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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

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Abstract – By means of the transfer matrix technique, interface-induced Rashba 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 which contain internal structure inversion asymmetry introduced by the insertion of $Al_xGa_{1-x}As$ step potential is investigated theoretically in the absence of electric field and magnetic field. The dependence of spin splitting on the well width, step width and Al concentration is investigated in detail. We find that the sign of the first excited subband spin splitting changes with well width and step width, and is opposite to that of the ground subband under certain conditions. The sign and strength of the spin splitting are shown to be sensitive to the components of the envelope function at three interfaces.

Recently, the Rashba effect in quantum wells (QWs) is of high interest due to its role in novel spintronic devices [1,2]. It is caused by structure inversion asymmetry (SIA) which can be controlled by an external electric field [3,4] as well as band structure engineering [5]. By using the complete five-level $k \cdot p$ approach to the band structure of III-V compounds, Pfeffer and Zawadzki [6] emphasized that the SIA splitting is not directly related to the electric field in the conduction band, but rather it is caused by the offsets of valence bands at the interfaces. When some researchers reported the electric-field–induced spin splitting, they showed that the value of Rashba parameter largely depends on the interface contribution [7–9] by which the band structure can be manipulated greatly. Except for the external electric field, the structure inversion symmetry can also be destroyed by asymmetrical structure design, such as the asymmetrical QW with different left and right barrier materials [10,11]. In the present paper, the asymmetrical structure design is used to investigate the interface-induced Rashba spin splitting which is called interface Rashba effect.

Different from the well structure with different barrier materials, in the present paper, we introduce an $Al_xGa_{1-x}As$ layer into the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ symmetry QW to destroy the structure inversion symmetry by a step potential. The corresponding spin splitting is a kind of Rashba spin splitting which is different from the case of no-common-atom QWs in which the interface-related spin splitting term has the same structure as the k-linear term deriving from the bulk inversion asymmetry [12]. As shown in the inset of fig. 1(a), instead of the two-interfaces arrangement in the asymmetrical QW with different barrier materials, there exist three interfaces in our well structure. The introduction of the step potential and one more interface results in many novel characters in the spin splitting of conduction subbands which will be shown in detail in this paper. The effect of the insertion of an $InP/In_{0.53}Ga_{0.47}As$ interface on the Rashba spin splitting in $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ quantum wells has been reported [13]. While the effect of the step QW structure on the Rashba effect, the origin of the interface-related Rashba spin splitting and how to control the SIA of the step QWs are unknown, and these are the focuses of this paper.

Generally the Rashba effect on spin splitting in the conduction band can be described by a Rashba Hamiltonian:

$$H_R = \alpha(z)(\sigma_x k_y - \sigma_y k_x), \tag{1}$$

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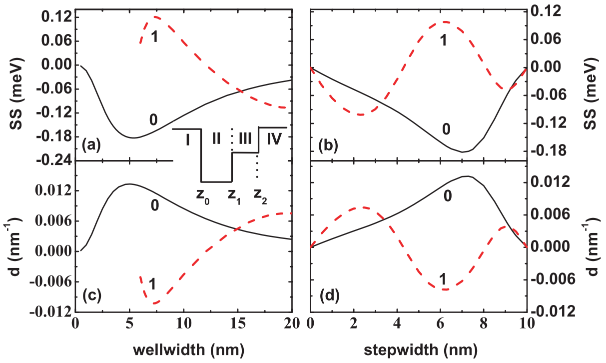

Fig. 1: Spin splitting (SS) and difference of electron probability density of the ground (0) and the first excited (1) subbands of $GaAs/Al_{0.15}Ga_{0.85}As/Al_{0.3}Ga_{0.7}As$ step quantum well at $k = 0.2 \times 10^6\,cm^{-1}$ as a function of the total well width (where the step width is half of the total well width) ((a) and (c)) and of the step width of a 10 nm wide quantum well ((b) and (d)). The inset shows the schematic conduction energy band diagram of the $GaAs/Al_xGa_{1-x}As/Al_{0.3}Ga_{0.7}As$ step quantum wells.

where $\alpha(z)$ is the Rashba coefficient, k_x and k_y are the wave vectors, σ_x and σ_y denote the spin Pauli matrices. When spin splitting is introduced by a uniform electric field, $\alpha(z)$ is a constant proportional to the electric field [10,14–16]:

$$\alpha(z) = \alpha_{so} e \langle E \rangle, \tag{2}$$

where α_{so} is the Rashba spin orbit coupling parameter, E is the electric field. For an abrupt interface like GaAs/AlGaAs, $\alpha(z)$ should have the form [5,6,9]

$$\alpha(z) = P\delta(z - z_0), \tag{3}$$

where z_0 is the position of the interface, the δ-function clearly shows that the Rashba effect (spin-orbit coupling) is localized at the interface. The interface parameter P is related to the difference of band parameters across the interface [5,6,16–18]. For a $GaAs/Al_xGa_{1-x}As$ interface, it is reasonable to assume that P is proportional to x. Therefore, for the $Al_{0.3}Ga_{0.7}As/GaAs/Al_xGa_{1-x}As/Al_{0.3}Ga_{0.7}As$ step QW with internal SIA shown in the inset of fig. 1(a) in the absence of electric field and magnetic field, the Rashba coefficient can be written as

$$\alpha_I(z) = P\delta(z - z_0) - \frac{x}{x_0} P\delta(z - z_1) - \left(1 - \frac{x}{x_0}\right) P\delta(z - z_2), \tag{4}$$

where P is the interface parameter for the $GaAs/Al_{0.3}Ga_{0.7}As$ interface, x and x_0 stand for the Al concentration in the step and barrier, respectively, and z_i is the position of the i-th interface. In the following calculation, z_0 is set to be 0, x_0 is set to be 0.3, the coordinate of the interface is controlled by the step width and well width, the heights of the offsets at the interfaces are controlled by the concentration of Al in the $Al_xGa_{1-x}As$ step. The contribution of the barrier is given as the band offsets weighted by the probability density of the conduction electrons at the interfaces [7].

For [001]-oriented step QWs, only considering the interface contribution to the Rashba effect, the conduction Hamiltonian can be written as

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + V(z) + \alpha_I(z)(\sigma_x k_y - \sigma_y k_x), \tag{5}$$

where m^* is the electron effective mass, $V(z)$ is the confinement potential. In z-direction, the electron wave function can be written as

$$\Psi^{\pm}(z) = \begin{bmatrix} A^+ \\ A^- \end{bmatrix} e^{ikz} + \begin{bmatrix} B^+ \\ B^- \end{bmatrix} e^{-ikz}. \tag{6}$$

In regions II ($0 < z < z_1$) and III ($z_1 < z < z_2$), $A^{\pm}$ and $B^{\pm}$ are constants to be determined, in regions I ($z < 0$) and IV ($z > z2$), $B^{\pm}$ and $A^{\pm}$ are set to be zero, respectively. The electron wave vectors in the z-direction in both barriers regions are determined by $k = i\sqrt{\frac{2m^*}{\hbar^2}(V_2 - E)}$, while in the well regions II and III, they are determined by $k = \sqrt{\frac{2m^*}{\hbar^2}E}$ and $k = \sqrt{\frac{2m^*}{\hbar^2}(E - V_1)}$, respectively. The electron effective mass m^* is determined by the linear interpolation of GaAs ($0.0667m_e$) and AlAs ($0.15m_e$). From integration across the interface, we obtain the boundary conditions

$$\Psi^{\pm}(z)|_{z_i+0} = \Psi^{\pm}(z)|_{z_i-0}, \tag{7}$$

and

$$-\frac{\hbar^2}{2m^*_{z_i+0}}\frac{\partial \Psi^{\pm}(z)}{\partial z}|_{z_i+0} = -\frac{\hbar^2}{2m^*_{z_i-0}}\frac{\partial \Psi^{\pm}(z)}{\partial z}|_{z_i-0} + Q_i(k_y \pm ik_x)\Psi^{\mp}|_{z_i-0}, \tag{8}$$

in which Q_i is, respectively, $-P$, $\frac{x}{x_0}P$ and $(1 - \frac{x}{x_0})P$ at the i-th interface. We relate the coefficients of wave functions in both barriers by the above boundary conditions to obtain the transfer matrix and solve the spin-dependent eigenenergies $E_n^{\pm}$ numerically, the spin splitting can be written as $\Delta E_n = E_n^+ - E_n^-$.

Now we are in the position to perform the numerical calculation about the Rashba spin splitting under the step-like confinement potential. By simulating the results of ref. [10] and ref. [16], we extract $P \approx -30\,meV \cdot nm^2$. For simplicity, we let $k_y = 0$, so the parallel wave vector $k_{//}$ can be labeled by $k_x = 2.0 \times 10^6\,cm^{-1}$.

First of all, by changing the total well width and the step width for a given well width of the step QW, we take 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 as an example to find the origin of the Rashba spin splitting. In fig. 1(a) we plot the spin splitting as a function of the total well width, where the step width is half of the total well width. For a narrow well, only the ground subband is present in it, with the increasing of the well width, the spin splitting of the ground subband whose sign is always negative first increases to a negative maximum up to when it is close to a critical well width where the first exited subband falls into the well, and then, turns down. While for the first exited subband, what should be noted is the sign of spin splitting which is opposite to that of the ground subband for a narrow well. With the increasing of well width, the spin splitting decreases from the positive maximum, and finally changes its sign from positive to negative. The sign changing of the first excited subband spin splitting of the step QW is the most distinct character different from that of the asymmetry QW with different barrier materials [10,11] in which the sign of the first excited subband spin splitting is always positive; this implies that the $Al_{0.15}Ga_{0.85}As/Al_{0.3}Ga_{0.7}As$ interface of the step QW plays a very important effect on the sign of the spin splitting of the step QW. Compared with the asymmetrical QW, another difference is that the spin splitting appears in narrower well due to the better confinement effect of the existence of the $Al_{0.15}Ga_{0.85}As/Al_{0.3}Ga_{0.7}As$ interface.

Due to the introduction of the step, another merit of the step QW is that the spin splitting can be controlled by the step width, which cannot be realized by the asymmetrical QW. In fig. 1(b) we show the spin splitting of the ground and the first excited subband as a function of the step width for the 10 nm wide QW. The spin splitting of the excited subband can be larger or smaller than that of the ground subband depending on the well structure. When the step width equals zero or ten, the QW is a symmetrical $GaAs/Al_{0.3}Ga_{0.7}As$ or $Al_{0.15}Ga_{0.85}As/Al_{0.3}Ga_{0.7}As$ QW, respectively, the structure inversion symmetry of which is preserved. Accordingly, no spin splitting can be observed in fig. 1(b) for the two extreme cases. With the step width increasing from zero to ten, the spin splitting of the ground subband presents a negative single peak when the width of the $Al_{0.15}Ga_{0.85}As$ step is about 7.5 nm, which means that a 7.5 nm width step contributes to the optimal SIA of the 10 nm width step QW. The fact that a narrower GaAs layer is helpful to obtain a bigger spin splitting may be a hint for designing the structure of the QWs such as to obtain big spin splitting. While for the first excited subband, a distinct character to be noted is that the spin splitting changes its sign between negative and positive and presents an oscillation behavior with the increasing of the step width.

The origin of the spin spitting of such a step QW can be traced down to the introduction of the step potential and one more interface. Due to the existence of the step, the former and latter interface of the step QW cannot transform into each other by a mirror reflection in the well plane, therefore, the interface contributions to Rashba effect caused by the abrupt change of the potential at the interfaces with opposite signs and different magnitude cannot cancel out each other. The contribution of the Rashba Hamiltonian to spin splitting can be treated as a perturbation. The n-th subband spin splitting calculated by the first-order degenerate perturbation theory can be

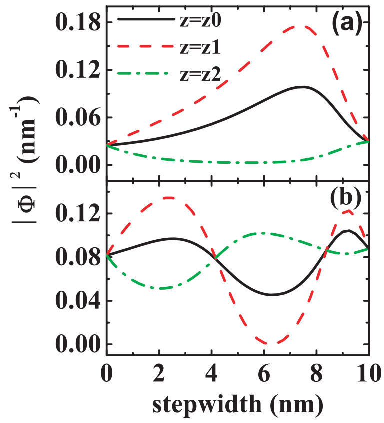

Fig. 2: Electron probability density at three interfaces of the ground (a) and the first excited (b) subbands as a function of the step width of a 10 nm wide $GaAs/Al_{0.15}Ga_{0.85}As/Al_{0.3}Ga_{0.7}As$ step quantum well.

written as

$$\Delta E_n=2k_xP\left[\left(1-\frac{x}{x_0}\right)|\psi_n^0(z_2)|^2+\frac{x}{x_0}|\psi_n^0(z_1)|^2-|\psi_n^0(z_0)|^2\right], \tag{9}$$

which is tightly related to the difference of electron probability density between the two right interfaces and the left interface. We introduce

$$d_n=\left(1-\frac{x}{x_0}\right)|\psi_n^0(z_2)|^2+\frac{x}{x_0}|\psi_n^0(z_1)|^2-|\psi_n^0(z_0)|^2 \tag{10}$$

to describe the probability density difference of the n-th $(n=0,1)$ subband electron between the two right interfaces and the left interface. Where $\psi_n^0(z_i)$ is the zeroth-order envelope function of the n-th subband at the i-th interface. It is easy to find that ΔE_n linearly depends on d_n under the first-order perturbation approximation. d_n as a function of the total well width and the step width of a 10 nm wide QW are shown in fig. 1(c) and (d), respectively. One can see that the dependences of d_n and of the spin splitting on the well width and step width are similar, so that, the dependence of the spin splitting on the total well width and step width for a given well width can be well explained by the behavior of d_n as shown in fig. 1(c) and (d).

Now we will show how the well structure influences the electron probability density in the step QW. In fig. 2(a) and (b) we plot the electron probability density at three interfaces of the ground and the first excited subbands as a function of the step width of the 10 nm wide QW, respectively. When the QW is symmetrical, the electron probability densities at both interfaces are equal to each other due to the symmetrical penetration of the wave function into both barriers. The existence of the step results in the asymmetrical penetration of the wave function into the barriers, therefore, the electron probability density at the three interfaces changes with

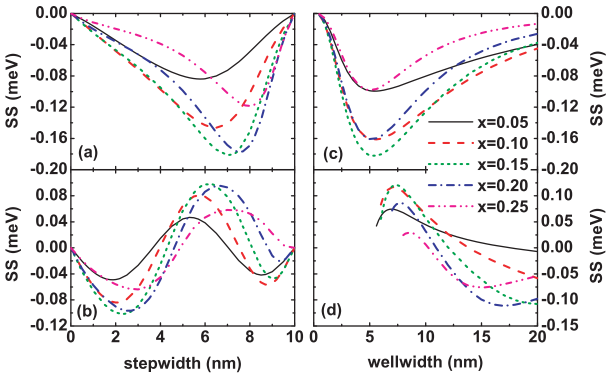

Fig. 3: Spin splitting (SS) of the ground and the first excited subbands of $GaAs/Al_xGa_{1-x}As/Al_{0.3}Ga_{0.7}As$ step quantum wells at $k = 0.2 \times 10^6 cm^{-1}$ as a function of the step width of a 10 nm wide quantum well ((a) and (b)) and the total well width (where the step width is half of the total well width) ((c) and (d)).

the step width. It is easy to note that the changing of the electron probability density at the z_0 and z_1 interfaces with the step width is similar to the spin splitting changing with the step width, and the changing at the z_1 interface is more pronounced than that at the z_0 interface, the changing of the electron probability density at the z_2 interface is opposite to that of the z_0 and z_1 interfaces. The combined effect of the three interfaces results in the sign changing of the spin splitting of the excited subband. Therefore, as mentioned above, the spin splitting of the step QW is tightly related to the electron probability density at the three interfaces, *i.e.* the wave function at the three interfaces. The quantitative understanding of the excited subbands spin splitting behavior provides an approach to implementing a spintronic device which can manipulate the sign of the electron spin splitting by its energy or by the well width and the step width of the QW.

In order to complete the picture of the spin splitting induced by the interface Rashba effect, we focus on the Al concentration in the $Al_xGa_{1-x}As$ step which influences the degree of SIA by controlling the band offset at the interfaces. For the Al concentrations $x = 0.05$, 0.10, 0.15, 0.20 and 0.25, we plot in fig. 3(a) and (b) the spin splitting depending on the step width of the 10 nm wide QW. Obviously, when $x = 0$ or 0.3, the QW is symmetric, so to improve the degree of SIA of the QW, the value of x cannot be too close to those two x values, as a result, the greatest amplitude of spin splitting as a function of step width occurs at $x = 0.15$. The band offset of the $GaAs/Al_{0.15}Ga_{0.85}As$ interface is almost half of that of $GaAs/Al_{0.3}Ga_{0.7}As$ interface, which is far from symmetry and induces the biggest spin splitting. In fig. 3(c) and (d) we plot the spin splitting of the ground subbands and the first excited subbands as a function of the well width, respectively. We can come to the same conclusion that $x = 0.15$ contributes to the biggest spin splitting. Furthermore, One can note that, especially from fig. 3(c), the narrower QW is more sensitive to the Al concentration in the step. We should mention that the novel behavior of sign changing of the excited subband spin splitting is kept when changing the Al concentration from 0.05 to 0.25.

The sign changing of the first excited subbands may result in many novel effects. Some experiments would be needed to fully test the results we calculated. The spin splitting has important effect on the spin-orientation–induced circular photogalvanic effect (CPGE) [19], so CPGE can be utilized to investigate the sign changing of the excited subbands spin splitting, the magnitude and sign of the resulting photocurrent may be different depending on the well structure. The method proposed by Lorenz Meier and Gian Salis *et al.* [20] can be applied to extract the magnitude and sign of the excited subbands spin splitting. By the means of Shubnikov-de Haas oscillations, the magnitude of the ground and the excited subbands can also be determined [21].

In summary, we have investigated theoretically the 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 QWs which contains built-in SIA in the absence of electric field and magnetic field. Due to the introduction of the $Al_xGa_{1-x}As$ step and the $Al_xGa_{1-x}As/Al_{0.3}Ga_{0.7}As$ interface into the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ QW, the resulting interface Rashba effect induces spin splitting of conduction subbands which can be well controlled by the well width, step width and the concentration of Al in the $Al_xGa_{1-x}As$ step. To realize an optimal spin splitting, the three parameters should match each other till the greatest degree of SIA is obtained. Especially, a narrower GaAs layer contributes to a bigger spin splitting of the ground subband, among all Al concentrations in the step less than 0.3, $x = 0.15$ can result in the biggest spin splitting of the ground subband for the 10 nm wide step QW with 7.5 nm wide step. The sign changing of the spin splitting is the most distinct character of the step QWs. The sign of the ground subband is always negative, and the sign of the excited subband changes with the well width and step width. When the step width is half of the well width, for a narrow well, the sign of the spin splitting of the first excited subband is just opposite to that of the ground state. For a given well width, with the variation of the step width, the spin splitting of the first excited subband presents an oscillation behavior, the sign of which shifts between negative and positive. This will be an advantage in designing the spintronic devices. We also demonstrate that the sign and the magnitude of the spin splitting of the step QW is governed by the electron probability at the three interfaces. These results may give some hints about how a QW should be design for a desired spin splitting.

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