# Spin–orbit coupling effects on the in-plane optical anisotropy of semiconductor quantum wells*

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We theoretically study the influence of the spin–orbit coupling (SOC) on the in-plane optical anisotropy (IPOA) induced by in-plane uniaxial strain and interface asymmetry in (001) GaAs/AlGaAs quantum wells (QWs) with different well width. It is found that the SOC has more significant impact on the IPOA for the transition of the first valence subband of heavy hole to the first conduction band (1H1E) than that of 1L1E. The reason has been discussed. The IPOA of (001) InGaAs/InP QWs has been measured by reflectance difference spectroscopy, whose amplitude is about one order larger than that of GaAs/AlGaAs QWs. The anisotropic interface potential parameters of InGaAs/InP QWs are also determined. The influence of the SOC effect on the IPOA of InGaAs/InP QWs when the QWs are under tensile, compressive or zero biaxial strain are also investigated in theory. Our results demonstrate that the SOC has significant effect on the IPOA especially for semiconductor QWs with small well width, and therefore cannot be ignored.

**Keywords:** spin–orbit coupling, in-plane optical anisotropy, InGaAs/InP quantum well, GaAs/AlGaAs quantum well

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## 1. Introduction

It is well known that in-plane optical anisotropy (IPOA) of (001)-grown zinc-blende quantum wells (QWs) can be induced when the symmetry is reduced from $D_{2d}$ to $C_{2v}$.[1–6] There are many factors that can induce this symmetry reduction effect (SRE), such as anisotropic-chemical-bond arrangement at the interfaces,[1] uniaxial strain along the [110] direction,[4,7–9] segregation effect of atoms,[6,10] and anisotropic interface structures.[11–13] These SREs introduce coupling of the heavy-hole (HH) bands and light-hole (LH) bands, which results in IPOA of QWs. Ivchenko *et al.* studied the IPOA induced by the coupling of HH and LH by tight-binding model,[14] while Krebs *et al.* investigated it by introducing "B" and "F" operators into the traditional $\boldsymbol{k}\cdot\boldsymbol{p}$ theory.[1] Then, Chen *et al.* studied it by using perturbation theory incorporating the effect of $C_{2v}$ interface symmetry based on the envelope function approximation.[11] It is worth noting that, these SREs will also introduce the coupling between the HH, LH bands and the spin–orbit spin-off (SO) bands. However, no report has concerned the influence of the coupling between HH, LH, and SO bands on the IPOA of QWs so far.

In this paper, we theoretically study the influence of the spin–orbit coupling (SOC), i.e., the coupling between HH, LH bands and the SO bands, on the IPOA induced by in-plane uniaxial strain and interface asymmetry in (001)-oriented GaAs/AlGaAs QWs with different well widths. We find that the SOC has more significant impact on the IPOA for the transition of 1H1E (the first valence subband of heavy hole to the first conduction band) than that of 1L1E (the first valence subband of light hole to the first conduction band). The IPOA of (001) InGaAs/InP QWs has been measured by reflectance difference spectroscopy, whose amplitude is about one order larger than that of GaAs/AlGaAs QWs. The anisotropic interface potential parameters of InGaAs/InP QWs are also determined. Then, we also theoretically investigate the influence of the SOC effect on the IPOA in (001)-oriented InGaAs/InP QWs under tensile, zero, and compressive biaxial strain with different well width. Our results demonstrate that the SOC has significant effect on the IPOA especially for semiconductor QWs with small well width, and therefore cannot be ignored.

## 2. Theory

Based on the theory of Luttinger–Kohn and Bir–Pikus, and adopting the hole mixing induced by strain and the two interfaces as perturbation, the valence-band structure of a semiconductor can be described by the following 4×4 Hamiltonian in the envelop-function approach:[11,15]

$$\boldsymbol{H} = \boldsymbol{H}_0 + \boldsymbol{H}', \tag{1}$$

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where

$$\boldsymbol{H}_0 = \begin{pmatrix} P+Q & 0 & 0 & 0 \\ 0 & P-Q & 0 & 0 \\ 0 & 0 & P-Q & 0 \\ 0 & 0 & 0 & P+Q \end{pmatrix},$$

and

$$\boldsymbol{H}' = \begin{pmatrix} 0 & -S & R & 0 \\ -S^\dagger & 0 & 0 & R \\ R^\dagger & 0 & 0 & S \\ 0 & R^\dagger & S^\dagger & 0 \end{pmatrix},$$

with

$$\begin{aligned} P &= P_k + P_\epsilon, Q = Q_k + Q_\epsilon, \\ R &= R_k + R_\epsilon + R_{\rm in}, \ S = S_k + S_\epsilon, \\ P_k &= \left(\frac{\hbar^2}{2m_0}\right)\gamma_1(k_x^2+k_y^2+k_z^2), \\ Q_k &= \left(\frac{\hbar^2}{2m_0}\right)\gamma_2(k_x^2+k_y^2-2k_z^2), \\ R_k &= \left(\frac{\hbar^2}{2m_0}\right)\sqrt{3}[-\gamma_2(k_x^2-k_y^2)+2{\rm i}\gamma_3 k_x k_y], \\ S_k &= \left(\frac{\hbar^2}{2m_0}\right)2\sqrt{3}\gamma_3(k_x-{\rm i}k_y)k_z, \\ P_\epsilon &= -a_{\rm v}(\epsilon_{xx}+\epsilon_{yy}+\epsilon_{zz}), \\ Q_\epsilon &= -\frac{b}{2}(\epsilon_{xx}+\epsilon_{yy}-2\epsilon_{zz}), \\ R_\epsilon &= \frac{\sqrt{3}}{2}b(\epsilon_{xx}-\epsilon_{yy})-{\rm i}d\epsilon_{xy}, \\ S_\epsilon &= -d(\epsilon_{zx}-{\rm i}\epsilon_{yz}), \\ R_{\rm in} &= P_1\delta(z-w/2)-P_2\delta(z+w/2). \end{aligned}$$

Here $\epsilon_{ij}$ is the strain tensor; $\gamma_1$, $\gamma_2$, and $\gamma_3$ are the Luttinger parameters; $a_{\rm v}$, $b$, and $d$ are the Bir–Pikus deformation potentials; $\Delta$ is the spin–orbit spin-off energy; $P_1$ and $P_2$ are the interface potential parameters of the upper and lower interfaces, respectively, which are used to describe the effect of $C_{2v}$ interface symmetry; $z = \pm w/2$ indicates the positions of the interfaces. Here, $x \parallel [100]$ and $y \parallel [010]$. The bases for the Hamiltonian $\boldsymbol{H}$ are $|3/2,3/2\rangle, |3/2,1/2\rangle, |3/2,-1/2\rangle$, and $|3/2,-3/2\rangle$. It can be seen from the Hamiltonian $\boldsymbol{H}'$ that, the strain and interface potential can introduce the coupling of the heavy and light holes.

Actually, the strain and interface potential will also result in the coupling of the SO bands with heavy- and light-holes bands. If this coupling is taken into account, the valence-band structure should be described by the following $6\times 6$ Hamiltonian:[11,15]

$$\boldsymbol{H} = \boldsymbol{H}_0 + \boldsymbol{H}', \tag{2}$$

where

$$\boldsymbol{H}_0 = \begin{pmatrix} P+Q & 0 & 0 & 0 & 0 & 0 \\ 0 & P-Q & 0 & 0 & 0 & 0 \\ 0 & 0 & P-Q & 0 & 0 & 0 \\ 0 & 0 & 0 & P+Q & 0 & 0 \\ 0 & 0 & 0 & 0 & P+\Delta & 0 \\ 0 & 0 & 0 & 0 & 0 & P-\Delta \end{pmatrix},$$

and

$$\boldsymbol{H}' = \begin{pmatrix} 0 & -S & R & 0 & -\frac{1}{\sqrt{2}}S & \sqrt{2}R \\ -S^\dagger & 0 & 0 & R & -\sqrt{2}Q & \sqrt{\frac{3}{2}}S \\ R^\dagger & 0 & 0 & S & \sqrt{\frac{3}{2}}S^\dagger & \sqrt{2}Q \\ 0 & R^\dagger & S^\dagger & 0 & -\sqrt{2}R^\dagger & -\frac{1}{\sqrt{2}}S^\dagger \\ -\frac{1}{\sqrt{2}}S^\dagger & -\sqrt{2}Q & \sqrt{\frac{3}{2}}S & -\sqrt{2}R & 0 & 0 \\ \sqrt{2}R^\dagger & \sqrt{\frac{3}{2}}S^\dagger & \sqrt{2}Q & -\frac{1}{\sqrt{2}}S & 0 & 0 \end{pmatrix},$$

with the bases $|3/2,3/2\rangle$, $|3/2,1/2\rangle$, $|3/2,-1/2\rangle$, $|3/2,-3/2\rangle$, $|1/2,1/2\rangle$, and $|1/2,-1/2\rangle$.

For a QW grown along [001] ($z$) direction, the energies and the envelope functions of valence subbands can be obtained by solving the effective-mass equation

$$\sum_\nu [H_{\mu\nu} + V_{\rm h}(z)\delta_{\mu\nu}]F_\nu(\boldsymbol{k}_\parallel, z) = E(\boldsymbol{k}_\parallel)F_\mu(\boldsymbol{k}_\parallel, z), \tag{3}$$

where $\mu,\nu \in \{|3/2,3/2\rangle, |3/2,1/2\rangle, |3/2,-1/2\rangle, |3/2,-3/2\rangle, |1/2,1/2\rangle, |1/2,-1/2\rangle\}$ for 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, and $\mu,\nu \in \{|3/2,3/2\rangle, |3/2,1/2\rangle, |3/2,-1/2\rangle, |3/2,-3/2\rangle\}$ for 4-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory. Here $\boldsymbol{H}$ is the Luttinger–Kohn Hamiltonian described by Eq. (1) (for 4-band) or Eq. (2) (for 6-band), and $V_{\rm h}(z)$ is the quantum-well potential for holes. The envelope function component $F_\nu$ can be written as[15]

$$F_\nu(\boldsymbol{k}_\parallel, \boldsymbol{r}) = F_\nu(\boldsymbol{k}_\parallel, z)\,{\rm e}^{{\rm i}\boldsymbol{k}_\parallel\cdot\boldsymbol{\rho}}, \tag{4}$$

where $\boldsymbol{k}_\parallel = k_x\hat{\boldsymbol{x}} + k_y\hat{\boldsymbol{y}}$, and $\boldsymbol{\rho} = x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}}$. The wave vector $k_z$ is interpreted as a differential operator $-{\rm i}\partial/\partial z$. Since excitonic effect is dominant for interband transition in an undoped QW sample, we can evaluate the IPOA of the sample by only taking into account the contribution of anisotropy at $k = 0$.[16] Thus, adopting $k_x = k_y = 0$, $k_z = -{\rm i}\partial/\partial z$, and using the finite difference method, we can obtain the energies and envelope functions of holes numerically. Similarly, the energies and envelope functions of electrons can be obtained by the single band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory. Then the IPOA can be calculated, which is described by the anisotropic transition probability $\Delta M = M_{110} - M_{1\bar{1}0}$. Here $M_{110}$ denotes the transition probability when the incident light is polarized along the [110] direction, i.e., for the transition 1H1E, $M_{110}^{\rm 1H1E} = \langle f_{\rm 1E}|\mathscr{P}_{110}|f_{\rm 1H}\rangle$,

where $f_{1E}$ ($f_{1H}$) is the envelope function of the first electron subband (the first heavy-hole subband), and $\mathscr{P}_{110}$ is the operator describing the transition probability when the incident light is polarized along the [110] direction.

In order to see clearly the influence of the uniaxial strain and interface potential on the IPOA when the SOC effect is taken into account, we discuss them separately. In Section 3, we will first discuss the IPOA induced by uniaxial strain and interface potential in the lattice matched GaAs/$Al_xGa_{1-x}$As QWs, and then we determine the interface potential in InGaAs/InP QWs, and further theoretically study the influence of the SOC effect on the IPOA when the QWs are under tensile, compressive, or zero biaxial strain.

## 3. Results and discussion

### 3.1. GaAs/AlGaAs quantum well

For GaAs/$Al_xGa_{1-x}$As QWs, we should first evaluate the value of the interface potential $P_0$. According to Ref. [11], $P_0 = 400$ meV·Å for AlAs/GaAs interface. Thus, for $Al_{0.34}Ga_{0.66}$As/GaAs QW, $P_0$ can be adopted to be 136 meV·Å by linear interpolation.[11] If we only consider the uniaxial strain along the [110] direction, we have

$$\begin{aligned} \epsilon_{xx} &= \epsilon_{yy} = \epsilon_{zz} = \epsilon_{yz} = \epsilon_{xz} = 0, \\ \epsilon_{xy} &\neq 0, \\ P_1 &= P_2 = P_0. \end{aligned} \tag{5}$$

If we only consider the effect of interface potential, we have

$$\begin{aligned} \epsilon_{ij} &= 0, \quad (i,j = x,y,z), \\ P_1 &\neq P_2 = P_0, \end{aligned} \tag{6}$$

and $\Delta P = P_1 - P_2$ is used to characterize the asymmetry degree of the two interfaces. Figure 1 shows the calculated interface- and uniaxial strain-induced anisotropic transition probabilities $\Delta M$ of 1H1E, 1L1E and their ratio in GaAs/$Al_{0.34}Ga_{0.66}$As QWs as a function of well width. The solid and dashed lines indicate the results calculated by 4-band and 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, respectively. It can be seen that, the interface-induced anisotropic transition probability $\Delta M$ decreases as the the well width is increased, while that induced by uniaxial strain firstly decreases and reaches a minimum at well width about 2 nm, and then increases almost linearly with the well width. SOC will introduce additional IPOA, and its value depends on the well width. Figure 1(c) displays the ratio of $\Delta M$ of 1H1E to that of 1L1E, from which we can see that the variation trend of the value of $\Delta M_{1H1E}/\Delta M_{1L1E}$ induced by uniaxial strain is different from that induced by interface. That is, the former one increases with the increasing well width, while the latter one decreases with the well width. Besides, the ratio $\Delta M_{1H1E}/\Delta M_{1L1E}$ obtained by 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory with the SOC effect taken into account is larger than that obtained by 4-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, which indicates that the SOC has more significant influence on the IPOA for 1H1E than that for 1L1E.

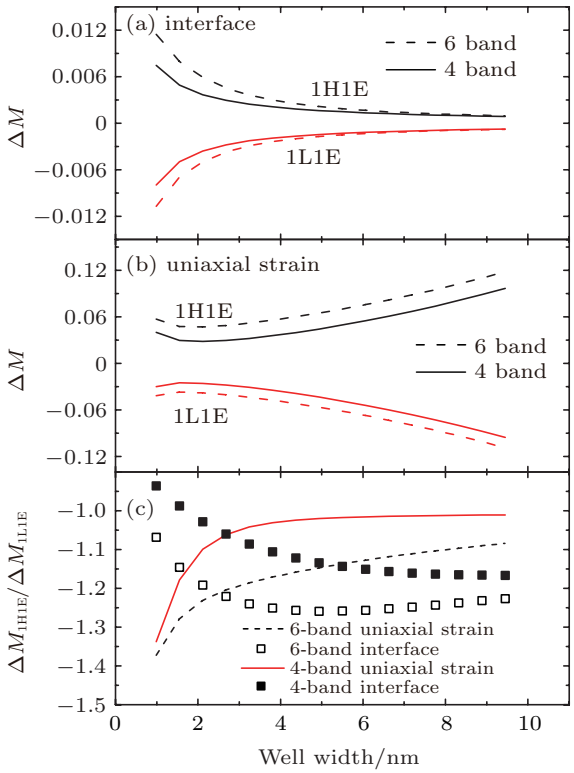



**Fig. 1.** (color online) Calculated (a) interface- and (b) uniaxial strain-induced anisotropic transition probabilities $\Delta M$ ($\Delta M = M_{110} - M_{1\bar{1}0}$) of 1H1E and 1L1E in GaAs/$Al_{0.34}Ga_{0.66}$As QWs vs well width. The solid and dashed lines are the results calculated by 4-band and 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, respectively. (c) The ratio of $\Delta M$ of 1H1E to that of 1L1E as a function of well width. The dashed and solid lines indicate the results obtained by 6-band and 4-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory when we only consider the influence of biaxial strain, respectively. The lines and squares denote the results induced by uniaxial strain and interface potential, respectively.

A perturbation approach can help us understand the above results. If there is a mixing between $k$ state and $k'$ state caused by the perturbation potential $\Delta V$, then under the first-order approximation, the envelope function of the $k$ state can be written as

$$\psi_k(x) = \psi_k^{(0)} + \psi_k^{(1)}(x), \tag{7}$$

$$\psi_k^{(1)}(x) = \sum_{k'\neq k} \frac{\langle k'|\Delta V|k\rangle}{\varepsilon_k^{(0)} - \varepsilon_{k'}^{(0)}} \psi_{k'}^{(0)}. \tag{8}$$

Here $\psi_k^{(0)}$ is the pure state wave function without hole mixing effect, $\varepsilon_k^{(0)}$ is the energy of the $k$ state without hole mixing effect, and $\langle k'|\Delta V|k\rangle$ is the hole-mixing strength between $k'$ state and $k$ state. Thus, if the SOC effect is taken into account, the wave function of 1H and 1L can be described by

$$\psi_{1H} = \frac{\langle 1L|\Delta V_1|1H\rangle}{\varepsilon_{1H}^{(0)} - \varepsilon_{1L}^{(0)}} \psi_{1L}^{(0)} + \frac{\langle SO|\Delta V_2|1H\rangle}{\varepsilon_{1H}^{(0)} - \varepsilon_{SO}^{(0)}} \psi_{SO}^{(0)} + \psi_{1H}^{(0)}, \tag{9}$$

$$\psi_{1L} = \frac{\langle 1H|\Delta V_1|1L\rangle}{\varepsilon_{1L}^{(0)} - \varepsilon_{1H}^{(0)}} \psi_{1H}^{(0)}$$

$$+\frac{\langle \mathrm{SO}|\Delta V_3|1\mathrm{L}\rangle}{\varepsilon_{1\mathrm{L}}^{(0)}-\varepsilon_{\mathrm{SO}}^{(0)}}\psi_{\mathrm{SO}}^{(0)}+\psi_{1\mathrm{L}}^{(0)}. \tag{10}$$

Here $\Delta V_i$ $(i=1,2,3)$ are the elements that will introduce hole-mixing effect, and they are given by

$$\Delta V_1 = R_\epsilon + R_{\mathrm{in}}, \tag{11}$$

$$\Delta V_2 = \sqrt{2}(R_\epsilon + R_{\mathrm{in}}), \tag{12}$$

$$\Delta V_3 = \sqrt{2}(Q_k + Q_\epsilon). \tag{13}$$

According to the perturbation approach,[11] if there is a mixing between subband of $m$H and $n$L ($m$H denotes the subband of $m$th heavy hole) caused by $\Delta V$, the anisotropic transition strength of $m$H1E is proportional to

$$\frac{\langle 1\mathrm{E}|m\mathrm{H}\rangle\langle m\mathrm{H}|\Delta V|n\mathrm{L}\rangle\langle n\mathrm{L}|1\mathrm{E}\rangle}{|\varepsilon_{m\mathrm{H}}-\varepsilon_{n\mathrm{L}}|}, \tag{14}$$

where $\langle 1\mathrm{E}|m\mathrm{H}\rangle$ is the overlap integral of 1E and $m$H subband. Thus, taking into account the SOC effect, we can express the anisotropic transition probability of 1H1E and 1L1E as

$$\Delta M_{1\mathrm{H1E}} = \frac{2\sqrt{3}}{3}\frac{\langle 1\mathrm{L}|\Delta V_1|1\mathrm{H}\rangle}{\varepsilon_{1\mathrm{H}}^{(0)}-\varepsilon_{1\mathrm{L}}^{(0)}} + \frac{2\sqrt{6}}{3}\frac{\langle \mathrm{SO}|\Delta V_2|1\mathrm{H}\rangle}{\varepsilon_{1\mathrm{H}}^{(0)}-\varepsilon_{\mathrm{SO}}^{(0)}}, \tag{15}$$

$$\Delta M_{1\mathrm{L1E}} = \frac{2\sqrt{3}}{3}\frac{\langle 1\mathrm{H}|\Delta V_1|1\mathrm{L}\rangle}{\varepsilon_{1\mathrm{L}}^{(0)}-\varepsilon_{1\mathrm{H}}^{(0)}} + \frac{2\sqrt{6}}{3}\frac{\langle \mathrm{SO}|\Delta V_3|1\mathrm{L}\rangle}{\varepsilon_{1\mathrm{L}}^{(0)}-\varepsilon_{\mathrm{SO}}^{(0)}} \times \frac{\langle 1\mathrm{H}|\Delta V_1|1\mathrm{L}\rangle}{\varepsilon_{1\mathrm{L}}^{(0)}-\varepsilon_{1\mathrm{H}}^{(0)}}. \tag{16}$$

It can be seen that SOC will introduce additional contribution to the anisotropic transition probability $\Delta M$. Specifically speaking, it influences $\Delta M$ in two ways. Firstly, the SO band will push the HH and LH bands upward, and make them closer to each other. Since $\Delta M$ of 1H1E or 1L1E is inversely proportional to the energy difference between subband of 1H and 1L, SOC effect will lead to larger $\Delta M$. Secondly, SOC will introduce additional coupling between SO band and 1H or 1L bands, thus resulting in larger $\Delta M$. According to Eqs. (15) and (16), the additional contributions to $\Delta M$ induced by SOC are

$$\Delta M_{\mathrm{SO}} = \frac{2\sqrt{6}}{3}\frac{\langle \mathrm{SO}|\Delta V_2|1\mathrm{H}\rangle}{\varepsilon_{1\mathrm{H}}^{(0)}-\varepsilon_{\mathrm{SO}}^{(0)}}, \quad \text{for 1H1E}, \tag{17}$$

$$\Delta M_{\mathrm{SO}} = \frac{2\sqrt{6}}{3}\frac{\langle \mathrm{SO}|\Delta V_3|1\mathrm{L}\rangle}{\varepsilon_{1\mathrm{L}}^{(0)}-\varepsilon_{\mathrm{SO}}^{(0)}}\frac{\langle 1\mathrm{H}|\Delta V_1|1\mathrm{L}\rangle}{\varepsilon_{1\mathrm{L}}^{(0)}-\varepsilon_{1\mathrm{H}}^{(0)}}, \quad \text{for 1L1E}. \tag{18}$$

Thus, denoting

$$\Delta M_{1\mathrm{L}} = \frac{2\sqrt{3}}{3}\frac{\langle 1\mathrm{L}|\Delta V_1|1\mathrm{H}\rangle}{\varepsilon_{1\mathrm{H}}^{(0)}-\varepsilon_{1\mathrm{L}}^{(0)}},$$

and according to Eqs. (15) and (17), we have, for 1H1E,

$$\frac{\Delta M_{1\mathrm{L}}}{\Delta M_{\mathrm{SO}}} \approx \frac{\Delta V_1}{\sqrt{2}\Delta V_2}\frac{|\varepsilon_{1\mathrm{H}}-\varepsilon_{\mathrm{SO}}|}{|\varepsilon_{1\mathrm{H}}-\varepsilon_{1\mathrm{L}}|}, \tag{19}$$

and

$$\frac{\Delta M_{\mathrm{SO}}}{\Delta M_{\mathrm{total}}} \approx \frac{1}{\left[1+\frac{1}{2}\frac{|\varepsilon_{1\mathrm{H}}-\varepsilon_{\mathrm{SO}}|}{|\varepsilon_{1\mathrm{H}}-\varepsilon_{1\mathrm{L}}|}\right]}. \tag{20}$$

Here, $\Delta M_{\mathrm{total}} = \Delta M_{1\mathrm{L}} + \Delta M_{\mathrm{SO}}$. Thus, we can estimate the contribution of SOC to the total $\Delta M$ for 1H1E by Eq. (20). In the following, we will discuss how the SOC effect influence the $\Delta M$ by the two ways mentioned above, respectively.

Figure 2 shows the energy difference between 1L and 1H obtained by 4-band and 6-bank $\boldsymbol{k}\cdot\boldsymbol{p}$ theory for GaAs/$Al_{0.34}Ga_{0.66}$As QW, respectively. The lines and squares indicate the results induced by the uniaxial strain and interface potential, respectively. It can be seen that, there is no distinct difference for $\varepsilon_{1\mathrm{L}}-\varepsilon_{1\mathrm{H}}$ between that induced by uniaxial strain and interface potential. However, the value of $\varepsilon_{1\mathrm{L}}-\varepsilon_{1\mathrm{H}}$ obtained by 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory is smaller than that obtained by 4-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory when the well width is smaller than 5.3 nm, indicating that the SOC effect reduces the energy difference between 1L and 1H for this range of well width. The value of $\varepsilon_{1\mathrm{L}}-\varepsilon_{1\mathrm{H}}$ obtained by 6-band theory shows the maximum difference (about 5 meV) than that obtained by 4-band theory when the well width is 2 nm. However, when the well width is larger than 5.3 nm, the value of $\varepsilon_{1\mathrm{L}}-\varepsilon_{1\mathrm{H}}$ obtained by 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory is a little larger than that obtained by 4-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory.

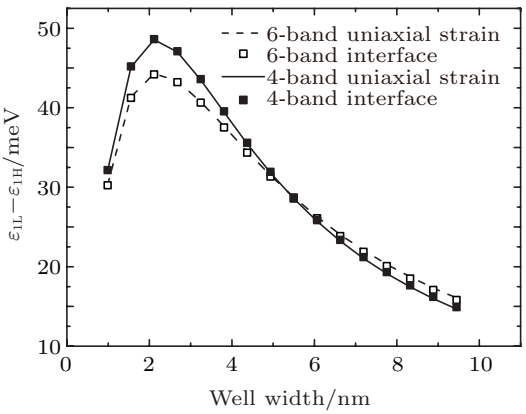



**Fig. 2.** Energy difference between 1L and 1H obtained by 6-band and 4-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory. The lines and squares indicate the results induced by the uniaxial strain and interface potential, respectively.

Figure 3 shows the ratio of $\Delta M_{\mathrm{SO}}$ contributed by SOC effect to the total $\Delta M$ as a function of well width. The lines and squares are the numerical results obtained by $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, while the "triangles on line" are the results obtained by Eq. (20). It can be seen that, the value of the ratio $\Delta M_{\mathrm{SO}}/\Delta M_{\mathrm{total}}$ depends on the well width for both 1H1E and 1L1E. Their values first increase with the well width and reach a maximum when the well width is 2 nm, and then decrease with the well width. When the well width is about 2 nm, the SOC effect will lead to about 24% increasement for the $\Delta M$

for 1H1E, while about 10% increasement for 1L1E. This implies that the SOC has more significant impact on the IPOA for the transition of 1H1E than that of 1L1E, which can be attributed to the fact that the additional contribution $\Delta M$ induced by SOC for 1L1E is nearly one order smaller than that for 1H1E, as shown in Eqs. (17) and (18). Besides, there is no significant difference for $\Delta M_{\rm SO}/\Delta M_{\rm total}$ between that induced by uniaxial strain and interface potential. In addition, for 1H1E, the value of $\Delta M_{\rm SO}/\Delta M_{\rm total}$ estimated by Eq. (20) is about 25% larger than that obtained numerically by $\boldsymbol{k}\cdot\boldsymbol{p}$ theory when the well width is smaller than 2 nm, while about 15% smaller when the well width is larger than 2 nm. Therefore, equation (20) provides us a convenient method to estimate the degree of the influence of SOC to the IPOA.

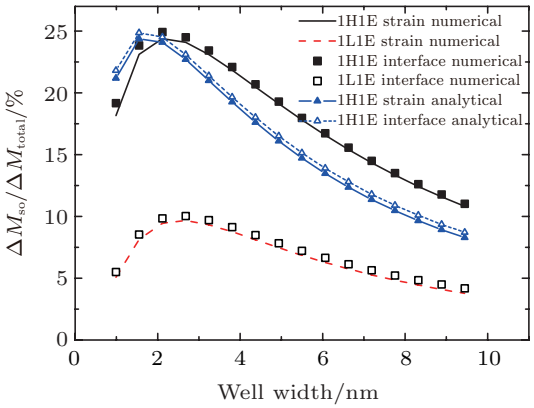



**Fig. 3.** (color online) The ratio of $\Delta M_{\rm SO}$ contributed by SOC effect to the total $\Delta M$ as a function of well width. The lines and squares are the numerical results obtained by $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, while the "triangles on line" are the results obtained by Eq. (20).

### 3.2. InP/InGaAs quantum well

Now let us look at the influence of the SOC effect on the IPOA in $In_xGa_{1-x}As$/InP QWs, in which the well and the barrier do not share common atoms. Firstly, we should estimate the interface potential parameter. In order to obtain this value, we measure the IPOA of an $In_{0.57}Ga_{0.43}As$/InP QW with a well width of 2 nm by reflectance difference spectroscopy (RDS). RDS is an interface-sensitive and non-destructive technique, and it can measure precisely the relative reflectance difference between the [110] and [1$\bar{1}$0] direction,[17] i.e., $\Delta r/r = 2(r_{110}-r_{1\bar{1}0})/(r_{110}+r_{1\bar{1}0})$. It is first invented by Aspnes [17] and further developed into $\mu$RDS with sub-μm spatial resolution by Cardona and co-workers.[19] The setup of the RDS is described in Ref. [18]. The reflectance spectra can be obtained at the same time with the RDS measurements.[3] Thus, we can obtain the $\Delta R/R$ spectra. Here $R$ is the reflectivity of the sample and $\Delta R$ is the reflectivity difference between samples with and without QW layers. The degree of polarization (DP) of a particular transition, which is defined as $(M_{110}-M_{1\bar{1}0})/(M_{110}+M_{1\bar{1}0})$ in the literature ($M_{110}$ denotes the transition probability when the light of incidence is polarized along [110] direction), can be obtained from the $\Delta r/r$ and $\Delta R/R$ spectra by the following equation:[11]

$$\mathrm{DP} = \frac{|\Delta r/r|}{|\Delta R/R|}. \tag{21}$$

Figure 4 shows the reflectance difference (RD) spectrum $\Delta r/r$ and $\Delta R/R$ spectrum of an $In_{0.57}Ga_{0.43}As$/InP QW with a well width of 2 nm measured at room temperature. Thus, we obtain the DP value for the transition of 1H1E is 17.4% by Eq. (21). This value is much larger than that obtained in a GaAs/AlGaAs QW (0.7%),[11] due to the inherent non-equivalence of the interface bonds in the "no-common-atom" InGaAs/InP QW.[2,11] Since the chemical bond on the upper interface is different from that on the lower interface, we can assume that $P_1 \neq P_2$. Thus, assuming that one of the interface potential ($P_1$ or $P_2$) equal to the theoretically estimated interface potential $P_0$, we can obtain the other interface potential by fitting the theoretical DP to the measured DP. Hence, we should firstly theoretically estimate the interface potential parameter $P_0$ by the boundary conditions (BC), the perturbed interface potential (HBF), the averaged hybrid energy difference of interface (AHE) and lattice mismatch models.[20] Given that BC model is equivalent to HBF model, we only need to consider one of them. Thus using HBF, AHE, and lattice mismatch model and adding them up, we obtain the value of $P_0 = 415$ meV·Å for $In_xGa_{1-x}As$/InP QW with $x = 0.57$. Adopting $P_2 = P_0$, we only need to determine the parameter $P_1$ by fittings. By careful calculation, we find that if we adopt $P_1 = 520$ meV·Å, i.e., $\Delta P = P_1 - P_2 = 105$ meV·Å, the DP value can be well fitted by 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, while the DP value obtained by 4-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory is much smaller (about 66% smaller) than that obtained in experiments. This indicates that the SOC effect play an important role in the IPOA of the InGaAs/InP QW.

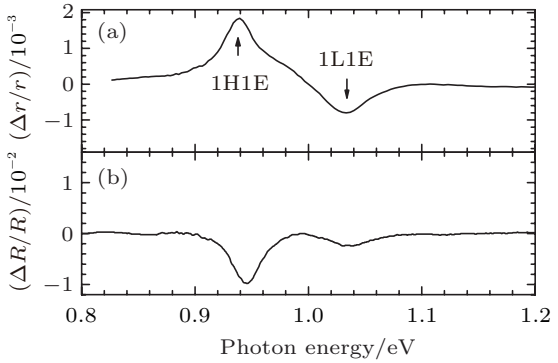



**Fig. 4.** (a) RD spectrum and (b) $\Delta R/R$ spectrum of a $In_{0.57}Ga_{0.43}As$/InP QW with a well width of 2 nm measured at room temperature.

Obtaining the interface potential parameter, we can theoretically investigate the influence of the SOC effect on the IPOA when the QW is under tensile, compressive and zero strain. When the indium (In) concentrations are $x = 0.46$, 0.468, 0.57, the $In_xGa_{1-x}As$/InP QWs are under compressive,

zero strain, and tensile biaxial strain, respectively. The biaxial strain can be calculated by the following equations:

$$\epsilon_{xx} = \epsilon_{yy} = \frac{a_0 - a}{a}, \tag{22}$$

$$\epsilon_{zz} = -\frac{2C_{12}}{C_{11}}\epsilon_{xx}, \tag{23}$$

where $a_0$ and $a$ are the lattice constants of the substrate and the layer material, and $C_{11}$ and $C_{12}$ are the stiffness constants. Then the biaxial strain for InGaAs/InP QWs with the investigated In concentration are

$$\begin{aligned}
\epsilon_{xx} &= \epsilon_{yy} = -5.54 \times 10^{-4}, \epsilon_{zz} = 5.47 \times 10^{-4}, \quad \text{for} x = 0.46, \\
\epsilon_{xx} &= \epsilon_{yy} = \epsilon_{zz} = 0, \quad \text{for} x = 0.468, \\
\epsilon_{xx} &= \epsilon_{yy} = 7.1 \times 10^{-3}, \epsilon_{zz} = -6.9 \times 10^{-3}, \quad \text{for} x = 0.57.
\end{aligned}$$

It is worth noting that, if we only consider the biaxial strain, i.e., $\epsilon_{xx} = \epsilon_{yy} \neq 0$, $\epsilon_{ij} = 0$ $(i \neq j)$, and $P_1 = P_2$, the IPOA for 1H1E and 1L1E are all zero whether the SOC effect is taken into account or not, according to Eqs. (17) and (18). Therefore, the biaxial strain alone is not enough to introduce IPOA of the 1H1E and 1L1E. There must exist some other factors, such as inequivalent upper and lower interface, or shear strain, to bring in IPOA into QWs. Since there exists inherent non-equivalence of interface bonds in the two interface of the "no-common-atom" InGaAs/InP QWs, which can be described by the interface potential (i.e., $P_2 \neq P_1$), we should consider the interface potential together with the biaxial strain. Using HBF, AHE, and lattice mismatch model, we estimate the interface potential $P_0$ are 336, 334, and 415 meV·Å for $x = 0.46$, 0.468, and 0.57, respectively. Then, adopting $P_2 = P_0$, $P_1 = P_2 + \Delta P$ ($\Delta P = 105$ meV·Å), we can theoretically calculate the anisotropic transition probability $\Delta M$ by 4-band (solid lines for 1H1E, "filled squares on line" for 1L1E ) and 6-band (dashed lines for 1L1E, "open squares on line" for 1L1E) $\boldsymbol{k} \cdot \boldsymbol{p}$ theory when the In concentrations are 0.46, 0.468, and 0.57, respectively, in an $In_xGa_{1-x}As$/InP QW with the well width of 2 nm, which are shown in Fig. 5. Here we assume that the value of $\Delta P$ is the same when the In concentrations are $x = 0.46$, 0.468, and 0.57. It can be seen that, in the $In_xGa_{1-x}As$/InP QW, the SOC effect will make the $\Delta M$ value nearly twice as large as that obtained by the model without SOC effect. This can also be attributed to the following two reasons, (i) SOC effect reduces the energy difference between 1HH and 1LH, and (ii) SOC effect introduces additional coupling between 1H (or 1L) with the SO bands, thus enhance the IPOA of the sample. The influence of the first reason can be seen in Fig. 6, which shows the energies of valence subband 1HH and 1LH, and the energy difference between 1HH and 1LH of an $In_xGa_{1-x}As$/InP QW as a function of well width for $x = 0.46$, 0.468, and 0.57, respectively. The dotted and solid lines indicate the results with and without SOC effect, respectively. It can be seen that the HH and LH bands are pushed upward by the SO band due to the quantum-mechanical level repulsion. Besides, the SOC effect also makes the 1HH and 1LH closer to each other especially when the well width is small, which will enhance the IPOA of the sample according to the Eqs. (17) and (18). Figure 7 displays the ratio of $\Delta M_{SO}$ contributed by SOC effect to the total $\Delta M$ as a function of well width obtained by $\boldsymbol{k} \cdot \boldsymbol{p}$ theory. It can be seen that the SOC effect will make the $\Delta M$ enhance about 40% for 1H1E and about 20% for 1L1E when the In concentration is 0.46 or 0.468 at well width of 2 nm. As the increase of well width, the ratio of $\Delta M_{SO}$ to $\Delta M_{total}$ decreases. From Fig. 5, we can see that, there is a sign reversion for the $\Delta M$ of 1H1E and 1L1E at a particular well width when the In concentration is 0.57. This is because at this particular well width (6.4 nm for 4-band, and 4.8 nm for 6-band), there exists an anticrossing of energies for 1HH and 1LH bands, which can be clearly seen in Fig. 6(c). Obviously, the value of $\Delta M$ will be greatly enhanced when the well width is close to this critical well width, and the SOC effect will reduce this critical well width. From above discussions, we find that SOC effect has significant influences on the IPOA of the InGaAs/InP QWs especially for the transition of 1H1E and for QWs with small well width.

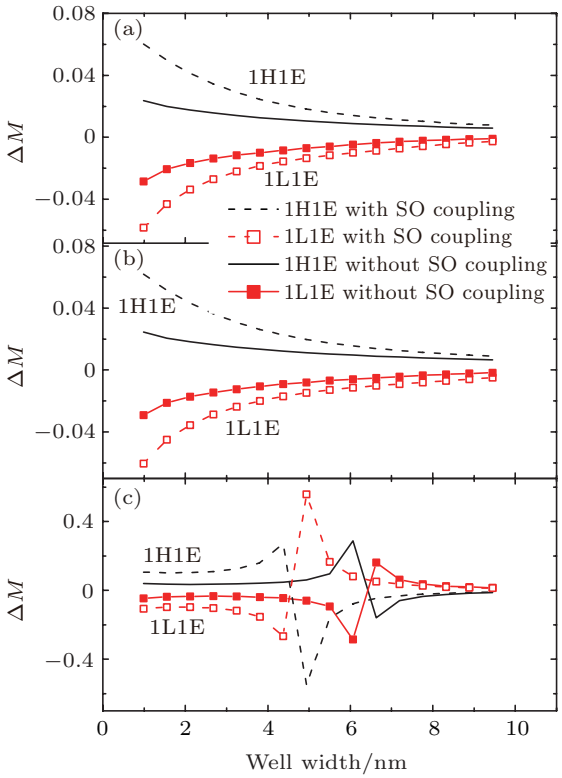



**Fig. 5.** (color online) The anisotropic transition probability $\Delta M$ obtained by 4-band (without SO coupling) and 6-band (with SO coupling) $\boldsymbol{k} \cdot \boldsymbol{p}$ theory when the In concentration is (a) 0.46, (b) 0.468, and (c) 0.57, respectively, in an $In_xGa_{1-x}As$/InP QW with the well width of 2 nm.

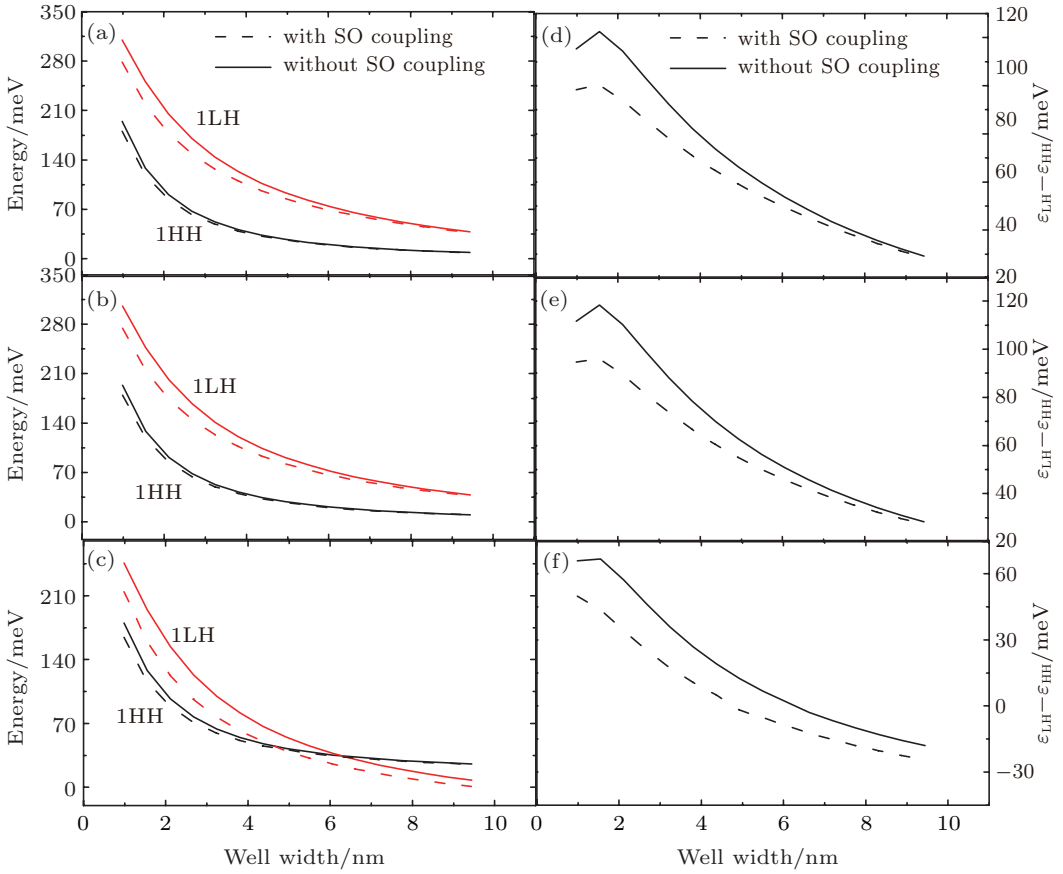



**Fig. 6.** (color online) The energies of valence subband 1HH and 1LH of an $In_xGa_{1-x}As/InP$ QW as a function of well width for (a) $x = 0.46$, (b) 0.468, and (c) 0.57, respectively. The energy difference between 1L and 1H of an $In_xGa_{1-x}As/InP$ QW as a function of well width for (d) $x = 0.46$, (e) 0.468, and (f) 0.57, respectively. The solid and dotted lines are the results obtained by 4-band and 6-band $\boldsymbol{k}\cdot\boldsymbol{p}$ theory, respectively.

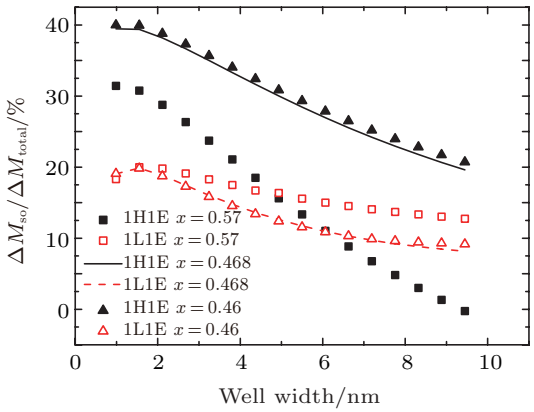



**Fig. 7.** (color online) The ratio of $\Delta M_{SO}$ contributed by SOC effect to the total $\Delta M$ as a function of well width obtained by $\boldsymbol{k}\cdot\boldsymbol{p}$ theory. The squares, lines and triangles indicate the results corresponding to the In concentration of 0.57, 0.468, and 0.46, respectively.

## 4. Conclusions

In conclusion, we theoretically study the influence of the SOC effect on the IPOA induced by in-plane uniaxial strain and interface asymmetry in (001) GaAs/AlGaAs QWs with different well width. It is found that the SOC has significant impact on the IPOA, especially for the transition of 1H1E. This is because (1) the SOC effect reduce the energy difference between 1HH and 1LH, and (2) the SOC effect introduces additional hole mixing effect between 1H (or 1L) and SO bands. The IPOA of (001) InGaAs/InP QWs has been measured by reflectance difference spectroscopy, whose amplitude is about one order larger than that of GaAs/AlGaAs QWs. The anisotropic interface potential parameters of InGaAs/InP QWs are also determined by fitting the theoretical calculated DP to that measured by experiments. We also theoretically investigate the influence of the SOC on the IPOA in the InGaAs/InP QWs when the QWs are under tensile, compressive or zero biaxial strain. Our results demonstrate that the SOC has significant effect on the IPOA especially for semiconductor QWs with small well width, and therefore cannot be ignored.

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