phys. stat. sol. (b) **226**, No. 1, 175–184 (2001)

Spin–Orbit Energy State Splitting in Semiconductor Cylindrical and Spherical Quantum Dots

O. VOSKOBOYNIKOV (a, b), C. P. LEE (a), and O. TRETYAK (b)

(a) National Chiao Tung University, 1001 Ta Hsueh Rd., Hsinchu, 300, Taiwan

(b) Kiev Taras Shevchenko University, 64 Volodymirska st., 01033 Kiev, Ukraine

(Received February 15, 2001; in revised form May 2, 2001; accepted May 4, 2001)

Subject classification: 71.70.Ej; 73.21.La; S7.12; S7.13

We present a theoretical study of the spin–orbit interaction impact on electron energy states in small cylindrical and spherical quantum dots. The investigation is based on the effective one-electronic band Hamiltonian and the spin dependent boundary conditions. It has been demonstrated that the spin–orbit interaction can significantly modify the energy spectrum of InAs and InSb quantum dots. The splitting can provide a situation where only the lowest spin split energy states are bound in the dot. A reasonable agreement was found with data from more sophisticated theoretical models for the spherical quantum dots which is available in the literature.

1. Introduction

The study of semiconductor quantum dots (QDs) and nanocrystals in recent years has been of a great interest from experimental and theoretical points of view (see [1–3] and references therein). The interest originates from an ultimate limit of size quantization in solids in those objects. For an ideal QD the electron spectrum consists of a set of discrete levels and the level density is a set of δ-functions. This makes the semiconductor quantum dots very attractive for possible applications in micro and nano-optoelectronics [2]. On the other hand, unique electronic characteristics of the QDs make it possible to model atomic physics in macroscopic systems experimentally and theoretically [4]. Thus, the electron energy level hierarchy in QDs is an object of extensive investigations.

The electron spin plays an important role in the QD design, and spin effects can significantly alter the electron energy spectrum [5–7]. An additional interest in the spin dependent energy structure of semiconductor QDs is produced by a new branch of semiconductor electronics, the so called "spintronics" [8, 9]. In semiconductor spintronics devices, the carrier generation, recombination, and transport will be controlled by the electron spin polarization as well as the electron charge. Obviously, a study of the electron spin-dependent confinement in semiconductor QDs can be an essential part of the semiconductor spintronics development.

The spin–orbit interaction has been used successfully to interpret many experimental results in various quantum structures of III–V semiconductors, quantum wells and wires [10–21]. It has been found that this interaction can change the electronic properties of those structures essentially. In this paper, we investigate the spin–orbit interaction impact on QD energy states of narrow gap semiconductors such as InAs and InSb. Different methods have been used in recent theoretical investigations of QDs (see e.g. [4, 22–28] and references therein). In this study we use the effective one-band spin-dependent Hamiltonian with the spin-dependent boundary conditions [14, 15]. Cou-

 0370-1972/01/22607-0175 $ 17.50+.50/0

lomb interaction between electrons is neglected for simplification. However, it has been shown recently (see e.g. [29]), that the electron–electron interaction in systems with a strong confinement can lead to a reinforcement of the spin–orbit interaction. In addition, we will show that the spin–orbit interaction plays an important and interesting role in relatively small QDs where the Coulomb interaction can be described by means of perturbation theory. It will be clear from the following that principal consequences of the spin–orbit interaction can be discussed with the used simplifications.

The QDs size, shape, and material parameters are obviously important for the electron energy state determination. We consider cylindrical and spherical QDs with hard-wall confinement potential that is induced by the discontinuity of the conduction band edge of the systems. This model is commonly used in calculations of the electron energy states in QDs [26]. The symmetry allows us to solve the three-dimensional Schrödinger equation with a small number of additional approximations. In the same time the basic structure parameters (such as the energy gaps, effective masses, band offsets etc.) are affected by different factors (strain in the system, for instance) and are often poorly known. The parameters for cylindrical QDs vary within a wide range in the modern literature [24, 25]. In our calculations we adjust the parameters in accordance to available information. As a reference, we consider spherical QDs, which can be produced by means of colloidal chemistry techniques [23, 30]. For the last mentioned type of QDs we can use well adjusted material parameters.

The paper is organized as following. Section 2 begins with an introduction to the effective one band spin-dependent Hamiltonian and the spin-dependent boundary conditions used for quantum heterostructures. Section 3 describes lines of calculations for cylindrical and Section 4 for spherical QDs. Section 5 is devoted to the discussion of the calculated results. Conclusions are drawn in Section 6.

2. Effective Hamiltonian and Spin-Dependent Boundary Conditions

We will consider electrons confined in three-dimensional quantum structures and use the approximate one-band effective Hamiltonian [15],

$$\hat{H} = \hat{H}_0 + \hat{V}_{\mathrm{so}}(\mathbf{r})\,. \tag{1}$$

In Eq. (1) H_0 is the system Hamiltonian without spin–orbit interaction [31],

$$\hat{H}_0 = -\frac{\hbar^2}{2}\,\nabla_{\mathbf{r}}\left(\frac{1}{m(E,\mathbf{r})}\right)\nabla_{\mathbf{r}} + V(\mathbf{r})\,,$$

where $\nabla_{\mathbf{r}}$ stands for the spatial gradient, $m(E,\mathbf{r})$ is the energy and position dependent electron effective mass,

$$\frac{1}{m(E,\mathbf{r})} = \frac{2P^2}{3\hbar^2}\left[\frac{2}{E + E_{\mathrm{g}}(\mathbf{r}) - V(\mathbf{r})} + \frac{1}{E + E_{\mathrm{g}}(\mathbf{r}) + \Delta(\mathbf{r}) - V(\mathbf{r})}\right],$$

$V(\mathbf{r})$ is the confinement potential, $E_{\mathrm{g}}(\mathbf{r})$ and $\Delta(\mathbf{r})$ stand for the position dependent band gap and the spin–orbit splitting in the valence band, respectively, and P is the conventional momentum matrix element [31, 32]. The spin–orbit interaction for the conduct-

ing band electrons $V_{so}(\mathbf{r})$ is described by [15, 33, 34]

$$\hat{V}_{so}(\mathbf{r}) = i\nabla\beta(E,\mathbf{r})\cdot[\hat{\boldsymbol{\sigma}}\times\nabla]\,, \tag{2}$$

where

$$\beta(E,\mathbf{r}) = \frac{P^2}{3}\left[\frac{1}{E+E_g(\mathbf{r})-V(\mathbf{r})} - \frac{1}{E+E_g(\mathbf{r})+\Delta(\mathbf{r})-V(\mathbf{r})}\right],$$

is the spin–orbit coupling parameter, and $\hat{\boldsymbol{\sigma}} = \{\sigma_x\sigma_y\sigma_z\}$ is the vector of the Pauli matrices.

For systems with a sharp discontinuity of the conduction band edges between the QD (material 1) and the semiconductor matrix (material 2) the hard-wall confinement potential can be presented as

$$V(\mathbf{r}) = \begin{cases} 0; & \mathbf{r}\in 1\,, \\ V_0; & \mathbf{r}\in 2\,. \end{cases}$$

From integration of the Schrödinger equation with Hamiltonian (1) along the direction perpendicular to the interface ($\mathbf{r}_n$) we obtain the spin dependent Ben Daniel-Duke boundary conditions for the electron wave function $\Psi(\mathbf{r})$,

$$\Psi_A(\mathbf{r}_s) = \Psi_B(\mathbf{r}_s)\,,$$
$$\left\{\frac{\hbar^2}{2m(E,\mathbf{r}_s)}\,\nabla - i\beta(E,\mathbf{r}_s)\,[\hat{\boldsymbol{\sigma}}\times\nabla]\right\}_n \Psi(\mathbf{r}_s) = \text{const.}\,, \tag{3}$$

where $\mathbf{r}_s$ denotes the position of the system interface. The boundary conditions above obviously depend on the electron spin and originate from the difference of the spin–orbit interaction parameters in different materials

.

3. Cylindrical QDs

When the quantum dot has a disk shape of radius ρ_0 and thickness z_0 we solve the problem with cylindrical coordinates (ρ,ϕ,z). The origin of the system lies in the center of the disk and the z-axis is chosen along the rotation axis. Because of the cylindrical symmetry the wave function can be represented as

$$\Psi(r) = \Phi(R,z)\exp(il\phi)\,,$$

where $l = 0, \pm1, \pm2, \ldots$ is the electron orbital quantum number. To derive the equation for $\Phi(R,z)$ we will use the adiabatic approximation [26, 27, 35], when an approximate wave function can be taken in the form

$$\Phi(R,z) \simeq R(\rho)\,Z(z)\,.$$

First, we consider the ground state of the z-direction electron motion and solve the one-dimensional quantum well problem. The wave function of the ground state has the form

$$Z(z) = \begin{cases} A\cos(kz)\,; & |z| < z_0/2\,, \\ B\exp(-\varkappa|z|)\,; & |z| \geq z_0/2 \end{cases}, \tag{4}$$

where

$$k(E_\rho, E_z) = \frac{\sqrt{2m_1(E_\rho + E_z)\,E_z}}{\hbar}$$
$$\varkappa(E_\rho, E_z) = \frac{\sqrt{2m_2(E_\rho + E_z)\,(V_0 - E_z)}}{\hbar}\,,$$

$m_i(E)$ is the energy dependent electron effective mass inside $(i = 1)$ and outside $(i = 2)$ the dot, E_ρ and E_z are the effective energies of the ρ- and z-direction motions (the total electron energy is $E = E_\rho + E_z$). From the Ben-Daniel Duke boundary conditions we can obtain the transcendental equation

$$\tan\left[\frac{k(E_\rho, E_z)\,z_0}{2}\right] = \frac{m_1(E)}{m_2(E)}\,\frac{\varkappa(E_\rho, E_z)}{k(E_\rho, E_z)}\,. \tag{5}$$

Equation (5) gives the dependence E_z (E_ρ) in an implicit form. We substitute the wave function (4) (after proper normalization) in the three-dimensional Schrödinger equation and then integrate out the z-coordinate by taking the average

$$\int \mathrm{d}z\, Z^*(z)\,\hat{H}Z(z) = \hat{H}_\rho\,.$$

The quasi-one-dimensional Schrödinger equation in the ρ-direction (we neglect the electron kinetic energy contribution from the z-dependent part for $\rho \geq \rho_0$ [35]) is given in the form

$$-\frac{\hbar^2}{2\tilde{m}_1(E_\rho, E_z)}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{\mathrm{d}}{\rho\,\mathrm{d}\rho} - \frac{l^2}{\rho^2}\right) R_1(\rho) = E_\rho R_1(\rho)\,; \qquad \rho < \rho_0,$$
$$-\frac{\hbar^2}{2m_2(E_\rho + E_z)}\left(\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{\mathrm{d}}{\rho\mathrm{d}\rho} - \frac{l^2}{\rho^2}\right) R_2(\rho)$$
$$= \left[E_\rho + E_z(E_\rho) - V_0\right] R_2(\rho)\,; \qquad \rho \geq \rho_0\,, \tag{6}$$

and the spin-dependent boundary conditions (3) become of the form

$$R_1(\rho_0) = R_2(\rho_0)\,,$$
$$\frac{1}{\tilde{m}_1}\,\frac{\mathrm{d}R_1}{\mathrm{d}\rho}\bigg|_{\rho_0} - \frac{1}{m_2}\,\frac{\mathrm{d}R_2}{\mathrm{d}\rho}\bigg|_{\rho_0} + 2\sigma\,\widetilde{\Delta\beta}\,\frac{l}{\hbar^2\rho_0}\,R_1(\rho_0) = 0\,. \tag{7}$$

In Eqs. (6) and (7)

$$\frac{1}{\tilde{m}_1(E_\rho, E_z)} = \frac{1}{C_1 + C_2}\left[\frac{C_1}{m_1(E)} + \frac{C_2}{m_2(E)}\right],$$
$$\widetilde{\Delta\beta}(E_\rho, E_z) = \frac{C_1[\beta_1(E) - \beta_2(E)]}{C_1 + C_2}\,,$$

where

$$C_1 = \frac{z_0}{2} + \frac{m_2(E)}{\varkappa(E_\rho, E_z)\,m_1(E)}\,\sin^2\left[\frac{k(E_\rho, E_z)\,z_0}{2}\right],$$
$$C_2 = \frac{1}{\varkappa(E_\rho, E_z)}\,\cos^2\left[\frac{k(E_\rho, E_z)\,z_0}{2}\right],$$

and $\sigma = \pm 1$ refers to the spin polarization along the z-axis. Equation (6) with the boundary conditions (7) are used to obtain the function $R(\rho)$. A formal solution of Eq. (6) is well known as the following:

$$R_1(\rho) = A\mathrm{J}_{|l|}\left[p(E_\rho, E_z)\,\rho\right],$$
$$R_2(\rho) = B\mathrm{K}_{|l|}\left[\gamma(E_\rho, E_z)\,\rho\right],$$

where J_n and K_n are the Bessel function and the modified Bessel function, respectively, and

$$p(E_\rho, E_z) = \frac{\sqrt{2\tilde{m}_1(E_\rho, E_z)\,E_\rho}}{\hbar},$$
$$\gamma(E_\rho, E_z) = \frac{\sqrt{2m_2(E_\rho, E_z)\,(V_0 - E_\rho - E_z)}}{\hbar}.$$

After using the boundary conditions (7), the equation that gives the electron energy states of the dot is found to be

$$\frac{p}{\tilde{m}_1}\left[\frac{|l|}{p\rho_0}\,\mathrm{J}_{|l|}(p\rho_0) - \mathrm{J}_{|l|+1}(p\rho_0)\right]\mathrm{K}_{|l|}(\gamma\rho_0)$$
$$-\frac{\gamma}{m_2}\left[\frac{|l|}{\gamma\rho_0}\,\mathrm{K}_{|l|}(\gamma\rho_0) - \mathrm{K}_{|l|+1}(\gamma\rho_0)\,\mathrm{J}_{|l|}(p\rho_0)\right]$$
$$+2\sigma\,\widetilde{\Delta\beta}\,\frac{l}{\hbar^2\rho_0}\,\mathrm{J}_{|l|}(p\rho_0)\,\mathrm{K}_{|l|}(\gamma\rho_0) = 0. \tag{8}$$

Equation (8) is the second equation we need besides Eq. (5) to solve the problem and to obtain the "self-consistent" value of the total energy $E = E_z + E_\rho$. The energy is a complicated function of the dot parameters, the electron angular momentum, and spin. The energy spectrum of the dot consists of a set of discrete levels numerated by a set of numbers $\{n, l, \sigma\}$, where n is the n-th solution of (8) with fixed l and σ. States having the same value of n and parallel (antiparallel) orbital momentum and spin remain twofold degenerate (the known Kramers degeneracy). But n-th states with antiparallel orbital momentum and spin are separated from the n-th states with parallel orbital momentum and spin.

4. Spherical QDs

When the dots have spherical shapes the solution of the three-dimensional Schrödinger equation solution can be obtained in spherical coordinates (r, θ, ϕ). The spherical symmetry of the problem allows us to write the electron wave function as

$$\Psi(\mathbf{r}) = f_l(r)\,\mathrm{Y}_{lm}(\theta, \phi), \tag{9}$$

where $f_l(r)$ is the radial wave function and $\mathrm{Y}_{lm}(\theta, \phi)$ is the spherical harmonics, m is the projection of the angular momentum along the z-direction. Substituting (9) into the three-dimensional Schrödinger equation with the Hamiltonian (1) we find the equation

$$-\frac{\hbar^2}{2m_1(E)}\left[\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\,r^2\,\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2}\right]f_{1l}(r) = Ef_{1l}(r); \qquad r < r_0,$$
$$-\frac{\hbar^2}{2m_2(E)}\left[\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\,r^2\,\frac{\mathrm{d}}{\mathrm{d}r} - \frac{l(l+1)}{r^2}\right]f_{2l}(r) = (E - V_0)\,f_{2l}(r); \qquad r \geq r_0, \tag{10}$$

where r_0 is the sphere radius. The spin dependent boundary conditions (3) for the spherical QD can be written as

$$
\begin{aligned}
& f_{1l}(r_0) = f_{2l}(r_0)\,, \\
& \frac{\hbar^2}{m_1(E)}\,\frac{\mathrm{d}}{\mathrm{d}r}\,f_{1l}(r)\bigg|_{r_0} - \frac{\hbar^2}{m_2(E)}\,\frac{\mathrm{d}}{\mathrm{d}r}\,f_{2l}(r)\bigg|_{r_0} \\
& + \frac{2[\beta_1(E)-\beta_2(E)]}{r_0}\left[j(j+1)-l(l+1)-\frac{3}{4}\right] f_{1l}(r_0) = 0\,,
\end{aligned}
\tag{11}
$$

where j is the total angular momentum quantum number ($j = \left|l \pm \frac{1}{2}\right|$ for states with spin-up and spin-down, respectively).

The radial function for the dot and barrier regions are given, respectively, by

$$
\begin{aligned}
& f_{1l}(r) = D\,\sqrt{\frac{1}{\lambda r}}\;\mathrm{J}_{l+\frac{1}{2}}(\lambda r)\,, \\
& f_{2l}(r) = C\,\sqrt{\frac{1}{\mu r}}\;\mathrm{K}_{l+\frac{1}{2}}(\mu r)\,,
\end{aligned}
\tag{12}
$$

where

$$
\lambda(E) = \frac{\sqrt{2m_1(E)\,E}}{\hbar}\,,
$$

and

$$
\mu(E) = \frac{\sqrt{2m_2(E)\,(V_0 - E)}}{\hbar}\,.
$$

Substitution of (12) into (11) gives the following equation for the electron energy states in the dot:

$$
\begin{aligned}
& \frac{1}{m_1}\,[l\mathrm{J}_{l+\frac{1}{2}}(\lambda r_0) - \lambda r_0 \mathrm{J}_{l+\frac{3}{2}}(\lambda r_0)\,\mathrm{K}_{l+\frac{1}{2}}(\mu r_0)] \\
& - \frac{1}{m_2}\,[l\mathrm{K}_{l+\frac{1}{2}}(\mu r_0) - \mu r_0 \mathrm{K}_{l+\frac{3}{2}}(\mu r_0)\,\mathrm{J}_{l+\frac{1}{2}}(\lambda r_0)] \\
& + \frac{2[\beta_1-\beta_2]}{\hbar^2}\left[j(j+1)-l(l+1)-\frac{3}{4}\right]\mathrm{J}_{l+\frac{1}{2}}(\lambda r_0)\,\mathrm{K}_{l+\frac{1}{2}}(\mu r_0) = 0\,.
\end{aligned}
\tag{13}
$$

We can numerate the electron energy states by a set of numbers $\{n, j, l, m\}$, where n numerates solutions of Eq. (13) with fixed j and l. States having the same value of n, l, and j remain $(2l+1)$-fold degenerated [36]. But, the electron energy states with the same n , l, and m and different j (different spin) are split.

5. Calculation Results and Discussion

The energy of the electron states are found by numerically solving the system of Eqs. (5) and (8) for cylindrical QDs and Eq. (13) for spherical ones.

For cylindrical QDs we use a conventional notation for the electron energy states: $n_\rho L_\sigma$, where n_ρ denotes the n-th solution of Eq. (8), $L = \mathrm{S}, \mathrm{P}, \mathrm{D}, \ldots$ presents the abso-

lute value of l, and $\sigma = \pm 1$ refers to the electron spin directions in respect to the electron angular momentum direction. For all calculations we choose the lowest energy state in the z-direction.

For the calculation of the electron energy spectra of InAs cylindrical QDs in GaAs matrix we tuned the band parameters to take into account effects of strain in small InAs quantum dots. In accordance with the results of [25] we use tuned semiconductor band structure parameters for InAs: the energy gap is $E_{1g} = 0.52$ eV, spin–orbit splitting is $\Delta_1 = 0.48$ eV, $m_1(0) = 0.022m_0$ (m_0 is the free electron mass). For GaAs we choose: $E_{2g} = 1.52$ eV, $\Delta_2 = 0.34$ eV, $m_2(0) = 0.067m_0$ [31]. The band offset is taken as $V_0 = 0.55$ eV [25]. It should be noted, that the chosen E_{1g} makes the spin–orbit effect weaker but it is more realistic for strained QDs.

The spin splitting effect is obviously zero for the lowest energy state $1S_{\pm 1}$ as it follows from Eq. (8). The dependence on the dot size for the energy splitting of the state 1P

$$\Delta E_{1P} = E_{1P_{+1}} - E_{1P_{-1}}$$

is shown in Fig. 1. The theory demonstrates a valuable spin splitting for small QDs. The splitting is strongly dependent on the dot size and decreases rapidly when the size increases. For dots of small height the spin splitting is small. This is a result of electron wave function penetration into the barrier along the z-direction. For quantum dots with a small height the averaged effective mass $\tilde{m}_1$ is lager than the electron effective mass in InAs. At the same time, the difference $\Delta\beta$ is smaller than $\beta_1 - \beta_2$. When z_0 increases the difference also increases and then becomes z independent. When ρ_0 decreases (with fixed z_0) the confined electron energy becomes higher and the electron wave function penetration into the barrier becomes lager. That is the reason why the spin spliting ΔE_{1P} dependence on ρ_0 with fixed z_0 demonstrates a nonmonotonic behavior [15]. Certainly, the spin splitting impact becomes stronger for the states with $|l| > 1$.

An interesting consequence of the spin–orbit interaction is the possibility to choose a size of the dot when only one set of the spin split states is situated below the dot's top energy V_0 and another one is situated above V_0. In fact, one can obtain a dot of a critical size $\{\rho_0^{c1}, z_0^{c1}\}$ when only the $1P_{-1}$ electronic states are bound. When we reach the critical size and continue to reduce $\{\rho_0, z_0\}$, the states $1P_{-1}$ become unbound very soon at $\{\rho_0^c, z_0^c\}$. Therefore, the range of the dot sizes when only the $1P_{-1}$ energy states are bound is very narrow. The size ranges are presented in Table 1.

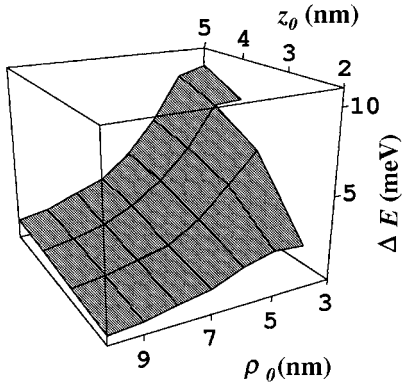

Fig. 1. Spin splitting (ΔE_{1P}) for InAs cylindrical quantum dots versus dot sizes

The spin splitting effect is significantly stronger in InSb QDs. We calculated the energy spectrum for the system where InSb dots are embedded in CdTe matrix. For this calculation we use the following band structure parameters: for InSb: $E_{1g} = 0.24$ eV, $\Delta_1 = 0.81$ eV, $m_1(0) = 0.014m_0$; for CdTe: $E_{2g} = 1.61$ eV, $\Delta_2 = 0.81$ eV, $m_2(0) = 0.11m_0$. The band offset

Table 1
Size ranges

dot	InAs		InSb	
z_0 (nm)	ρ_0^{c1} (nm)	ρ_0^{c}(nm)	ρ_0^{c1}(nm)	ρ_0^{c}(nm)
1.5	4.6	4.5	6.0	5.5
2.0	3.9	3.8	5.5	4.9
3.0	3.6	3.4	5.0	4.4
4.0	3.2	3.0	4.8	4.1
5.0	3.1	2.9	4.7	4.0

is taken as $V_0 = 0.35$ eV [37]. Figure 2 shows the spin–orbit splitting for the structure. The situation when only the $1P_{-1}$ states are bound can be reached with a set of lager $\{\rho_0^{c1}, z_0^{c1}\}$ and with a wider range of dot sizes (see Table 1).

We use spherical QDs as a reference to verify our calculated results. The calculations were performed for InAs spherical QDs embedded in a noncrystalline polymer matrix and spherical nanocrystals of InSb. For those systems we can avoid additional approximations concerning the dot material parameters. We also can compare our results with those obtained by means of more sophisticated models [22, 23]. For the spherical QDs we use the standard atomic notation for the energy states: nL_J, where n denotes the main quantum number and J is the total angular momentum quantum number. The size dependence of the spin splitting between the $1P_{1/2}$ and $1P_{3/2}$ energy states

$$\Delta E_{1P} = E_{1P_{3/2}} - E_{1P_{1/2}}$$

for InAs QDs is presented in Fig. 3 (we choose $E_{1g} = 0.42$ eV, $\Delta_1 = 0.38$ eV, $m_1(0) = 0.024m_0$, $m_2 = m_0$, $\beta_2 = 0$, $V_0 = 2$ eV [23]). Our calculation results are in a reasonable agreement with results obtained by other methods [23]. Figure 4 shows the $1P_{1/2}$ and $1P_{3/2}$ electron energy states for InSb nanocrystals ($E_{1g} = 0.24$ eV, $\Delta_1 = 0.8$ eV,

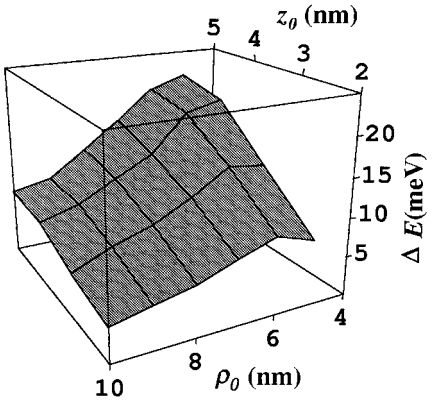

Fig. 2

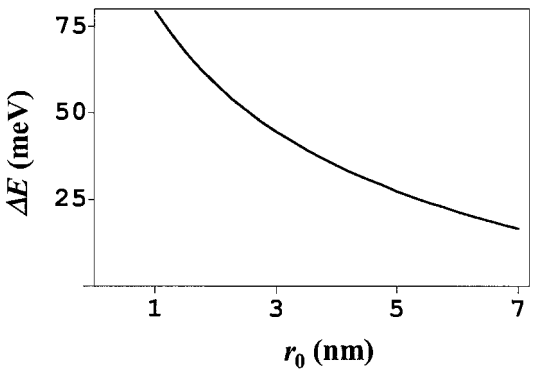

Fig. 3

Fig. 2. Spin splitting (ΔE_{1P}) for InSb cylindrical quantum dots versus dot sizes

Fig. 3. Spin splitting (ΔE_{1P}) for spherical InAs monocrystal versus the dot radius

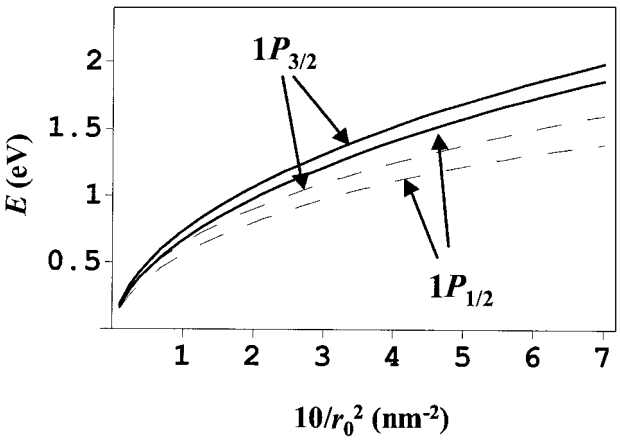

Fig. 4. Size dependence of $E_{1P_{1/2}}$ and $E_{1P_{3/2}}$ energy states in InSb spherical nanocrystals. Present results (solid lines) in comparison with calculated results from Ref. [22] (dashed lines)

$E_{1p} = 23.5$ eV, $m_2 = m_0$, $\beta_2 = 0$, $V_0 = 4.59$ eV that corresponds to the InSb electron affinity). The spin splitting in our model is found to be smaller than that in Ref. [22] and can be taken as the lower limit for estimations. That demonstrate our model capabilities in evaluations of the spin–orbit interaction impact. The simple one-band nonparabolic approximation reproduces major features beside giving reasonable estimations of the spin splitting in semiconductor QDs.

6. Conclusions

We have studied theoretically the spin–orbit interaction impact on the electron energy states in small semiconductor quantum dots. Our calculations are based on the effective one-electronic band Hamiltonian and spin dependent boundary conditions. The spin–orbit splitting in cylindrical and spherical quantum dots has been investigated. Our results show that the spin–orbit interaction can significantly modify the electron energy spectrum of InAs and InSb narrow gap semiconductor QDs. The modification heavily depends on the dot size and shape. The spin splitting in the cylindrical quantum dots demonstrates the nonmonotonic dependence on the dot sizes. In addition, the spin–orbit interaction can provide in cylindrical quantum dots a situation where only the lowest spin split energy states are bound in the dot. The spin splitting effect is quite large for small InSb QDs and can be proposed for experimental investigations.

Finally, we would like to point out that our model of calculations can be used as the starting point in estimations of the spin–orbit interaction effects in semiconductor QDs. To make proper quantitative calculations one should solve the three-dimensional Schrödinger equation and use the self-consistent potential within the multiband approach.

Acknowledgement This work was supported by the National Science Council of Taiwan under contract number NSC89-2218-E009-055.

References

[1] D. Bimberg, M. Grundmann, F. Heinrichdorff et al., Thin Solid Films **367**, 235 (2000).
[2] D. Bimberg, Semicond. **33**, 951 (1999).
[3] N. N. Ledentsov, V. M. Ustinov, V. A. Shchukin et al., Semicond. **32**, 343 (1998).

[4] P. A. Maksym and T. Chakraborty, Phys. Rev. Lett. **65**, 108 (1990).
[5] O. Steffens, M. Suhrke, and U. Rössler, Physica B **256–258**, 147 (1998).
[6] S. Tarucha, T. Honda, D. G. Austing et al., Physica E **3**, 112 (1998).
[7] H. Tamura, Physica B **249–251**, 210 (1998).
[8] S. Datta and B. Das, Appl. Phys. Lett. **56**, 665 (1990).
[9] B. E. Kane, Nature **393**, 133 (1998).
[10] G. Dresselhaus, Phys. Rev. **100**, 580 (1955).
[11] Yu. A. Bychkov and E. I. Rashba, J. Phys. C **17**, 6039 (1984).
[12] Can-Ming Hu, J. Nitta, T. Akazaki, J. Osaka, P. Pfeffer, and W. Zawadzki, Phys. Rev. B **60**, 7736 (1999).
[13] D. Richards and B. Jusserand, Phys. Rev. B **59**, R2506 (1999).
[14] E. A. de Andrada e Silva, Phys. Rev. B **60**, 8859 (1999).
[15] E. A. de Andrada e Silva, G. C. La Rocca, and F. Bassani, Phys. Rev. B **55**, 16 293 (1997).
[16] A. Voskoboynikov, Shiue Shin Liu, C. P. Lee, and O. Tretyak, J. Appl. Phys. **87**, 387 (2000).
[17] A. G. Malshukov and K. A. Chao, Phys. Rev. B **61**, R2413 (2000).
[18] P. N. Racec, T. Stoica, C. Popescu, M. Lepsa, and Th. G. van de Roer, Phys. Rev. B **56**, 3595 (1997).
[19] A. V. Moroz and C. H. W. Barnes, Phys. Rev. B **61**, R2464 (2000); Phys. Rev. B **60**, 14 272 (2000).
[20] E. Silveira, M. K. Kelly, C. E. Nebel, G. Böhm, G. Abstreiter, and M. Stutzmann, Physica E **2**, 929 (1998).
[21] L. I. Magaril and A. V. Chaplik, JETP Lett. **70**, 615 (1999); Zh. Eksp. Teor. Fiz. **115**, 1478 (1999) [JETP **88**, 815 (1999)].
[22] Al. L. Efros and M. Rosen, Phys. Rev. B **58**, 7120 (1998).
[23] U. Banin, C. J. Lee, A. A. Guzelian et al., J. Chem. Phys. **109**, 2306 (1998).
[24] A. J. Williamson and A. Zunger, Phys. Rev. B **61**, 1978 (2000); Phys. Rev. B **59**, 15 819 (1999).
[25] C. Pryor, Phys. Rev. B **60**, 2869 (1999).
[26] F. M. Peeters and V. A. Schweigert, Phys. Rev. B **53**, 1468 (1996).
[27] A. Wojs, P. Hawrylak, S. Farad et al., Phys. Rev. B **54**, 5604 (1996).
[28] P. C. Serel and K. J. Vahala, Phys. Rev. B **42**, 3690 (1990).
[29] Guang-Hong Chen and M. E. Raikh, Phys. Rev. B **60**, 4826 (1999).
[30] A. A. Guzelia, U. Banin, A. V. Kadavanich et al., Appl. Phys. Lett. **69**, 1432 (1996).
[31] G. Bastard, Wave Mechanics Applied to Semiconductor Heterostructures, Les Edition de Physique, Les Ulis 1988.
[32] E. O. Kane, J. Phys. Chem. Solids **1**, 249 (1957).
[33] T. Darnhofer and U. Rössler, Phys. Rev. B **47**, 16020 (1993).
[34] Th. Schäpers, G. Engels, J. Lange et al., J. Appl. Phys. **83**, 4324 (1998).
[35] G. Lamouche and Y. Lépine, Phys. Rev. B **51**, 1950 (1995).
[36] L. D. Landau and E. M. Lifshitz, Quantum Mechanics. Non-Relativistic Theory, Pergamon Press, London/Oxford 1977.
[37] E. T. Yu, J. O. McCaldin, and T. C. McGill, Solid State Phys. **46**, 2 (1992).