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Citation: Journal of Applied Physics 108, 083718 (2010); doi: 10.1063/1.3484042
View online: http://dx.doi.org/10.1063/1.3484042
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/108/8?ver=pdfcov
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Nonmagnetic semiconductor spin transistor
Spin-degenerate surface and the resonant spin lifetime transistor in wurtzite structures

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(Received 15 June 2010; accepted 28 July 2010; published online 27 October 2010)

Spin-splitting energies of wurtzite AlN and InN are calculated using the linear combination of atomic orbital method, and the data are analyzed utilizing the two-band k·p model. It is found that in the k·p scheme, a spin-degenerate surface exists in the wurtzite Brillouin zone. Consequently, the D’yakonov-Perel’ spin relaxation mechanism can be effectively suppressed for all spin components in the [001]-grown wurtzite quantum wells (QWs) at a resonant condition through application of appropriate strain or a suitable gate bias. Therefore, wurtzite QWs (e.g., InGaN/AlGaN and GaN/AlGaN) are potential structures for spintronic devices such as the resonant spin lifetime transistor.

parameters used for wurtzite InN, due to lack of established results, are obtained by directly fitting the first-principle calculation data. The nearest-neighbor LCAO parameters for both wurtzite AlN and InN in this study are listed in Table I. The spin-splitting energy of the lowest conduction band can be obtained after the eigenvalues of the above Hamiltonian are solved.

The spin-orbital component of the two-band $k \cdot p$ Hamiltonian for the wurtzite structure from our analytical derivation can be written as

$$H_{SO}(\vec{k}) = [\alpha_R - \gamma_{\nu z}(k_z^2 - b k_x^2)](\sigma_x k_y - \sigma_y k_x),$$

which is consistent with the derivation from the group theories. Here $\alpha_R$, $\gamma_{\nu z}$, and $b$ are evaluated by fitting the spin-splitting energy and the minimum-spin-splitting (MSS) surface data from LCAO results. The parameters obtained through these processes for AlN and InN are listed in Table II.

Figure 1 shows the calculated results of spin-splitting energy along $\Gamma M$ on several $k_z$-planes from both the LCAO method and the two-band model. As can be seen, the results from the two-band model are highly in agreement with those from the LCAO method. This indicates the spin-splitting energy and the MSS surface in wurtzite structure can be well described by the two-band $k \cdot p$ Hamiltonian. Most importantly, in the $k \cdot p$ scheme, the spin-degenerate surface does exist in the wurtzite Brillouin zone. Figure 2 shows that the spin-degenerate surface evaluated by two-band $k \cdot p$ model is highly in agreement with the MSS surface calculated by the LCAO method. The insets of Fig. 2 schematically depict that the spin-degenerate surface for the real wurtzite AlN (InN) has the shape of a hyperboloid of two sheets (a hyperboloid of one sheet). The two-sheet hyperboloidal spin-degenerate surface of AlN has been confirmed by our first-principle calculation. As for InN, the characteristics of its spin-degenerate surface are currently under investigation, and will be reported in the near future.

The working principle of the RSL transistor is related to the DP relaxation mechanism. When spin splitting vanishes, the scattering process due to this mechanism is suppressed and the spin lifetime increases dramatically. Consequently, the spin direction of the charge current can be maintained when electrons pass through the channel, and therefore resistance is reduced in the transistor. As a result, it is important to study the relation between the spin-degenerate surface and the spin lifetime. In the two-band $k \cdot p$ model, the inversion-asymmetry term of the two-dimensional Hamiltonian for [001]-grown wurtzite QWs can be written as $H_{IA}(k) = [\alpha_R - \gamma_{\nu z}(k_z^2 - b k_x^2)](\sigma_x k_y - \sigma_y k_x)$, and the effective spin-splitting

![Image](image_url)

**TABLE I.** Nearest-neighbor tight binding parameters (in eV) for wurtzite AlN and InN. When crystal field is included, the nearest-neighbor couplings in the bond along the [001] direction (in parentheses) are different from those in other bonds (see Ref. 14). The values of lattice constants ($c,a$) and the internal parameter ($\gamma$) were given in Ref. 15. For the ideal wurtzite, $V_{\langle x,y,0 \rangle} = \frac{3}{4} E_{pp}$, $V_{\langle u,vc \rangle} = \frac{3}{4} E_{pp}$, $V_{\langle pa,sc \rangle} = \frac{3}{4} E_{pp}$, $V_{\langle x,y \rangle} = \frac{3}{4} (E_{pp} + 2E_{pp})$.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>AlN</th>
<th>InN</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{so}$</td>
<td>$-12.104$</td>
<td>$-11.900$</td>
</tr>
<tr>
<td>$E_{po}$</td>
<td>$3.581$</td>
<td>$5.000$</td>
</tr>
<tr>
<td>$E_{pc}$</td>
<td>$-0.096$</td>
<td>$-2.600$</td>
</tr>
<tr>
<td>$E_{pe}$</td>
<td>$9.419$</td>
<td>$8.000$</td>
</tr>
<tr>
<td>$E_{pp}(E_{pp})$</td>
<td>$-2.694$ ($-2.730$)</td>
<td>$-1.685$ ($-1.619$)</td>
</tr>
<tr>
<td>$E_{pp}(E_{pp})$</td>
<td>$3.466$ (4.001)</td>
<td>$1.764$ (1.695)</td>
</tr>
<tr>
<td>$E_{pp}(E_{pp})$</td>
<td>$4.178$ (4.823)</td>
<td>$2.789$ (2.680)</td>
</tr>
<tr>
<td>$E_{pp}(E_{pp})$</td>
<td>$5.823$ (5.683)</td>
<td>$3.077$ (2.956)</td>
</tr>
<tr>
<td>$E_{pp}(E_{pp})$</td>
<td>$-0.685$ ($-0.668$)</td>
<td>$-0.769$ ($-0.739$)</td>
</tr>
</tbody>
</table>

**FIG. 1.** (Color online) Spin-splitting energy for wurtzite AlN calculated by the LCAO method and fitting by the two-band $k \cdot p$ model on different planes (a) $k_z=0.25 \pi /c$, (b) $k_z=0.30 \pi /c$, and (c) $k_z=0.35 \pi /c$.

**FIG. 2.** (Color online) Projections of the MSS surface (solid curve) and the reference spin-degenerate surface (dashed curve) onto the plane of $k_z=0$ for (a) AlN and (b) InN. The equations of the reference spin-degenerate surface for AlN (InN) is $k_z^2=3.767 k_x^2-0.275 k_x^2+4.885 k_y^2+0.121$. The insets depict the projections of the three-dimensional MSS surfaces onto the $k_x-k_z$ plane.
energy becomes \( \delta E(k) = 2(\alpha_I k_y - \gamma_{w} k_y^2) \), where \( \alpha_R + \gamma_w b(k_0^2) \) and \( \alpha_R \) is the coefficient of the Rashba linear- \( k \) term. Clearly, a spin-degenerate Fermi surface denoted by \( \alpha_R + \gamma_w b(k_0^2) = 0 \) can be achieved in the two-dimensional electron gases (2DEGs) of wurtzite heterostructures, by varying gate voltage, crystal field, or biaxial strain (corresponding to \( \alpha_R \)). QW width (corresponding to \( b(k_0^2) \)), or carrier concentration (corresponding to \( k_F \)).\(^{17\sim19} \) At relatively small carrier concentration, the cubic- \( k \) term \( H_{IA,3}(k) = -\gamma_w k_y^2(\sigma_x k_y - \sigma_y k_x) \) can be neglected, and therefore the inversion-asymmetry term of the two-dimensional Hamiltonian for [001]-grown wurtzite QWs can be approximated by the linear- \( k \) term \( H_{IA}(k) = H_{IA,1}(k) = \alpha_I(\sigma_x k_y - \sigma_y k_x) \). Since the linear- \( k \) term \( H_{IA,1}(k) \) of the wurtzite [001] structures is identical to that of the zinc-blende [111] structures (see Eq. 5 of Ref. 4), the spin relaxation time given in Eq. 6 of Ref. 4 also holds here

\[
\tau_x = \tau_\parallel = \frac{\hbar^2}{2\tilde{\tau}_1 R_{IA}} \frac{1}{\alpha_x \alpha_y},
\]

where the tilde indicates a magnitude evaluated at a given energy and \( \tilde{\tau}_1 \) is the effective time for field reversal due to the harmonic \( \ell = 1 \) of the scattering cross section, and in general \( \tau_\parallel(E) = \theta(\phi, E)(1 - \cos l \phi) d\phi \).\(^{4} \) However, when the cubic- \( k \) term is also taken into account, the spin lifetimes obtained here will be different from those in Eq. 10 of Ref. 4, due to \( H_{IA,1}(k) \) in [001] wurtzite is different from that in [111] zinc-blende (see Eq. 9 in Ref. 4). The spin lifetimes obtained here are

\[
\tau_x = \tau_\parallel = \frac{\hbar^2}{2\tilde{\tau}_1 k_0^2 (\alpha_x - \gamma_{w} k_y^2)^2}, \tag{4}
\]

As pointed out in Ref. 4, including the \( k_0^6 \) term in the denominator of Eq. (4) is not correct in general. However, the \( k_0^6 \) term is still kept here, since it is correct in the special case when \( \alpha_x = 0 \).

The spin lifetimes \( \tau = \tilde{\tau}(\kappa) \) (i.e., \( x, y, z \)) calculated by Eq. (4) for InN are plotted as functions of \( -\alpha_R/\alpha_x \) \( (\alpha_x = \gamma_{w} b(k_0^2) - \gamma_{wc} k_y^2) \) in Fig. 3, with \( k_0 = k_F = 0.01 \) Å\(^{-1} \), \( \tilde{\tau}_1 = 1 \) ps, \( \gamma_{wc} = -353.576 \) meV Å\(^3 \), \( b = 4.885 \), and \( \langle k_y^2 \rangle = 0.0439 \) Å\(^{-2} \). It is seen that all three spin lifetime components show a resonant behavior when the Fermi surface is spin-degenerate (i.e., \( \alpha_R = -\alpha_x \)). Such results demonstrate that the DP spin relaxation mechanism can be effectively suppressed for all three spin lifetime components in [001]-grown wurtzite QWs at the resonant condition through appropriate device design or application of a suitable gate bias. The spin lifetime \( \bar{\tau}_z(=\bar{\tau}_x) \) for [111]-grown zinc-blende QWs with the cubic- \( k \) term \( H_{IA,3}(k) \) included in the Hamiltonian can be expressed in the following form:

\[
\bar{\tau}_z = \bar{\tau}_x = \frac{\hbar^2}{2\tilde{\tau}_1 k_0^2 \alpha_{IA}} \frac{1}{\alpha_{IA} - \gamma_{wc} k_y^2} \left( \frac{\tilde{\tau}_1}{\gamma_{wc} k_y^2} + \left( \sqrt{\frac{\tilde{\tau}_1}{\gamma_{wc} k_y^2}} \right)^2 \right), \tag{5}
\]

where \( \gamma_{wc} = \gamma/(2\sqrt{3}) \) and \( \gamma \) is the coefficient of the cubic- \( k \) term in the BIA Hamiltonian for zinc-blende in Ref. 4. Apparently, \( \bar{\tau}_z(=\bar{\tau}_x) \) of [111]-grown zinc-blende QWs always exhibits a finite value as long as \( k_0 \) and \( \alpha_{IA} \) are not equal to zero at the same time. By contrast, the spin lifetime of [001]-grown wurtzite QWs diverges when \( \alpha_{IA} = -\gamma_{wc} k_y^2 \), according to Eq. (4). This difference suggests that, from the perspective of achieving the resonant condition with less constraint, the [001]-grown wurtzite QW is a more suitable structure for fabricating the RSL transistor.

Figure 4 depicts that the shape of the spin-degenerate surface can be manipulated via strain or gate bias. For 2DEGs in InN/InAlN QWs, when the compressive strain is applied along the \( x-y \) plane, the curvature of the spin-degenerate surface can be altered and overlapped with the Fermi surface to achieve the resonant condition. By contrast, the spin direction can be maintained across the channel of the RSL transistor.

Phenomena related to the spin-degenerate surface indeed have been observed experimentally by Lo et al., since they observed a dramatic change on the spin-splitting energy from 0 to 10 meV at the Fermi surface by varying carrier concentrations in the 2DEGs of GaN/AlGaN wurtzite heterostructures.\(^{18\sim20} \) Moreover, the spin-splitting energies at the Fermi surface of wurtzite III-nitride QWs (e.g., InGaN/ AlGaN and InN/AlInN) can also be controlled by gate volt-
These observations imply that wurtzite III-nitride QWs, whose spin splitting at the Fermi surface can be degenerate and very sensitive to gate voltage through appropriate sample design, are potential candidates for the RSL transistor.

In conclusion, spin-splitting data of wurtzite AlN and InN calculated by the LCAO method have been analyzed through the two-band $k \cdot p$ model. It is found a spin-degenerate surface does exist in the wurtzite Brillouin zone in the $k \cdot p$ scheme. As a result, the DP spin relaxation mechanism can be effectively suppressed for all spin lifetime components in $/H_20851$/H_20852/grown wurtzite QWs at resonance, which can be achieved through the application of appropriate strain, gate bias, or optical illumination. Therefore, not only zinc-blende but also wurtzite III-nitride (e.g., InGaN/AlGaN and GaN/AlGaN) QWs are promising structures for spintronic devices such as the RSL transistor.

This project was supported by the National Science Council of Taiwan and Academia Sinica.