The S- and P-states have no significant qualitative changes in the shape of the wave functions with increasing the electric field, except that they become slightly shifted due to the competition between the field action and the quantum confinement. The wave function of the WL-state is strongly modified in polarized structures. Our results reveal that the Stark shift of electron energies can be fitted with a quadratic dependence on the electric field, the linear and quadratic terms corresponding to the dipole moment and static electron polarizability. Their estimated values reasonable agree with those calculated.

1. Introduction

In recent years, quantum dots (QDs) have been extensively studied due to their potential applications in high performance devices. Therefore, a great deal of works has been performed on the electronic structures, impurity states and their binding energies, and optical properties [1–12] of QDs with different shapes of the confinement potential.

Particularly, self-assembled QDs obtained by the epitaxial growth of heterostructures with lattice mismatch between the substrate and the active layer have attracted considerable interest. In the Stranski-Krastanov fabrication process of these structures, 3D dot islands having various sizes and shapes are formed on a residual thin layer known as wetting layer (WL). Although initially in the theoretical works the WL and its role have been ignored due to the complexity of the calculation, the experiments and recent theoretical studies revealed its effects on the optical and electronic properties of QDs. An exhaustive description of the experimental and theoretical researches related to the WL influence on the electronic structure and performances of QD based devices can be found in [13] and references therein.

On the other hand, the application of external perturbations, such as the electric and magnetic fields, hydrostatic pressure, and temperature changes can provide much valuable information about the confined states in QDs. Moreover, these perturbations allow tuning the energy spectrum and optical properties for tailoring new electro-optical devices. Of particular interest is the action of an electric field on the carriers distribution and energy levels in QDs, the so-called Stark shift. It is well known that the quantum-confined Stark effect on the exciton energy in a semiconductor self-assembled QD [14] leads to a shift of the excitonic peak in absorption or photoluminescence spectra given by:

$$\Delta E(F) = E(F) - E(F=0) = -\vec{p}\cdot\vec{F} - \frac{1}{2}\beta F^2 \quad (1)$$

This quadratic form follows from a second-order perturbation theory with $\vec{p}$ the dipole moment and β the polarizability of the system [15]. Assuming that the donor impurity behaves like an exciton with infinite hole effective mass [16], it is expected that the field dependence of the Stark shift of the exciton energy to be also valid for the Stark shift of the donor energy. Zeng et al. [16] prove the validity of this hypothesis for hydrogenic donors in a self-assembled GaAs/AlGaAs quantum dot subjected to a tilted electric field. They found that ΔE has a quadratic decrease with the applied electric field for any field orientation. The results are in agreement with the symmetry consideration which implies the absence of the permanent dipole moment in the systems with

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inversion symmetry with respect to applied field direction. However, it is of interest to study the dependence of the impurity states energy on the electric field in structures without symmetry and the QD/WL can be such a system.

A number of studies have focused on the influence of the QD/WL size and shape on their electronic and optical properties. For example, Seravalli et al. [17] have investigated wetting layer states in InAs/InGaAs metamorphic quantum dot nanostructures. A comparison between semi-spheroid- and dome-shaped quantum dots coupled to wetting layer was presented by Shahzadeh and Sabaeian [18]. In the study of electronic properties and intersubband P-to-S transition features they found that, although there are different trends for these quantities in the studied structures, all the results coincide at a dot height of 7 nm, when both sets of values become identical. The theoretical results on the intersubband electronic and optical properties of three-dimensional self-assembled pyramid-shaped InAs/GaAs quantum dots (QDs) coupled to WL have been reported in Refs. [19,20].

Parvizi and Rezaei [21] have studied the effects of the shape and size on the intersubband electromagnetically induced transparency in strained truncated pyramid-shaped InAs/GaAs quantum dot. They found that the width of the transparency window can be tuned by the WL thickness and the depth of this window can be enhanced by increase of the QD height.

The influence of the structure parameters: QD height, base dimension length and WL thickness on the both z- and in-plane polarized intersubband transition in the same QD/WL structure have been recently reported [22]. Very little attention has been paid, however, to the changes in the energy spectrum of carriers in these structures due to the impurity centers and external applied fields. Within the effective mass approximation Dezhkam and Zakery [23] have obtained the electronic structure and the expressions for the absorptions and dispersions of the probe pulse in an InAs hemispherical quantum dot embedded in a GaAs barrier, with hydrogenic impurity located at the origin. Sabaeian et al. [24] have discussed the dependence of energy eigenvalues of S- and P-states and interlevel P-to-S transition energy on applied vertical electric field on a semi-spheroid-shaped InAs/GaAs quantum dot coupled to its WL. The variations of the transition dipole moment and linear and nonlinear optical susceptibilities on bias voltage have been also investigated.

So far, to the best of our knowledge, studies have not been extended to investigate the energy shift of the impurity states and carriers polarization in a QD/WL under applied electric fields. In this context, in this paper we investigate the electric field effect on the donor levels in a three dimensional dome-shaped InAs/GaAs QD coupled to its wetting layer. It is also important to provide a quantitative relation connecting the Stark shift of the donor energy with the applied electric field in these structures. This becomes another major motivation of the present theoretical study.

The paper is organized as follows. In Section 2, we present our model and explain the general theory. Section 3 is dedicated to the discussion of the obtained results, and our conclusions are given in Section 4.

2. Theory

In order to calculate the electronic properties of QDs coupled to WL (QD/WL) the single-band Schrödinger equation in the framework of effective mass approximation was solved using a finite element method. A dome-shaped InAs/GaAs QD with radius of 7 nm under vertical electric fields was considered (see Fig. 1). The thick of WL was set at 2 nm.

The Hamiltonian of the system is given by [13,25]:

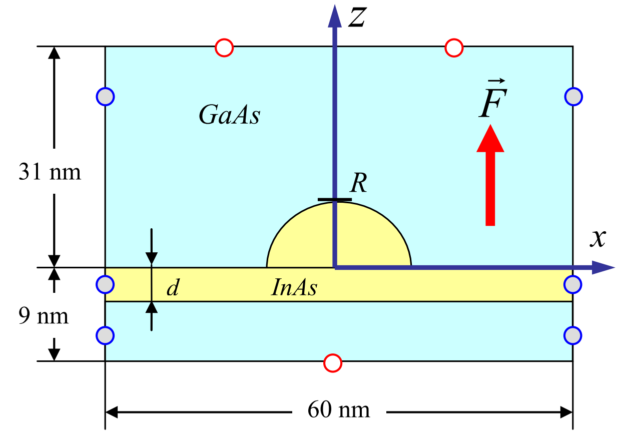

Fig. 1. The QD/WL cross-section in xOz plane. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$H = -\frac{\hbar^2}{2}\nabla\frac{1}{m^*(x,y,z)}\nabla + V(x,y,z) + eFz - \frac{e_0^2}{\varepsilon_r\sqrt{x^2+y^2+(z-z_i)^2+d_{cuttoff}^2}} \tag{2}$$

where the effective mass

$$m^*(x,y,z) = \begin{cases} m^*_{InAs}, & \text{in QD} \\ m^*_{GaAs}, & \text{elsewhere} \end{cases} \tag{3}$$

and

$$V(x,y,z) = \begin{cases} 0, & \text{in QD} \\ \Delta E_c, & \text{elsewhere} \end{cases} \tag{4}$$

is the potential energy. ΔE_c is the conduction band offset between the InAs and GaAs.

In the numerical calculations the values $m^*_{InAs} = 0.04m_0$, $m^*_{GaAs} = 0.067m_0$ and $\Delta E_c = 500$ meV are used. The third term represents the electrostatic potential induced by the electric field, F being its magnitude, and the last term is the Coulomb interaction between the electron and the donor impurity, located at $(0,\ 0,\ z_i)$. Because the impurity potential is singular at the origin we introduce a cut off distance to regularize it. According to Baskoutas et al. [26], we take for $d_{cuttoff}$ a fixed value below which the mean value of the Coulomb term does not changes. In the following, we choose $d_{cuttoff} = R\sqrt{10^{-5}}$ [26,27] where R is the dot radius.

In order to obtain the energy levels of the electron (E_e) and the donor (E_D) as well as the corresponding wave functions (WFs), the Schrödinger equation with the Hamiltonian given by Eq. (2) was solved by using the finite element method. Specialized software with nonlinear solver was used to solve the eigenvalues problem. Initially, a coarse predefinited tetragonal mesh is used, each maximal size in one direction being $1/10^{th}$ of the maximum distance in the geometry. We start with 1000 nodes. After the first iteration a WF coarse evaluation is obtained and a refinement grid is necessary. The mesh grid and implicit the finite element must be much smaller. The number of the finite elements becomes big and from numerical point of view, problems may occur for the models with large geometric scale. One way to reduce this problem is to split the geometry into subdomains which represent the various materials: the wetting layer (WL) and the hemispherical dome – i.e. InAs material – (yellow color in Fig. 1), and the other GaAs regions – (blue color in Fig. 1). Each region is meshed independently of each other. Consequently a finer mesh size is used for WL and