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Electron-hole transitions in self-assembled InAs/GaAs quantum dots: Effects of applied magnetic fields and hydrostatic pressure

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Abstract

A theoretical study of the effects of applied magnetic fields and hydrostatic pressure on the electron-hole transition energies in self-assembled InAs/GaAs quantum dots is presented. The effective-mass approximation and a model of a cylindrical-shaped quantum dot with in-plane parabolic potential have been used to describe the InAs/GaAs quantum dots. Present theoretical results are in quite good agreement with experimental measurements of the magnetic field and pressure dependence of the exciton transition energies in InAs/GaAs self-assembled quantum dots.
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Low-dimensionality semiconductor heterostructures constitute very interesting systems due both to their fundamental properties and potential applications in optoelectronics devices. Whereas quantum-well structures are already widely used in such devices, quantum-well wires and quantum dots (QDs) appear to be much more difficult to fabricate for these purposes. The formation of self-assembled quantum dots (SAQDs) by the Stranski-Krastanov growth mode has been demonstrated successfully in different material systems such as (Ga)InAs/(Al)GaAs or InP/GaInP heterostructures. By stopping the growth process in the initial state of formation of the nanostructure results in QDs free of defects and dislocations.

The understanding of the magnetic-field and pressure dependence of QD emission may be important for building efficient lasers. Itskevich et al. [1] have investigated the photoluminescence (PL) spectra of self-assembled InAs QDs embedded in a GaAs matrix in magnetic fields up to 23 T (applied in the growth direction) and under hydrostatic pressure up to 70 kbar. The sample [1] was grown by molecular-beam epitaxy on a ⟨100⟩ GaAs substrate, with the GaAs buffer layer grown at 600 °C, and 1.8 monolayers of InAs deposited at 450 °C after a growth interruption. The dots were capped at 450 °C by a 25-nm-thick GaAs layer. By measurements of the diamagnetic shift for the PL recombination line, Itskevich et al. [1] have concluded that the in-plane spatial extent of the carrier wave function in the InAs-dot is in the order of 60 Å. They have found that the pressure coefficient for the dot emission line is 9.1 ± 0.2 meV/kbar, and have attributed the dependence with the pressure to such effects as the change in the InAs energy gap, huge internal strain of the InAs dot, changes of the quantization energies of electrons and holes, and finally, in a minor scale, to changes in the Coulomb interaction energy and the small decrease of the dot size under compression.

In this work, we are concerned with the effects of an external magnetic field and hydrostatic pressure on the PL spectra in InAs/GaAs SAQDs. Calculations are made in the effective-mass approximation and a model of a cylindrical-shaped quantum dot with in-plane parabolic potentials has been used to describe the actual InAs/GaAs quantum dots. A detailed description of the theoretical treatment will be presented elsewhere. We take square potential-well barriers

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in the z-direction, and consider the relative motion of the carriers and that of the exciton center of mass as independent. The tangential and hydrostatic efforts due to the difference of lattice constants between the InAs-dot material and the GaAs-matrix material lift the degeneration between the heavy- and light-hole valence bands at $k=0$. In this work, we will concentrate in heavy-hole excitonic transitions.

We write the exciton envelope wave functions $F_m(\vec{\rho}, z_e, z_h)$ as a linear combination of products of single-particle f_k (z_e) and $f_{k'}$ (z_h) solutions of the effective-mass equation for electron or hole motion, respectively, along the z-axis of the QW, i.e. [2,3],

$$F_m(\vec{\rho}, z_e, z_h) = \sum_{k,k'} \psi^m_{k,k'}(\rho, \varphi) f_k(z_e) f_{k'}(z_h), \tag{1}$$

$$\psi^m_{k,k'}(\rho, \varphi) = \sum_j C^m_{k,k',j} \rho^{|m|} \, e^{im\varphi} \, e^{-\rho^2/\lambda_j^2}, \tag{2}$$

where the expansion in Eq. (2) is made in a restricted set of Gaussian functions with appropriate λ_j length parameters. Here we assume a cylindrical-shaped InAs QD model of radius R with in-plane infinite parabolic potential barrier, and the radius of the dot defined by $R=\sqrt{\hbar/\mu_{ex}\omega}$, where μ_{ex} is the exciton reduced effective mass and $\hbar\omega$ is the lateral confinement energy.

The strain effects on the geometric dimensions of the QD (h and R) may be obtained from the fractional change in volume associated with the hydrostatic pressure [4]. The parameters we have used in the present calculations are taken for the stressed InAs-QD and GaAs, respectively, as follows [5–10]: conduction effective masses $m_e=(0.040$ and $0.0665)$ in-growth direction heavy-hole effective masses $m_{hh,z}=(0.59$ and $0.377)$, in-plane heavy-hole effective masses $m_{hh,xy}=0.035$ and 0.112, conduction and valence band-offsets as $V(z)/[E_g(\text{GaAs})-E_g(\text{InAs})]=0.54$ and 0.46, static dielectric constants $\varepsilon=14.6$ and 12.35, the un-strained GaAs band gap pressure coefficient $\alpha=10.8$ meV/kbar, and the strained InAs-dot band gap pressure coefficient $\alpha=7.7$ meV/kbar.

In the process of growth, stress effects are generated in the interfaces of the well and barrier. A precise quantitative treatment of SAQDs should, therefore, include the size, shape, and stress effects which may be decomposed in hydrostatic and tangential components, as well as valence-band mixing, i.e. mixing between the light- and heavy-hole bands [12,13]. However, we note that, from the experimental work by Itskevich et al. [1], the actual shape and dimensions of the SAQDs are not precisely known, and therefore we have chosen to adopt a simple treatment of the problem, and to mimic the actual InAs/GaAs QDs with appropriate cylindrical QDs in which we consider in-plane parabolic potentials which would correspond to a given experimental measurement.

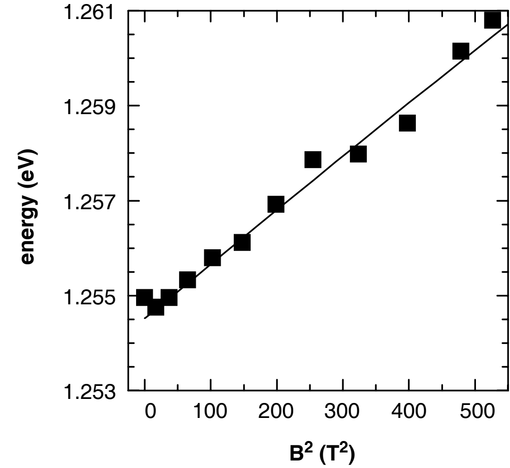

Fig. 1. Magnetic-field dependent correlated e–h energy transitions in parabolic-potential-cylindrical-shaped InAs QDs with $R=47.3$ and $h=10.1$ Å. Full squares are the experimental data from Itskevich et al. [1].

In Fig. 1, we report the theoretical results for the magnetic-field dependence of the correlated e–h energy transitions in parabolic-potential cylindrical-shaped InAs QDs [12,13]. The procedure we have followed consists in adjusting the dimensions of the theoretical structure so that the calculated correlated e–h transitions fit the zero-field experimental data from Itskevich et al. [1]. In this case, the dimensions were found as $R=47.3$ Å and $h=10.1$ Å. It is apparent from Fig. 1 that the present theoretical findings as functions of the magnetic field applied in the growth-direction are in good agreement with the experimental measurements of the e–h transition energy. A magnetic field up to 23 T leads to changes of the order of 6 meV, which is quite small as compared with the quantum-sized confinement energies of the carriers (magnitude order of 100 meV), and therefore, one may conclude that the adopted QD cylindrical confinement potential is quite adequate to quantitatively model the actual QDs in the experiment. It is worth noting that Itskevich et al. [1] have reported an anisotropic behaviour for the magnetic field-dependence of the PL energy line in their measurements. Again, the calculated results (cf. Fig. 1) suggest that the PL-line center dependence on the applied magnetic field along the axis of the QD cylinder is well modelled by the present parabolic cylindrical-shaped QD.

We have also performed calculations of the effects of hydrostatic pressure on the correlated e–h transition energies for parabolic-potential cylindrical-shaped InAs QDs. We notice that, at an hydrostatic pressure of the order of 9 kbar, experiment [1] with InAs SAQDs shows an increase of the e–h transition energy of about 80 meV, whereas the theoretical increment [10] in the energy gap for self-assembled InAs/GaAs QDs is 70 meV (for un-stressed InAs the pressure coefficient is 9.8 meV/kbar [9]). It is apparent, therefore, that the increase of the e–h transition

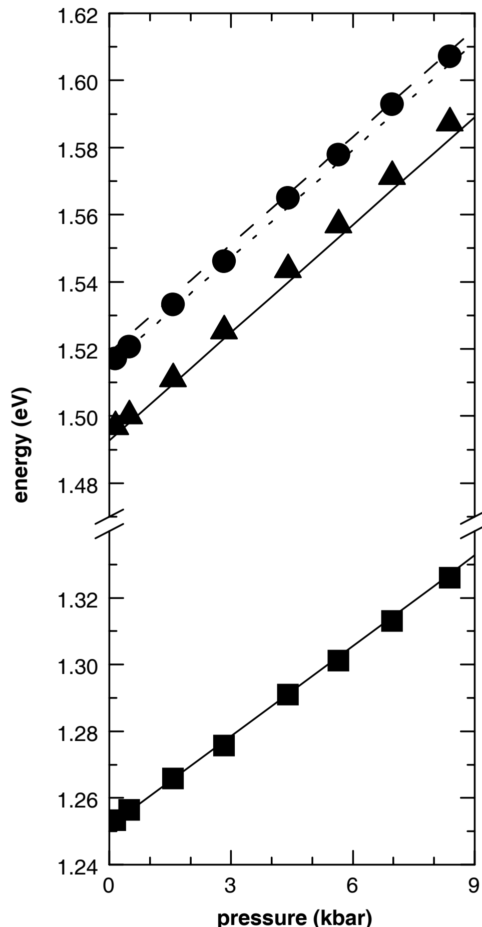

Fig. 2. Theoretical pressure-dependent conduction/valence-related (upper dotted line), bound exciton (upper dashed line), and acceptor (upper solid line) PL features in bulk GaAs. Also shown are the present theoretical results of the pressure-dependent correlated *e–h* energy transitions in parabolic-potential-cylindrical-shaped InAs QDs with $R=47.0$ and $h=10.2$ Å (lower full line). Full symbols are the experimental data from Itskevich et al. [1].

energy with applied hydrostatic pressure is essentially associated to the variation of the InAs energy gap. We first performed calculations for the pressure-dependent conduction/valence-, bound exciton-, and acceptor-PL features in bulk GaAs, with excellent agreement with experimental measurements [1], as seen in the upper part of Fig. 2, which also displays the present theoretical results of the pressure-dependent correlated *e–h* energy transitions in parabolic-potential cylindrical-shaped InAs QDs. In this case, the dimensions of the structure at atmospheric pressure are $R=47.0$ Å and $h=10.2$ Å. We note that the presence of the GaAs band gap results, at 9 kbar, in an increase of 15 meV in the height of the potential barrier for electrons, and 13 meV in the potential barrier for holes. The changes with stress in the electron and hole confinement potentials and radius and height of the structure lead to variations of the order of 10 meV, at 9 kbar, in the confinement energy of the *e–h* pair. The last two effects may give a small increasing of 10 meV in the *e–h* transition.

In conclusion, we have reported theoretical results of the applied magnetic-field and hydrostatic pressure effects on the transition energy for an *e–h* pair in InAs/GaAs SAQDs. We stress that the present model of a simple parabolic-potential cylindrical-shaped InAs QD clearly describes in an excellent quantitative form the experimental measurements by Itskevich et al. [1] on the effects of magnetic field and hydrostatic pressure on the electron-hole transition energies in InAs/GaAs SAQDs.

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