Gate-controlled spin splitting in GaN/AlN quantum wells

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The spin splitting of wurtzite GaN was calculated by $32 \times 32$ Hamiltonian with spin-orbital interaction. The band-folding effect generates two conduction bands $\Delta_{C1}$ and $\Delta_{C3}$ in which the $p$-wave probability shows a tremendous change where $k_z$ approaches the anticrossing zone. We found that a large spin splitting in GaN/AlN quantum wells is produced due to $\Delta_{C1}$-$\Delta_{C3}$ coupling, and is effectively controlled by electric field. Based on the mechanism and gate-controllable spin splitting, we proposed a $p$-wave-enhanced quantum well, In$_x$Ga$_{1-x}$/N, for the application of the spin-polarized field effect transistor designed by Datta and Das [Appl. Phys. Lett. 56, 665 (1990)]. © 2006 American Institute of Physics. [DOI: 10.1063/1.2178505]

Gate-controlled spin splitting in two-dimensional electron gas (2DEG) has been investigated in many zinc-blende III-V semiconductor quantum wells.1,2 The spin splitting in zinc-blende III-V compounds is induced by spin-orbital interaction3 as a result of inversion asymmetry; due to either bulk inversion asymmetry of the crystal potential (the $k^3$ term, called Dresselhaus effect),4 or structural inversion asymmetry of the electrostatic confinement potential (the linear-$k$ term, named Rashba effect).5 Ganiev et al.6 demonstrated the Rashba and Dresselhaus effects in zinc-blende InAs quantum well (QW), and showed that carriers confined to such a QW will experience an effective magnetic field that may induce spin precession. The manipulation of carrier spin in semiconductors is one of the interesting issues for spintronics. Dresselhaus and Rashba effects in zinc-blende III-V semiconductors have been successfully described by using an eight-band ($s^2p^6$) $k \cdot p$ model which includes the spin-orbital interaction and the coupling between conduction and valence bands.7 It is indicated that Dresselhaus and Rashba effects are strongly dependent on the spin-orbit split-off energy ($\Delta_{so}$) and the band gap ($E_g$) of material. In wurtzite GaN, the spin splitting due to Rashba effect is small, even though the crystal field energy ($\Delta_c$) is taken into account in the eight-band $k \cdot p$ model.8 This has been confirmed by Litvinov,9 who calculated the Rashba spin splitting of wurtzite GaN to be less than 1 meV. The spin splitting in wurtzite GaN due to Dresselhaus effect includes not only the $k^3$ term but also the linear-$k$ term due to the intrinsic wurtzite structural inversion asymmetry.10,11 However, the wurtzite GaN has a large $E_g$ but small $\Delta_{so}$ and $\Delta_c$.8 Therefore, the spin splitting due to either Dresselhaus or Rashba effects is small in wurtzite GaN. Recently, Tsubaki et al.12 and Lo et al.13 independently observed a large spin-splitting energy (greater than 5 meV) in the 2DEG of wurtzite GaN/AlGaN heterostructures, where the spin splitting is gate-controllable.12 Apparently, these experimental results cannot be explained by using the eight-band $k \cdot p$ model. In this letter, we show that the experimental results of Refs. 12 and 13 are due to a band-folding effect when the crystal symmetry of III-nitrides is changed from a cubic zinc-blende to a hexagonal wurtzite structure.14 Two conduction bands ($\Delta_{C1}$ and $\Delta_{C3}$) are generated as the wave vector along the zinc-blende $\Gamma$-$L$ [111] direction is folded back in the wurtzite $\Gamma$-$A$ [001] direction. A large gate-controllable spin splitting in GaN/AlN QW is achieved by the $\Delta_{C1}$-$\Delta_{C3}$ coupling, instead of the conduction-valence band coupling.

The spin-dependent full band structure is calculated by the linear combination of atomic orbitals (LCAO), based on the method used by Kobayashi et al.15 The Hamiltonian, we used, is a $32 \times 32$ spin-orbital coupling matrix: $H_{32 \times 32}=H_0+H_{SO}$. The non-zero matrix elements are used to solve the Schrodinger equation.1,3,6-15 The full band structure of wurtzite GaN is shown in Fig. 1. Here, $\Delta_{C1}$ and $\Delta_{C3}$ represent the lowest and second lowest conduction bands, respectively. For the two conduction bands, a band crossing occurs along $\Gamma$-$A$ direction,20 due to the fact that $\Gamma$-$A$ direction is the highest symmetrical orientation at $k_z$. This can be a mathematical saddle point. An anticrossing occurs when the symmetry is broken at $k_x$ or $k_y \neq 0$. The calculated density of states indicates that, near $\Gamma$-point, $\Delta_{C1}$ band is an $s$-like state, while $\Delta_{C3}$ band is a highly hybrid $sp^3$-state which has much higher $p$-wave probability than the $\Delta_{C1}$ band. This can be

![FIG. 1. The full band structure of GaN calculated by the LCAO method. The band folding effect generates two conduction bands ($\Delta_{C1}$ and $\Delta_{C3}$), which are crossing at the saddle point.](image-url)

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understood because the \( \Delta_{C^3} \)-point is indeed folded back from the highly hybrid-sp\(^3\) zinc-blende \( L_{C^1} \)-point.\(^{14} \) The full band structure of AlN and its density of states are also calculated, and no crossing occurs between \( \Delta_{C^1} \) and \( \Delta_{C^3} \) bands. The anticrossing between the \( \Delta_{C^1} \) and \( \Delta_{C^3} \) bands in GaN is shown in Fig. 2(a). The spin-splitting energies of \( \Delta_{C^1} \) (the solid lines) and \( \Delta_{C^3} \) bands (the dashed lines), denoted as \( \delta E(\Delta_{C^1}) \) and \( \delta E(\Delta_{C^3}) \), are plotted versus \( k_z \) at \( k_x = 0.12 \pi/c \) and \( k_y = 0.12 \pi/c \). It is noted that \( \Delta \)-band is traditionally assigned to the band along \( \Gamma-A \) direction (\( k_z = k_y = 0 \)) in wurtzite, but here we assign it, more generally, to those bands parallel to the \( \Gamma-A \) direction; i.e., for \( k_z = (k_x^2 + k_y^2)^{1/2} \) within the zone boundary. \( \delta E(\Delta_{C^1}) \) increases with increasing \( k_z \) and an abrupt jump (from 2.3 meV up to 5.7 meV) takes place at \( k_z \approx 0.384 \pi/c \) (marked anticrossing). After the jump, \( \delta E(\Delta_{C^1}) \) decreases with increasing \( k_z \) up to the zone boundary. On the contrary, \( \delta E(\Delta_{C^3}) \) decreases with increasing \( k_z \), followed by an abrupt drop (from 5.7 meV down to 2.3 meV) at \( k_z \approx 0.384 \pi/c \). It then increases with increasing \( k_z \) up to the zone boundary. The switch of \( \delta E(\Delta_{C^1}) \) and \( \delta E(\Delta_{C^3}) \) arises from the anticrossing of the \( \Delta_{C^1} \) and \( \Delta_{C^3} \) bands at \( k_z = 0.384 \pi/c \). Because the spin splitting is mainly due to the spin-orbital interaction of \( p \) wave, the probability of the density of states for the hybrid sp\(^3\)-wave in \( \Delta_{C^1} \) and \( \Delta_{C^3} \) bands is plotted in Fig. 2(b). For the \( \Delta_{C^1} \) (or \( \Delta_{C^3} \)) band, the probability of \( s \) wave is 96.2\% (or 54.6\%) at \( k_z = 0 \) and it decreases (or increases) as \( k_z \) increases. An abrupt drop (or jump) occurs at \( k_z = 0.384 \pi/c \) and then the probability of \( s \) wave in both bands goes to 60.6\% at the zone boundary. Similarly, the probability of a \( p \) wave is 3.8\% (or 45.4\%) for the \( \Delta_{C^1} \) (or \( \Delta_{C^3} \)) band at \( k_z = 0 \) and it increases (or decreases) with increasing \( k_z \). An abrupt jump (or drop) occurs at \( k_z = 0.384 \pi/c \) and then the probability of a \( p \) wave in both bands goes to 39.4\% at the zone boundary. The \( p \)-wave probability of the \( \Delta_{C^1} \) band increases with \( k_z \) before the anticrossing, therefore \( \delta E(\Delta_{C^1}) \) increases with \( k_z \). It shows an abrupt jump at the anticrossing, and then decreases with increasing \( k_z \). \( \delta E(\Delta_{C^1}) \) shows similar behavior. On the contrary, the \( p \)-wave probability of the \( \Delta_{C^3} \) band, and hence \( \delta E(\Delta_{C^3}) \), decreases with increasing \( k_z \) before the anticrossing. It shows an abrupt drop at the anticrossing, and then increases with increasing \( k_z \). \( \delta E(\Delta_{C^3}) \) shows similar behavior. Therefore, the spin-orbital interaction of the \( p \) waves in the \( \Delta_{C^1} \) and \( \Delta_{C^3} \) bands dominates the spin-splitting energies, \( \delta E(\Delta_{C^1}) \) and \( \delta E(\Delta_{C^3}) \).

The Schrödinger equation for the GaN/AlN QW with a long-range electric field is solved by \( H_{32} + \text{H}_{30} + \text{H}_{PE} \), where \( \text{H}_{PE} = \text{V}_{FE}(r) \text{I} \) is an operator for long-range electrical potential induced by either piezoelectric field or an applied external field, and \( \text{I} \) is a \( 32 \times 32 \) unitary matrix.\(^{21} \) The electric fields in the GaN well and AlN barrier are assumed to be linearly dependent on the layer thickness, and are set to be 100 mV/Å between two interfaces of the QWs. The calculation is carried out for the QWs with different well thicknesses (from one to ten layers). The QW ground subbands of \( \Delta_{C^1} \) and \( \Delta_{C^3} \) bands at the Fermi wave vector, \( k^F = (k_x^F, k_y^F) \), are denoted as \( \Delta_{C^1}(k^F) \) and \( \Delta_{C^3}(k^F) \), respectively. The spin-splitting energy of \( \Delta_{C^1}(k^F) \) subband at the Fermi wave vector of \( k^F = 0.12 \pi/c \) is plotted against well-thickness for the cases without electric field (empty circles), and with electric field (solid squares) in Fig. 3. The value \( k^F = (k_x^2 + k_y^2)^{1/2} = 0.12 \pi/c \) is referred to the carrier concentration of 2DEG, \( n_{2D} = 8.73 \times 10^{12} \text{cm}^{-2} \). It is shown that the spin-splitting energy of \( \Delta_{C^1}(k^F) \) increases with decreasing well thickness. This is because the \( p \)-wave probability of \( \Delta_{C^1}(k^F) \) increases as the well thickness decreases (as shown in the inset). The reduction of well thickness shifts up the ground subbands of \( \Delta_{C^1}(k^F) \) and \( \Delta_{C^3}(k^F) \), and hence the quantized wave vector \( k^F \) moves toward the anticrossing zone; e.g., see Fig. 2(a). When \( k^F \) approaches the anticrossing zone, the \( \Gamma_{C^1} \)-like \( \Delta_{C^1}(k^F) \) and \( \Gamma_{C^3} \)-like \( \Delta_{C^3}(k^F) \) will strongly couple with each other, and then turn into two highly mixing states: A \( p \)-wave-enhanced \( \Delta_{C^1}(k^F) \) and a \( p \)-wave-reduced \( \Delta_{C^3}(k^F) \). This coupling explains why the spin-splitting energy of \( \Delta_{C^1}(k^F) \) is capable of reaching a

**FIG. 2.** (a) The spin-splitting energies for \( \Delta_{C^1} \) and \( \Delta_{C^3} \) bands of wurtzite GaN, i.e., \( \delta E(\Delta_{C^1}) \) and \( \delta E(\Delta_{C^3}) \), respectively, are plotted against \( k_z \) for \( k_x = 0.12 \pi/c \) and \( k_y = 0 \). The anticrossing between \( \Delta_{C^1} \) (solid lines) and \( \Delta_{C^3} \) bands (dash lines) is shown. (b) The probabilities of the density of states for \( s \) and \( p \) waves in the two conduction bands.

**FIG. 3.** The spin-splitting energies of \( \Delta_{C^1}(k^F) \) are plotted against well thicknesses from one to ten layers GaN/AlN QWs at \( k^F = 0.12 \pi/c \), for the cases without electric field (open circles) and applied electric field (solid squares). The probabilities of the density of states for \( s \) and \( p \) waves in \( \Delta_{C^1}(k^F) \) and \( \Delta_{C^3}(k^F) \) are shown in the inset.
value as high as 4.4 meV in Fig. 3. On the other hand, if the quantized wave vector $k_z^F$ goes into the anticrossing zone, $\Delta c_1(k^F)$ will become more $p$ like than $\Delta c_3(k^F)$, and then a very large spin-splitting energy in $\Delta c_1(k^F)$ is expected. Thus the large controllable spin splitting of GaN/AlN QWs can be achieved due to the $\Delta c_1$-$\Delta c_3$ coupling.

In the spin-polarized field effect transistor proposed by Datta and Das, the precession of electron spin can be controlled with a gate voltage in the InGaAs/InAlAs 2DEG channel due to the Rashba spin-orbital interaction.\(^2,6\)

If we replace the InGaAs/AlInAs QW with an In\(_x\)Ga\(_{1-x}\)N/In\(_{y}\)Al\(_{1-y}\)N QW for the 2DEG channel, a larger spin splitting can be achieved due to the higher $p$-wave probability. According to the diagram of band gap versus lattice constant (Fig. 4), we can use wurtzite ZnO (lattice constant $a = 3.252 \text{ Å}$) as a substrate to grow an In\(_x\)Ga\(_{1-x}\)N/In\(_{y}\)Al\(_{1-y}\)N lattice-matched QW (e.g., $x = 0.27, y = 0.36$). From the bowing parameters of In\(_x\)Ga\(_{1-x}\)N and In\(_{y}\)Al\(_{1-y}\)N,\(^22\) the band-gap difference in the lattice-matched QW can reach $\Delta E_g = 1.2 \text{ eV}$. The $L_{c1}$ point in a zinc-blende structure is four-fold degenerate, whereas the $\Gamma_{c1}$ point in a wurtzite material is nondegenerate. In the In\(_x\)Ga\(_{1-x}\)N/In\(_{y}\)Al\(_{1-y}\)N QW structure, the band folding effect will lift off the four-fold degeneracy of $L$ point in zinc blende and will remove the complexity induced by the degeneracy. The physical properties of wide band-gap QW with a large band offset are also superior to the narrow band-gap QW for electronic device application. In addition to the large band offset and greater spin splitting, another advantage of the new QW structure is that its strain can be adjusted by alloy composition. Because the spin splitting can be tuned by strain as well, the device performance can be optimized by adjusting the indium composition ($x$) when fabricating the strain-layered QW. Based on the new mechanism for spin splitting analyzed in this letter, we proposed a $p$-wave-enhanced QW structure, In\(_x\)Ga\(_{1-x}\)N/In\(_{y}\)Al\(_{1-y}\)N, to fabricate the spin-polarized field effect transistor.\(^23,24\)

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