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Influence of strain on the Stark effect in InP/GaInP quantum discs

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Abstract

In InP/GaInP quantum discs it is shown that strain induces a type I to type II transition with increasing thickness of the disc. When an external electric field is applied along the cylindrical axis of the disc, the exciton energy exhibits a Stark effect, which for the light hole exciton becomes linear even for a small field value, while for the heavy hole it is more quadratic.

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1. Introduction

In recent years self-assembled quantum dots (QDs) have attracted considerable interest because they can be regarded as ideal model systems for quasi-zero-dimensional systems [1] and their promising advantages regarding opto-electronics [2]. Therefore, QDs are often called 'artificial atoms'. Many effects known from atomic physics were found in QDs, and of particular interest is the effect of an electric field on an exciton in a quantum dot, the so-called Stark shift. Recent experimental results [3,4] on InAs/GaAs QDs showed that the Stark shift exhibits an asymmetry in the presence of an electric field, due to a built-in dipole moment. Theoretical studies [5,6] have shown that the sign of this dipole moment in single dots depends on the composition gradient and/or strain effects, localizing the electron and hole in different regions of the quantum dot.

In this paper we study the Stark effect in type II QDs and extend our previous study on InP/GaInP QDs [7] to include the effects of strain. Our quantum dots are modelled by quantum discs of finite height and our calculations are based on a Hartree–Fock mesh calculation, done within the one-band model of the effective-mass approximation. InP/GaInP dots were also studied in Ref. [8]. However, the strain fields were not studied

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systematically as function of the height of the dot, nor was the Stark effect included.

2. Theoretical formalism

When self-assembled quantum dots are grown, strain is essential because it drives the QD growth process [1]. The strain in the material can change the band structure and possibly the effective mass. To calculate strain, we used a method based on Eshelby's theory [9] of inclusions and applied to quantum dots by Davies [10]. The elastic properties are assumed to be isotropic and homogeneous.

The procedure in the theory of inclusions consists in separating the total strain into different elements. One assumes that there is an infinite uniform sample of GaInP. From this sample, one removes the space that will form the quantum dot. This space is then transferred to a stress-free environment of InP. Since the lattice constant of InP is larger than the one of GaInP, the sphere will expand by a factor $\varepsilon_0 = a_{\mathrm{InP}}/a_{\mathrm{GaInP}} - 1$ (lattice mismatch). Then, a hydrostatic pressure is applied to reduce the volume of the sphere to its original volume. The compressed InP sphere is put in the cavity of the GaInP and allowed to relax. This causes a displacement in both the cavity and the surrounding material.

From the above argument it becomes clear that there are two different strains present in this approximation, first the strain caused by the hydrostatic compression and second the strain caused by the relaxation when the dot is inserted back into the cavity. The displacement vector $\vec{u}(\vec{r})$ due to the relaxation can easily be calculated [10] as an integral over the surface of the quantum dot:

$$\vec{u}(\vec{r}) = \frac{\varepsilon_0}{4\pi}\frac{1+v}{1-v}\oint \frac{\mathrm{d}\vec{S}'}{|\vec{r}-\vec{r}'|},$$

where v denotes the Poisson ratio for lateral contraction to longitudinal extension in a bar under terminal tension. For zinc-blende-type semiconductors it is known that $v \approx 1/3$. From this displacement, the corresponding strain tensor can easily be obtained by

$$\varepsilon_{i,j} = \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\bigg/2.$$

To take into account the strain due to the hydrostatic compression, an extra term $-\varepsilon_0$ needs to be added to the diagonal elements of the strain tensor inside the dot. This is due to the reduction of the lattice parameter in the dot material to the lattice parameter of the barrier material.

For our calculations the quantum dot is modelled by a disc of radius R and thickness d. We solved the Schrödinger equation within the one-band model of the effective mass approximation. By neglecting band mixing we obtain two sets of coupled equations, one for the heavy-hole and one for the light-hole exciton. The interaction between the electron and the hole is given by a Coulomb term in the potential. Within the effective mass approximation, the coupled single particle equations are given by

$$\left[H_{\mathrm{e,h}} + \int \frac{\rho_{\mathrm{h,e}}(\vec{r})}{|\vec{r}-\vec{r}'|}\,\mathrm{d}\vec{r}'\right]\psi_{\mathrm{e,h}}(\vec{r}) = E\psi_{\mathrm{e,h}}(\vec{r}), \quad (1)$$

with

$$H_{\mathrm{e,h}} = \frac{p_{\mathrm{e,h}}^2}{2m_{\mathrm{e,h}}} + V_{\mathrm{e,h}}(\vec{r}_{\mathrm{e,h}}) + S_{\mathrm{e,h}}(\vec{r}_{\mathrm{e,h}}) \mp eFz_{\mathrm{e,h}}, \quad (2)$$

where $H_{\mathrm{e,h}}$ and $V_{\mathrm{e,h}}$ are, respectively, the single electron (hole) Hamiltonian and confinement potentials, $S_{\mathrm{e,h}}$ is the conduction (respectively, valence) band deformation potential under the influence of the strain and F is the applied electric field. For the electron

$$S_{\mathrm{e}}(\vec{r}_{\mathrm{e}}) = a_{\mathrm{c}}(\varepsilon_{xx}(\vec{r}_{\mathrm{e}}) + \varepsilon_{yy}(\vec{r}_{\mathrm{e}}) + \varepsilon_{zz}(\vec{r}_{\mathrm{e}})) \quad (3)$$

with a_{c} the conduction band deformation potential [1]. The strain influences the heavy hole and the light hole differently and it can be calculated that

$$S_{\mathrm{h}}(\vec{r}_{\mathrm{h}}) = a_{\mathrm{v}}(\varepsilon_{xx}(\vec{r}_{\mathrm{e}}) + \varepsilon_{yy}(\vec{r}_{\mathrm{e}}) + \varepsilon_{zz}(\vec{r}_{\mathrm{e}})) \pm b(\varepsilon_{zz} + (\varepsilon_{xx} + \varepsilon_{yy})/2), \quad (4)$$

where the plus sign is used for the heavy hole and the minus sign for the light hole. The valence band deformation potentials are given by a_{v} and b [1].

These coupled single-particle equations are solved self-consistently using an iterative procedure. The exciton energy is given by

$$E_{\mathrm{tot}} = E_{\mathrm{e}} + E_{\mathrm{h}} + \frac{e^2}{4\pi\varepsilon}\int\int \frac{\rho_{\mathrm{e}}(\vec{r})\rho_{\mathrm{h}}(\vec{r}')}{|\vec{r}-\vec{r}'|}\,\mathrm{d}\vec{r}\,\mathrm{d}\vec{r}',$$