PERGAMON

Solid State Communications 119 (2001) 59–62

solid state communications

www.elsevier.com/locate/ssc

Electron energy state spin-orbit splitting in nanoscopic quantum rings

O. Voskoboynikov[a,b,*], H.C. Huang[a], C.F. Shi[a], C.P. Lee[a]

[a]*National Chiao Tung University, 1001 Ta Hsueh Road, Hsinchu 300, Taiwan, R.O.C.*
[b]*Kiev Taras Shevchenko University, 64 Volodymirska st., 252030 Kiev, Ukraine*

Received 26 March 2001; received in revised form 8 May 2001; accepted 14 May 2001 by H. Takayama

Abstract

The impact of spin-orbit interaction on the electron energy states in nanoscopic semiconductor quantum dots and rings is studied theoretically. The effective one-band Hamiltonian approximation with the spin-orbit coupling potential is used. It is shown that the spin-orbit interaction can produce a considerable spin splitting of excited electronic states at zero magnetic fields. We investigated changes in the spin splitting when the geometrical structure is gradually changed from a dot-like shape to a ring-like one. It has been found that the completion of the quantum ring geometry leads to the reversing of the splitting sign.

PACS: 68.65.+g; 71.70.Ej; 85.70.Vw

Keywords: A. Nanostructures; A. Semiconductors; D. Spin-orbit effects; D. Electronic states (localized)

The recent advances in nanoscopic semiconductor structure fabrication has allowed us to construct nanoscopic systems with a wide range of geometries. It produces a genuine explosion of researches on this topic. Electron quantum confinement effects are being under an extensive investigation for quantum wells, quantum wires, and quantum dots (see Refs. [1–4] and references therein). A new geometry of nanoscopic semiconductor quantum rings has been observed experimentally in recent works [5–8]. Although micro-scopic and meso-scopic metallic and semiconductor [1,9] quantum rings have been under a considerable attention for the recent decade, the recent development in semiconductor nanoscopic rings bridges the gap between quantum dots and meso-scopic ring structures.

The study of the electronic properties of nanoscopic rings have attracted a strong experimental and theoretical interests [5–8,10–14]. In contrast to the meso-scopic one the nanoscopic rings can not be described as a quasi-one-dimensional structure. The ring geometry makes this nanostructure very rich in physics including its far-infrared spectrum and its magnetic properties [15,16]. In addition, unusual optical and magnetic properties can be controlled by morphological changes during the nano-structure fabrication and by the number of electrons bound in a ring [5–8]. However, it can be seen from the literature that the agreement between the present day nanoscopic quantum ring theory and the experimental results is rather poor [16]. A good understanding of the spectroscopic and magnetic properties of the rings are still lacking.

In this study we discuss consequences of the spin-orbit coupling [17–19] between electron motion and the electron spin polarization in nanoscopic quantum rings. We show below that the spin-orbit interaction can play an important role in the formation of electron energy states in those nanoscopic quantum structures and lead to a significant revision of the electron energy spectrum even at zero magnetic field. We are particularly interested in a situation when the simply-connected geometry of quantum dots transforms to the multiply-connected geometry of quantum rings (a "dot to ring" transition). Our model allows us to calculate the electronic spin dependent energy structure of InAs/GaAs nanoscopic quantum dots and rings gradually within the "dot to ring" topology transition.

* Corresponding author. Present address: Department of Electronics Engineering and Institute of Electronics, National Chiao Tung University, 1001 Ta Hsueh Road, Hsinchu 300, Taiwan, R.O.C. Tel.: +886-3-5712121 ext. 54174; fax: +886-3-5724361.

E-mail address: vam@cc.nctu.edu.tw (O. Voskoboynikov).

0038-1098/01/$ - see front matter
PII: S0038-1098(01)00218-6

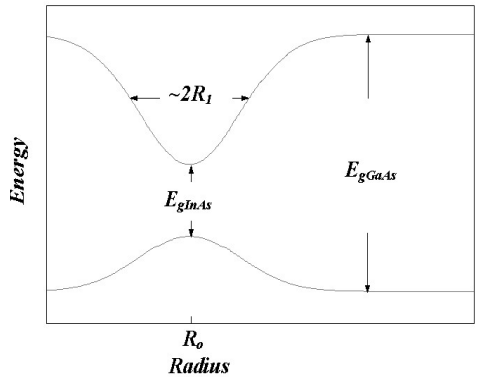

Fig. 1. Radial variation of the semiconductors band parameters in InAs/GaAs ring structures.

We describe here a quantum semiconductor structure with radial variations of the band structure parameters, as shown in Fig. 1. The structure is generated by the revolution of the radial variation around the z-axis. In our calculation we use the adiabatic approximation [20,21] and take the advantage of the fact that the electron wave function is strongly confined along z-direction. Obtained in experiments a typical height of nanoscopic quantum rings is about 2 nm [5,6]. The diameters of these rings are changed within a wide range but those are always an order of magnitude larger than the ring height [5–8]. This allows us to discuss only the ground energy state with respect to the electron motion along z-direction [21].

To calculate the electron energy state we use the effective one-electronic-zone Hamiltonian within the envelope function approximation [22–25]. The total electron wave function $\Phi_{n,l,s}(z,R)$ for the electron energy state with the orbital momentum l and spin s can be presented in the adiabatic approximation as:

$$\Phi_{nls}(z,R) \approx \Psi_0(z)F_{n,l,s}(R),$$

where $\Psi_0(z)$ satisfies the ground state z-component of the Schrödinger equation and n is the main quantum number for the electron radial motion. $F_{n,l,s}(R)$ is an eigen-function of the following effective Hamiltonian:

$$H = -\frac{\hbar^2}{2}\left[\frac{1}{R}\frac{d}{dR}\frac{R}{m(R,E)}\frac{d}{dR} - \frac{l^2}{m(R,E)R^2}\right] + V_c(R) + V_{so}(R,E), \quad (1)$$

where the coordinate and energy dependent electron effective mass can be presented as:

$$\frac{1}{m(R,E)} = \frac{P^2}{\hbar^2}\left[\frac{2}{E - E_c(R) + E_g(R)} + \frac{1}{E - E_c(R) + E_g(R) + \Delta(R)}\right], \quad (2)$$

E is the electron energy, $E_c(R)$, $E_g(R)$, and $\Delta(R)$ denote respectively the position-dependent electron band edge, the main band gap, and the spin-orbit splitting in the valent band. P is the momentum matrix element that is taken to be independent on R [22–24]. The material parameters of InAs/GaAs quantum structures are used for our evaluation. The confinement potential in the conduction band follows the well known rule $V_c(R) = E_c(R) = 0.7[E_g(R) - E_{gInAs}]$. The spin-orbit interaction potential is written in the cylindrical coordinates as:

$$V_{so}(R,E) = \frac{\sigma l}{R}\frac{d\beta(R,E)}{dR}, \quad (3)$$

where the spin-orbit coupling parameter β is [23–25]:

$$\beta(R,E) = \frac{P^2}{2}\left[\frac{1}{E - E_c(R) + E_g(R)} - \frac{1}{E - E_c(R) + E_g(R) + \Delta(R)}\right], \quad (4)$$

and $\sigma = \pm 1$ refers to the electron spin polarization along the z-axis. The coordinate dependence of the material band characteristics in $In_xGa_{1-x}As$ quantum structures is controlled by the composition parameter x, which is taken to be R-dependent and follows the distribution (see Fig. 1):

$$x(R) = \exp\left[-\left(\frac{R - R_0}{R_1}\right)^2\right]. \quad (5)$$

The key parameters of this model are the structure characteristic radius R_0 and the width of the confinement potential R_1. This "$x(R)$" model allows as to investigate the electron energy states of the structures starting from the quantum dot configuration ($R_0 = 0$). The position-dependent band parameters are then expressed using the following rule [26]:

$$E_g(R) = x(R)E_{gInAs} + [1 - x(R)]E_{gGaAs},$$

$$\Delta(R) = x(R)\Delta_{InAs} + [1 - x(R)]\Delta_{GaAs}.$$

The above model allows us to describe within one theoretical approach the "dot to ring" topology transition using one set of parameters $\{R_0,R_1\}$.

The Schrödinger equation with the Hamiltonian (1) was solved by using the nonuniform space grid method proposed in Ref. [21]. Because of the energy dependence of the effective mass and spin-orbit coupling parameter our calculation consists of iteration loops to reach a "self-consistent" energy solution. A feedback nonlinear iteration scheme is as follows: (i) set energy $E = 0$, (ii) compute effective mass m and spin-orbit coupling parameter β, (iii) solve Schrödinger equation for energy E, (iv) back to (ii). The iteration is terminated when a specified stopping criterion on energy is reached. We have found that for the above scheme the convergence criteria on energies (the maximum norm

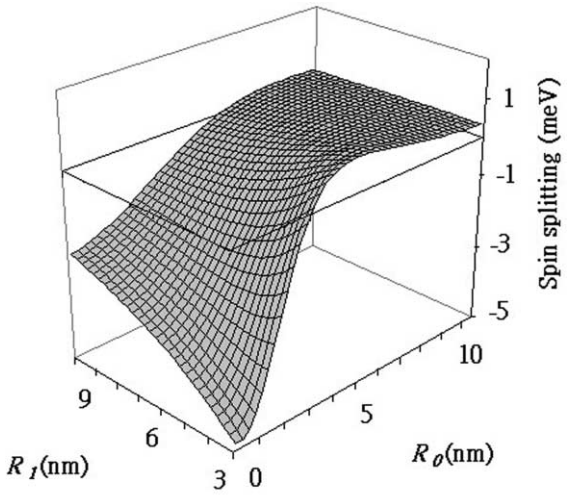

Fig. 2. Spin splitting as a function of the InAs/GaAs structure radial parameters ($E_{gInAs} = 0.42$ eV, $\Delta_{InAs} = 0.38$ eV, $E_{gGaAs} = 1.52$ eV, $\Delta_{GaAs} = 0.34$ eV, $P^2 = 0.89$ eV^{2}nm^2 [26]).

error is less than 10^{-7} eV) can be reached by only 8–10 iterative loops.

In this work the value of our main interest is the spin splitting in the electron energy states:

$$\Delta E_{n,l} = E_{n,l,+1} - E_{n,l,-1} \tag{6}$$

The dependence of $\Delta E_{n,l}$ on R_0 and R_1 is of primary concern in this study and we obtain a principal result for the lowest energy levels, when $n = 0$. It is clear from (3) that the spin-orbit splitting appears for states with $|l| \geq 1$.The spin-orbit interaction separates states with the same orbital momentum and different spin directions. However, the states with parallel spin and l (antiparallel spin and l) remain twofold degenerated. This is the well known Kramers degeneracy. For instance, when $d\beta(R,E)/dR \leq 0$ the doubly degenerated electron states with antiparallel directed spin and l have the higher energy. This level hierarchy obviously depends on the sign of the parameter $d\beta(R,E)/dR$.

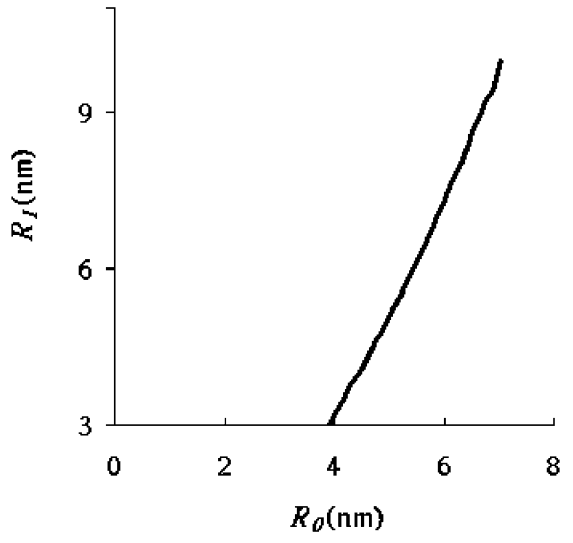

Fig. 3. Zero spin splitting line for InAs/GaAs "dot to ring" transition (parameters are the same as in Fig. 2).

Our calculation results demonstrate well-defined spin orbit splitting in electron states with non-zero angular momentum in small quantum dots and rings. In our model the spin splitting is a function of the two variables R_0 and R_1. Consequently, in $\{R_0,R_1\}$ plane we can investigate possible differences in the spin-orbit splitting for dot-like and ring-like structures. Fig. 2 presents our calculation results for the lowest spin-split energy level $|l| = 1$. The result demonstrates an observable splitting for relatively small dots and rings. An interesting consequence of the "dot to ring" topology transition (along the R_0 axis) is the change of the splitting sign. The sign inversion takes place when the parameter R_0 is large enough to complete the ring-like potential geometry for electrons. Starting from $R_0 = 0$ (the dot geometry) we have negative $d\beta(R,E)/dR$ for all R and E (see Eq. 3). When R_0 is increased a region with positive $d\beta(R,E)/dR$ appears (when $R \leq R_0$). Since the spin-orbit interaction is proportional to R^{-1} and the positive part of $d\beta(R,E)/dR$ becomes dominant when the ring structure starts to take shape. So the spin splitting changes sign as the dot changes to ring when R_0 increases. This is a direct consequence of the ring-like geometry completeness for the electron potential. In Fig. 3 we show a line on $\{R_0,R_1\}$ plane when the splitting is zero. It follows from Fig. 3 that the ring-like potential forming is complete when $R_0 \gtrsim R_1$.

In short summary, we have presented a theoretical study of the impact of the spin-orbit coupling on the electron energy structure of nanoscopic quantum dots and rings. The effective one-band Hamiltonian approximation with the spin-orbit coupling potential were employed to describe and evaluate this effect. Our results demonstrate that the system energy state hierarchy can be dependent on the electron spin polarization through the spin-orbit interaction. We have found that the spin-orbit splitting of the electron states can reach a considerable magnitude at zero magnetic fields. The electron state hierarchy can drastically change when the system geometry changes. An interesting "dot to ring" topology transition in the spin-splitting sign has been found. The completion of the ring-like structure leads to the splitting sign reversing. This can lead to unusual magnetic and magneto-optical properties of the structures.

The main goal of this paper is to demonstrate the spin-orbit interaction effects in the "dot to ring" topology transition. In our calculation, a simple model and conventional parameters of the semiconductor band structures are used. A real three dimensional calculation including the multi-electron effects should be performed to complete the investigation. However, the major finding: the spin-splitting at zero magnetic field and the reversing of the splitting sing are clear physical phenomena which are independent of the

model. We can conclude that the spin-orbit interaction offers not only rich physics but also possible useful device applications.

Acknowledgements

This work was supported by the National Science Council under contract number NSC 89-2218-E-009-055.

References

[1] D.K. Ferry, S.M. Goodnick, Transport in Nanostructures, Cambridge University Press, New York, 1997.
[2] M.J. Kelly, Low-dimensional Semiconductors: Material, Physics, Technology, Devices, Oxford University Press, Oxford, 1995.
[3] D. Bimberg, M. Grundmann, N.N. Ledentsov (Eds.), Quantum Dot Heterostructures, Wiley, Chichester, 1998.
[4] D. Bimberg, Semicond. 33 (1999) 951.
[5] J.M. Garcia, G. Mederios-Ribeiro, K. Schmidt, T. Ngo, J.L. Feng, A. Lorke, J.P. Kotthaus, P.M. Petroff, Appl. Phys. Lett. 71 (1997) 2014.
[6] A. Lorke, R.J. Luyken, A.O. Govorov, J.P. Kotthaus, J.M. Garcia, P.M. Petroff, Phys. Rev. Lett. 84 (2000) 2223.
[7] R.J. Waburton, C. Schäflein, D. Haft, F. Bickel, A. Lorke, K. Karrai, J.M. Garcia, W. Schoenfeld, P.M. Petroff, Physica E 9 (2000) 124.
[8] A. Lorke, R.J. Luyken, Physica B 256-258 (1998) 424.
[9] T. Ando, Y. Arakawa, K. Furuta, S. Komiyama, H. Nakashima (Eds.), Mesoscopic Physics and Electronics, Springer, Berlin, 1998.
[10] L. Wendler, V.M. Fomin, A.V. Chaplik, A.O. Govorov, Phys. Rev. B 54 (1996) 4794.
[11] O. Olendsky, C.S. Kim, O.H. Chung, C.S. Lee, Phys. Rev. B 55 (1997) 9834.
[12] W.C. Tan, J.C. Inkson, Phys. Rev. B 60 (1999) 5626.
[13] A. Bruno-Alfonso, A. Latgé, Phys. Rev. B 61 (2000) 15887.
[14] Z. Bartiecevic, M. Pacheco, A. Latgé, Phys. Rev. B 62 (2000) 6963.
[15] A. Emperador, M. Barrenco, E. Lipparini, M. Pi, Ll. Serra, Phys. Rev. B 59 (1999) 15301.
[16] A. Emperador, M. Pi, M. Barranco, A. Lorke, Phys. Rev. B 62 (2000) 4573.
[17] G. Dresselhaus, Phys. Rev. 100 (1955) 580.
[18] Yu.A. Bychkov, E.I. Rashba, J. Phys. C 17 (1984) 6039.
[19] G.E. Pikus, V.A. Marushchak, A.M. Titkov, Fiz. Tekh. Poluprovodn. 22 (1988) 185 [Sov. Phys. Semicond. 22 (1988) 115].
[20] G. Lamouche, Y. Lépin, Phys. Rev. B 51 (1995) 1950.
[21] F.M. Peeters, V.A. Schweigert, Phys. Rev. B 53 (1996) 1468.
[22] G. Bastard, Wave Mechanics Applied to Semiconductor Heterostructures, Halsted Press, New York, 1988.
[23] E.A. de Andrada e Silva, G.C. La Rocca, F. Bassani, Phys. Rev. B 50 (1994) 8523.
[24] E.A. de Andrada e Silva, G.C. La Rocca, F. Bassani, Phys. Rev. B 55 (1997) 16293.
[25] Th. Schäpers, G. Engels, J. Lange, Th. Klocke, M. Hollfelder, H. Lüth, J. Appl. Phys. 83 (1998) 4324.
[26] S.L. Chuang, Physics of Optoelectronic Devices, Wiley, New York, 1995.