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Determination of Quantum Dot Morphology from Magnetooptical Properties

V. Křápek[a,b,*], A. Schliwa[b] and D. Bimberg[b]

[a]Institute of Condensed Matter Physics, Faculty of Science, Masaryk University
Kotlářská 2, 611 37 Brno, Czech Republic

[b]Institut für Festkörperphysik, Technische Universität Berlin
Hardenbergstr. 36, 10623 Berlin, Germany

We present here the calculations of magnetooptical properties in InAs/GaAs quantum dots with different shapes, including excitonic effects. The influence of several structural parameters, such as vertical profile, aspect ratio, and basis squareness is discussed, as well as the possibility to retrieve the structural parameters from magnetooptical measurements.

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1. Introduction

Magnetic properties of quantum dots (QDs) are presently widely studied. Magnetophotoluminescence has been used in many studies of different properties of QD structures, including the morphology [1], or the impact of the elongation on the exchange interaction [2]. In order to understand correctly these effects, a detailed theory describing the electronic levels is necessary. We present here a systematic theoretical study of InAs/GaAs QD electronic structure in magnetic field for different dot shapes, we discuss particularly the effect of basis roundness/squareness, vertical profile, and aspect ratio to magnetooptical properties. Moreover, we discuss the possibility to retrieve the structural parameters from magnetooptical measurements.

The calculations of single particle states are carried out using the eight-band $k \cdot p$ theory [3, 4], including the influence of strain and first- and second-order piezoelectricity [5, 6]. A magnetic field is introduced through Peierl's substitution

*corresponding author; e-mail: krapek@physics.muni.cz

in the wave vector and by adding the Zeeman energy term [7]. The exciton energies are calculated using the configuration interaction (CI) method, expanding the wave function into a basis of the Slater determinants constructed from single-particle states. The accuracy of the results is limited mainly by neglection of distant bands in $k \cdot p$ theory; we estimate the error to be up to 5% for both absolute energies and energy shifts.

2. Results and discussion

As an example, we discuss here magnetooptical properties of the QD of lens shape with a height of 3 nm and a diameter of 20 nm. The evolution of the electron levels in magnetic field follows the Fock–Darwin (FD) pattern: we observe a diamagnetic shift of all states and a paramagnetic shift of states with non-zero orbital moment. Moreover, a splitting of double degenerate states with opposite spin occurs in non-zero field. The situation for hole levels, depicted in Fig. 1, is more complex. The holes are heavier than electrons and therefore experience the piezoelectric symmetry reduction more strongly. Moreover, band mixing, particularly of heavy and light holes, is more pronounced. The behaviour of ground state is similar to the electron case (diamagnetic shift and spin splitting). For excited states (of p-like structure), the following discrepancies with FD model occur: (a) There is a splitting of p-states at zero field with magnitude of 9 meV due to piezoelectricity. (b) The spin splitting is comparable to the bound state orbital moment splitting. (c) Excited states exhibit anticrossing behaviour (e.g. at 13 T in Fig. 1), which is connected to piezoelectricity. When the piezoelectric field is excluded from our model, the standard crossing behaviour is restored.

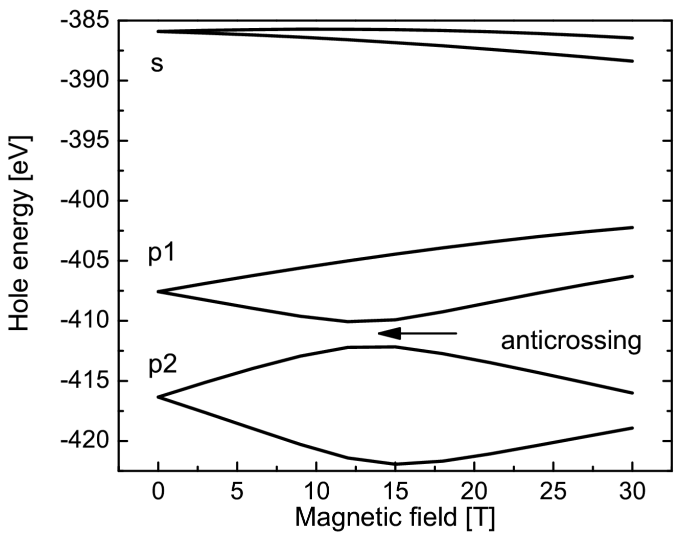

Fig. 1. The hole energies in lens-shaped quantum dot in a magnetic field.

The optical transition are calculated using the Fermi golden rule. The FD pattern for magnetic field is restored for them, since the energy shifts are significantly larger for electrons than for holes. In the following, we denote the transitions according to the approximate symmetry of involved states s-transition (for ground transition) and p-transition (excited transition between p-like states). We also average all energy shifts over two transitions with opposite spins. For the QD considered above and a magnetic field of 30 T, the diamagnetic shift of s-transition is 7.73 meV, and the diamagnetic shift and paramagnetic splitting of p-transitions are 12.72 meV and 77.10 meV, respectively. The FD model, with the effective mass fitted to s-transition ($m^* = 0.044$), gives the p-transition diamagnetic shift of 15.22 meV and paramagnetic splitting of 77.18 meV.

The direct Coulomb energy between the ground electron and hole state varies from –24.44 meV at 0 T to –25.11 meV at 30 T. This can be understood by considering the magnetic-field-induced additional confinement: the wave functions get squeezed and the Coulomb interaction is increased [8]. This effect decreases the diamagnetic shift effectively by approximately 10%. Another effect of the Coulomb interaction is the change (squeezing) of the wave functions due to the attraction of electron and hole. In our CI approach this is described by correlation, which is done by incorporating Slater determinants composed of higher states into the exciton wave function. Including the p-states into the basis (i.e., using 6 states for electrons and 6 for holes), we found a correlation energy of 0.55 meV, being almost constant for magnetic field ranging from 0 T to 30 T. This demonstrates the fact that the excitons are in a strong confinement regime in a considered dot; for larger QDs, the correlation effect would be more pronounced [4].

Next, we discuss the shape influence by reviewing of cone, lens, and cylinder-shaped QDs described within the single-band $k \cdot p$ theory. The sizes of the dots are tuned to the same lowest transition energies of 1.0 and 1.1 eV. The s-transition diamagnetic shift and p-transition paramagnetic splitting are equal for all QDs (at 30 T 12.6 meV and 107 meV, respectively). Differences occur in the p-transition diamagnetic shift, which is 20.2 meV for cylinder, 23.6 meV for lens, and 26.1 meV for cone. The FD model fitted to the s-transition diamagnetic shift predicts 25.2 meV, which is similar to the cone case. The ratio of diamagnetic shift of p- and s-transition is almost constant over the magnetic field ranging from 0 T to 30 T. The values of the ratio are 1.60 for cylinder, 1.87 for lens, and 2.07 for cone.

We further compare magnetooptical properties of the dots with five different shapes (cone, pyramid, lens, cylinder, box) and four values of aspect ratios A (1/6, 1/4, 1/3, 1/2), calculated within the eight-band $k \cdot p$ theory. The volume of all considered dots is constant (for example, the flattest box has a height of 2.82 nm and lateral dimension of 16.88 nm). The ground transition energies vary from 0.981 eV (box, $A = 1/6$) to 1.107 eV (lens and cylinder, $A = 1/2$). Higher aspect ratios mean always a higher ground transition energy. This increase is caused by the increase in strain, which overcomes a lower quantum confinement caused by increase in the lowest dimension (i.e., height). The increase is most pronounced for compact shapes like cylinder and box (from 0.981 eV to 1.089 eV for box), for the spread shapes (pyramid, cone, lens) is reduced (from 1.066 eV to 1.087 eV for pyramid). The energy differences between first excited and ground transition vary from 80 meV to 108 meV, slightly higher for compact shapes, increasing with transition energy.

Figure 2 displays the p-transition diamagnetic shift. The values of the shift are determined by transition energy and vertical profile, with clear differences between compact and spread shapes for transition energies below 1.06 eV. Therefore, the measurement of the shift allows a specification of the vertical profile. There is no significant difference between round and square-based dots. The s-transition diamagnetic shift is qualitatively similar to the p-transition, in contradiction to the single-band $k \cdot p$ theory. Higher values for spread shapes are mainly due to hole contributions.

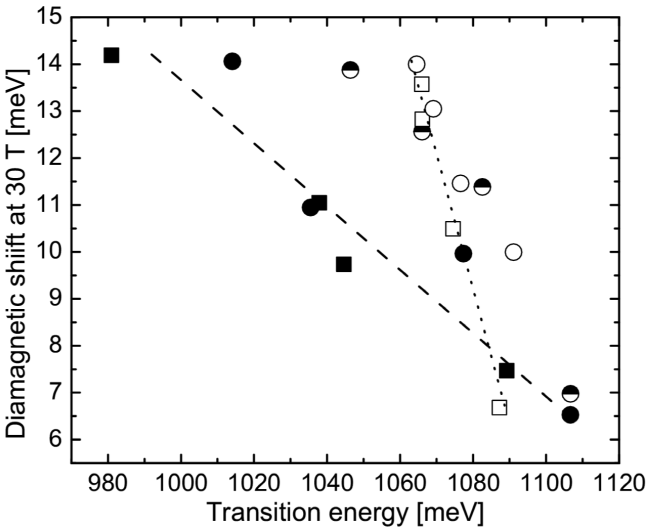

Fig. 2. The diamagnetic shift of p-transitions for box- (full squares), cylinder- (full circles), lens- (halffull circles), pyramid- (empty squares), and cone-shaped (empty circles) dots. Eye-guidelines are displayed for compact (dashed line) and spread (dotted line) QDs.

The paramagnetic splitting slightly decreases with increasing transition energy from 84 meV to 62 meV (with exception of pyramids). There is no clear effect of particular dot shape for lens, cone, cylinder and box. This is rather surprising in the case of the box, where the rotational symmetry is broken and a change in the paramagnetic splitting would be expected, as in the case of symmetry breaking by lateral elongation [9]. However, the finite effective mass of particles leads to smooth wave functions and a partial restoring of rotational symmetry, which explains the observed behaviour. The paramagnetic splitting in pyramids is reduced (for $A = 1/2$, it is 64 meV in cone, but only 39 meV in pyramid). This decrease is partially due to a broken rotational symmetry, but mainly due to a larger piezoelectric splitting of p-states in pyramids (for $A = 1/6$, where the piezoelectric splitting is small for both pyramid and cone, the difference in their paramagnetic splitting is as low as 5 meV).

3. Conclusions

In conclusion, the most important structural parameter influencing the magnetooptical properties is the vertical shape. From measurements of the diamagnetic shift we are able to distinguish between compact (box, cylinder) and spread (pyramid, cone, lens) QDs. A square basis leads to reduced paramagnetic splitting for pyramids; no such effect was found for boxes (it may be expected in larger dots). The aspect ratio influences zero-field energies, it has no observable effect to magnetooptical properties.

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