Effect of a step quantum well structure and an electric-field on the Rashba spin splitting*

Hao Yafei(郝亚非), Chen Yonghai(陈涌海)†, Hao Guodong(郝国栋), and Wang Zhanguo(王占国)

(Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China)

Abstract: Spin splitting of conduction subbands in $Al_{0.3}Ga_{0.7}As/GaAs/Al_xGa_{1-x}As/Al_{0.3}Ga_{0.7}As$ step quantum wells induced by interface and electric field related Rashba effects is investigated theoretically by the method of finite difference. The dependence of the spin splitting on the electric field and the well structure, which is controlled by the well width and the step width, is investigated in detail. Without an external electric field, the spin splitting is induced by an interface related Rashba term due to the built-in structure inversion asymmetry. Applying the external electric field to the step QW, the Rashba effect can be enhanced or weakened, depending on the well structure as well as the direction and the magnitude of the electric field. The spin splitting is mainly controlled by the interface related Rashba term under a negative and a stronger positive electric field, and the contribution of the electric field related Rashba term dominates in a small range of a weaker positive electric field. A method to determine the interface parameter is proposed. The results show that the step QWs might be used as spin switches.

Key words: Rashba effect; step quantum wells; electric field; interface
DOI: 10.1088/1674-4926/30/6/062001 **PACC:** 7170E; 7320D

1. Introduction

It has been shown that the Rashba spin-orbit coupling can be controlled by a gate voltage, which offers the possibility of altering the symmetry of the quantum well (QW)[1−3]. This provides an effective way to realize the so-called spin field effect transistor[4, 5] and other spintronic devices[6, 7]. However, it is proposed that the contribution of the potential jump at the well barrier interfaces to the Rashba spin-orbit coupling is larger than that of the vertical electric field in the well, which can be varied by the gate voltage[8−10], and the spin splitting is underestimated if the interface contribution is neglected[11]. In order to investigate the contribution of the band discontinuity to the Rashba spin splitting, many researchers focus on the asymmetrical QW with different barrier materials[12, 13]. However, the electron confinement is diminished in the asymmetrical QW compared with the symmetrical QW. In order to overcome the weakness, we focus our attention on the $Al_{0.3}Ga_{0.7}As/GaAs/Al_xGa_{1-x}As/Al_{0.3}Ga_{0.7}As$ step QW, which provides a good probe for the interface contribution to the spin splitting. The step QW contains a built-in structure inversion asymmetry (SIA), which is introduced by inserting the $Al_xGa_{1-x}As$ step into the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ symmetrical QW. The merit of the step QW is that it possesses an internal SIA, which induces a Rashba effect without any electric field or magnetic field as opposed to the case of the symmetrical QW, and the effect of the confining electrons is better than that of the asymmetrical QW. Applying an electric field, which is controlled by the gate voltage, to such a step QW may affect the SIA of the step QW. It has been reported that the introduction of an InP layer above the QW affects the spin-orbit interaction by the effect of the doping position[14]. In this paper, we will show the effect of the external electric field and the structure of the step QW, weighed by the well width and step width, on the spin splitting of the $Al_{0.3}Ga_{0.7}As/GaAs/Al_xGa_{1-x}As/Al_{0.3}Ga_{0.7}As$ step QW composed of intrinsic semiconductor materials. Moreover, we will give a method to determine the interface parameter, which is very important for the spin splitting of the asymmetrical structure.

2. Theory

For the [001]-grown step QW, the Hamiltonian describing the SIA contribution to the conduction subbands can be written as

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + V_0 + eFz + H_{so}, \tag{1}$$

where m^* is the electron effective mass, V_0 is the band offset, eFz is the potential induced by the external electric field, and H_{so} is the Rashba Hamiltonian containing the interface and electric field related Rashba terms, which can be written as

$$H_{so} = (\alpha_F + \alpha_I)(\sigma_x k_y - \sigma_y k_x), \tag{2}$$

---

* Project supported by the State Key Development Program for Basic Research of China (Nos. 2006CB921607, 2006CB604908) and the National Natural Science Foundation of China (No. 60625402).

† Corresponding author. Email: yhchen@red.semi.ac.cn

Received 15 December 2008, revised manuscript received 16 January 2009

where k_x and k_y are the wave vectors, σ_x and σ_y denote the spin Pauli matrices, and α_F and α_I are the electric field and interface related Rashba coefficients, respectively.

The electric field related Rashba coefficient α_F, which is proportional to the external electric field, depends on the constituting materials, which can be described by[15, 16]

$$\alpha_F = \frac{\hbar^2}{2m^*}\frac{\Delta}{E_g}\frac{2E_g+\Delta}{(E_g+\Delta)(3E_g+2\Delta)}eF, \tag{3}$$

where E_g is the band gap, Δ is the spin-orbit splitting energy, e is the electron charge, and F is the external electric field.

The interface related Rashba parameter α_I, which is determined by the materials at both sides of the interfaces and the well structure, should have a form of

$$\alpha_I = P\delta(z-z_1) - \frac{x}{x_0}P\delta(z-z_2) - (1-\frac{x}{x_0})P\delta(z-z_3), \tag{4}$$

where P is the interface parameter for the $Al_{0.3}Ga_{0.7}As/GaAs$ interface, x and $x_0 = 0.3$ are the Al concentrations in the step and the barrier material, respectively, and z_i ($i = 1, 2, 3$) is the position of the ith interface. The δ function clearly shows that the Rashba effect is localized at the interfaces[10, 17].

The Schrödinger equation, $H\psi = E\psi$, is solved by the method of finite difference, which can solve the interface and the electric field related Rashba effect in the same model simultaneously. We simulate the results of Refs. [12, 18] to extract the value of P and obtain $P \approx -30$ meV·nm^2 for the $Al_{0.3}Ga_{0.7}As/GaAs$ interface. In the following calculations, the center of the GaAs layer is set to be 0; for simplicity, we let $k_y = 0$, and the parallel wave vector is labeled by $k_x = 2.0 \times 10^6$ cm^{-1}.

3. Results and discussion

By altering the Al concentration in the $Al_xGa_{1-x}As$ step, particularly large spin splitting is obtained for the step QW with an $Al_{0.15}Ga_{0.85}As$ step; so, we take an $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.15}Ga_{0.85}As/Al_{0.3}Ga_{0.7}As$ step QW as an example to show how the electric field and the well structure, which is controlled by the well width and the step width, affect the spin splitting of the step QW. The electric field and interface related Rashba terms play different roles on the spin splitting of the step QW. In Fig. 1 we show the total spin splitting of the ground subband and the spin splitting induced by the interface and external electric field related Rashba terms, respectively, as a function of the well width and the step width. The interface induced spin splitting is opposite to the electric field induced spin splitting no matter whether the electric field is positive or negative. The magnitude of the interface induced spin splitting is much larger than that of the electric field induced spin splitting when the electric field is strong enough. So, the contribution of the electric field is canceled out by the interface contribution. As a result, the total spin splitting is mainly controlled by the interface contribution. This result agrees with some other experimental results[8, 9], in which it is discussed that the main contribution to the Rashba parameter originates from the interfaces of the quantum well rather than from the electric field.

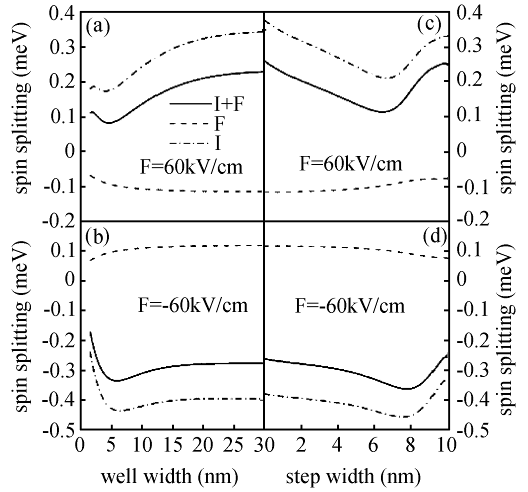

Fig. 1. Overall spin splitting (I+F) of the ground subbands and spin splitting induced, respectively, by interface (I) and electric field (F) related Rashba effects as a function of [(a), (b)] the well width (stepwidth = wellwidth/2) and [(c), (d)] the step width of the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.15}Ga_{0.85}As/Al_{0.3}Ga_{0.7}As$ step quantum well with an electric field of 60 and –60 kV/cm.

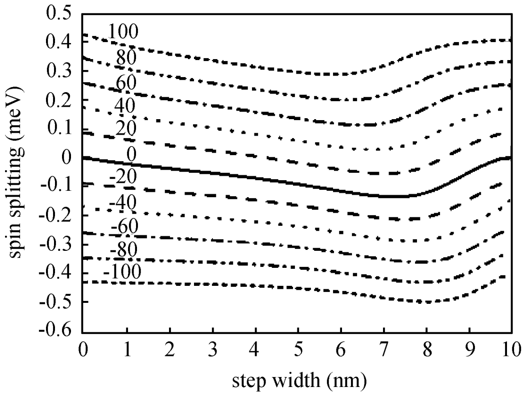

Fig. 2. Spin splitting of the ground subbands as a function of the step width of a 10nm-wide $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.15}Ga_{0.85}As/Al_{0.3}Ga_{0.7}As$ step quantum well with different electric fields.

In Fig. 2, we plot the overall spin splitting of the ground subbands as a function of the step width of a 10-nm-wide QW with different electric fields. Without an external electric field, the SIA of the step QW is controlled by the well structure, i.e., the step width. So, the spin splitting is caused only by the interface related Rashba term. Obviously, the step QW with a 0 or 10-nm-wide step is symmetrical, resulting in no spin splitting, and the degree of the SIA of the step QW with a 7.5-nm-wide step is most distinct, resulting in the largest spin splitting. For the situation of an electric field being applied to the step QW, the Rashba effect can be strengthened or weakened, depending on the direction and the magnitude of the electric field as well as the step width. For the step QW with a 0 or 10-nm-wide step, the Rashba effect appears due to the SIA induced by the electric field. Besides the two extreme cases, when a weaker

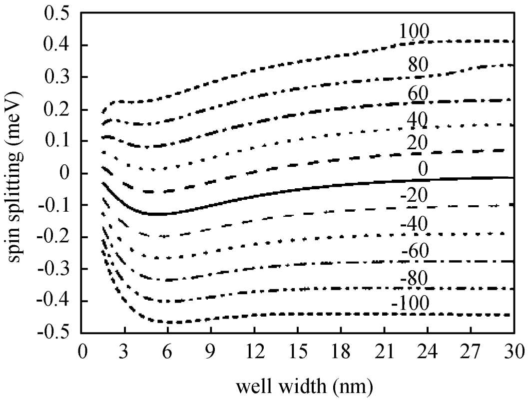

Fig. 3. Spin splitting of the ground subbands as a function of the well width of the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.15}Ga_{0.85}As/Al_{0.3}Ga_{0.7}As$ step quantum well at different electric fields.

positive electric field less than about 33 kV/cm is applied to the step QW, there exist two step widths for which the spin splitting is 0; so, the Rashba effect induced by interface is completely canceled out by the effect induced by the electric field. When the electric field is bigger than 33 kV/cm, the spin splitting is always positive, and the contribution of the interface to the Rashba effect is large enough and cannot be canceled out completely by the contribution of the electric filed. For a negative electric field, the spin splitting increases to more negative values when the electric field becomes more negative. So, the negative electric field can always strengthen the Rashba effect of the step QW.

In Fig. 3, we plot the spin splitting of the ground subbands as a function of the well width at different electric fields, where the step width is half of the well width. Without an external electric field, the spin splitting, which is controlled by the interface related Rashba effect, presents a negative maximum as a function of the well width. When a negative electric field is applied, the spin splitting is still negative and the magnitude of it increases with an increase of the electric field; in a large electric field, the spin splitting will saturate when the well width is larger than a critical value. If a positive electric field is applied to the step QW, similar to the spin splitting changing with the step width, the sign and the magnitude of the spin splitting depend on the magnitude of the electric field as well as the well width. An electric field between 0 and 37 kV/cm may result in zero spin splitting for two extreme well widths and electric fields larger than 37 kV/cm induce a positive spin splitting, which increases with an increase of the electric field. Therefore, for the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.15}Ga_{0.85}As/Al_{0.3}Ga_{0.7}As$ step QW, a weaker positive electric field, which can completely suppress the built-in SIA, must exist, and the magnitude of the electric field can be controlled by the well width and the step width of the step QW. The fact that spin splitting appears due to the built-in SIA without an external electric field and disappears under a weaker positive electric field may be applied to spin switches.

In Fig. 4, we plot the overall spin splitting of the ground subband and the spin splitting induced by the interface and the electric field related Rashba terms of the step QW as a function of the external electric field. The results show that the spin splitting induced by the external electric field related Rashba term is proportional to the electric filed, and the spin splitting induced by the interface related Rashba term can be tuned by the electric field by changing the electron probability density in the well. A negative electric field increases the electron probability density difference at three interfaces, resulting in a large interface related spin splitting. A weak positive electric field decreases the electron probability density difference at three interfaces until it becomes zero. Then, with an increasing of the positive electric field, the electron probability density difference at three interfaces is increased again, but with opposite sign, resulting in a sign change of the interface related spin splitting. The overall spin splitting, which is the sum of the two contributions, disappears when they have equal magnitude and opposite sign, which corresponds to the symmetrical confinement potential. Under negative and strong positive electric fields, the spin splitting induced by the interface and the electric field related Rashba terms are opposite to each other, and the contribution of the interface dominates, which is consistent with the result in Fig. 1. However, what should be noticed is that a small range of weak positive electric fields exist, in which the spin splitting induced by the electric field related Rashba term is larger than that induced by the interface related Rashba term.

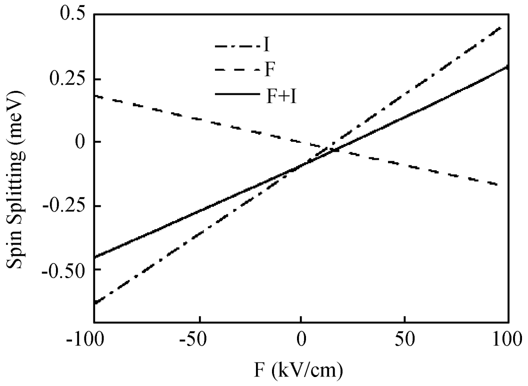

Fig. 4. Overall spin splitting of the ground subbands (F+I) and spin splitting induced, respectively, by interface (I) and electric field (F) related Rashba effects as a function of the external electric field of 10-nm-wide step QW with a 5-nm-wide step.

The value of P has an important effect on the total spin splitting. The exact value of it still needs to be determined by some experiments. Figure 5(a) presents the spin splitting without an external electric field; i.e., the spin splitting induced by the interface related Rashba effect. If the Rashba spin splitting can be extracted by some methods, e.g., the spin photocurrent or the Kerr rotation, the value of P can be determined by comparing the experimental results and the calculated results in Fig. 5(a). We have mentioned above that the electric field induced spin splitting can completely cancel out the interface induced spin splitting when applying an external electric field

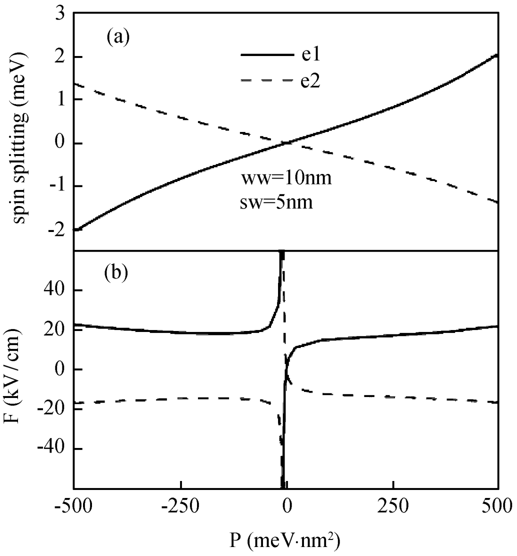

Fig. 5. (a) Spin splitting of the ground (e1) and the first excited (e2) subbands induced by the interface related Rashba term as a function of the interface parameter; (b) Electric field, which results in no spin splitting, as a function of the interface parameter.

to a given well structure. By determining such an electric field, the value of *P* can also be determined. In Fig. 5(b) we plot the electric field, which results in no spin splitting, as a function of *P* for the 10-nm-wide step QW with a 5-nm-wide step.

4. Conclusions

We have theoretically investigated the spin splitting of the $Al_{0.3}Ga_{0.7}As/GaAs/Al_xGa_{1-x}As/Al_{0.3}Ga_{0.7}As$ step QW induced by the interface and the electric field related Rashba terms. Without an external electric field, the spin splitting can be induced by the interface related Rashba term due to the built-in SIA, which is caused by the introduction of the $Al_xGa_{1-x}As$ step into the symmetrical $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ QW. When an external electric field is applied to the step QW, the SIA can be changed depending on the direction and the magnitude of the electric field. For the ground subbands, the negative electric field can lead to a more pronounced SIA, which results in a stronger Rashba effect. A weaker positive electric field weakens the SIA until it becomes a symmetrical confinement potential, and zero spin splitting appears for certain well widths or step widths. With the increase of the positive electric field, the SIA increases again. It is shown that the spin splitting of the step QW is mainly controlled by the interface related Rashba term under negative and stronger positive electric fields, and the contribution of the electric field related Rashba term dominates in a small range of weaker positive electric field. Such a step QW might be used in spin switches. We also proposed a method to determine the value of the interface parameter, which has an important effect on the spin splitting of the asymmetrical structure.

References

[1] Grundler D. Large Rashba splitting in InAs quantum wells due to electron wave function penetration into the barrier layers. Phys Rev Lett, 2000, 84: 6074

[2] Engels G, Lange J, Schäpers T, et al. Experimental and theoretical approach to spin splitting in modulation-doped $In_xGa_{1-x}As/InP$ quantum wells for B→0. Phys Rev B, 1997, 55: R1958

[3] Nitta J, Akazaki T, Takayanagi H. Gate control of spin-orbit interaction in an inverted $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ heterostructure. Phys Rev Lett, 1997, 78: 1335

[4] Datta S, Das B. Electonic analog of the electro-optic modulator. Appl Phys Lett, 1989, 56: 665

[5] Schliemann J, Egues J C, Loss D. Nonballistic spin-field-effect transistor. Phys Rev Lett, 2003, 90: 146801

[6] CartoixàX, Ting D Z Y, Chang Y C. A resonant spin lifetime transistor. Appl Phys Lett, 2003, 83: 1462

[7] Koga T, Nitta J, Takayanagi H. Spin-filter device based on the Rashba effect using a nonmagnetic resonant tunneling diode. Phys Rev Lett, 2002, 88: 126601

[8] Schäpers T, Engels G, Lange J, et al. Effect of the heterointerface on the spin splitting in modulation doped $In_xGa_{1-x}As/InP$ quantum wells for B→0. J Appl Phys, 1998, 83: 4324

[9] Sato Y, Kita T, Gozu S, et al. Large spontaneous spin splitting in gate-controlled two-dimensional electron gases at normal $In_{0.75}Ga_{0.25}As/In_{0.75}Al_{0.25}As$ heterojunctions. J Appl Phys, 2001, 89: 8017

[10] Pfeffer P, Zawadzki W. Spin splitting of conduction subbands in III-V heterostructures due to inversion asymmetry. Phys Rev B, 1998, 59: R5312

[11] Yang W, Chang K. Rashba spin splitting in biased semiconductor quantum wells. Phys Rev B, 2006, **73**: 113303

[12] De Andrada E, Silva E A, la Rocca G C, et al. Spin-orbit splitting of electronic states in semiconductor asymmetric quantum wells. Phys Rev B, 1997, 55: 16293

[13] Hasegawa M M, de Andrada E, Silva E A. Spin-orbit-split subbands in IV-VI asymmetric quantum wells. Phys Rev B, 2003, 68: 205309

[14] Lin Y, Koga T, Nitta J. Effect of $InP/In_{0.53}Ga_{0.47}As$ interface on spin-orbit interaction in $In_{0.52}Ga_{0.48}As/In_{0.53}Ga_{0.47}As$ heterostructures. Phys Rev B, 2005, 71: 045328

[15] Matsuyama T, Kürsten R, Mei*β*ner C, et al. Rashba spin splitting in inversion layer on p-type bulk InAs. Phys Rev B, 2000, 61: 15588

[16] De Andrada E, Silva E A, la Rocca G C, et al. Spin-split subbands and magneto-oscillations in III-V asymmetric heterostructures. Phys Rev B, 1994, 50: 8523

[17] Zawadzki W, Pfeffer P. Spin splitting of subband energies due to inversion asymmetry in semiconductor heterostructures. Semicond Sci Technol, 2004, 19: R1

[18] Yang W, Chang K. Nonlinear Rashba model and spin relaxation in quantum wells. Phys Rev B, 2006, 74: 193314