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Giant and zero electron g factors of dilute nitride semiconductor nanowires

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The electronic structures and electron g factors of $\text{InSb}_{1-s}\text{N}_s$ and $\text{GaAs}_{1-s}\text{N}_s$ nanowires and bulk material under the magnetic and electric fields are investigated by using the ten-band $k \cdot p$ model. The nitrogen doping has direct and indirect effects on the g factors. A giant g factor with absolute value larger than 900 is found in $\text{InSb}_{1-s}\text{N}_s$ bulk material. A transverse electric field can increase the g factors, which has obviously asymmetric effects on the g factors in different directions. An electric field tunable zero g factor is found in $\text{GaAs}_{1-s}\text{N}_s$ nanowires. © 2007 American Institute of Physics.
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Dilute nitride alloys of III-V semiconductors have progressed rapidly over recent years following the discovery of strong negative band gap bowing effects.¹ There are many investigations on $\text{GaAs}_{1-s}\text{N}_s$ (Ref. 1) and $\text{InSb}_{1-s}\text{N}_s$ (Refs. 2 and 3) alloys. Meanwhile, semiconductor nanowires are synthesized in a large range of materials and radii by several methods,^{4,5} and the method to dope nitrogen in semiconductor nanowires is archived.⁶

Nowadays, the electron g factors of semiconductor nanostructures are widely investigated.⁷⁻⁹ The g factors depend sensitively and asymmetrically on the shape and size of the nanostructures.⁹ The effect of the electric field on the g factors is also studied.¹⁰ It is well known that in dilute magnetic semiconductors (DMSs), one can obtain giant g factors by tuning the temperature and magnetic field.^{11,12} On the other hand, the magnetic field tunable zero g factor was found in DMS quantum dot.¹³ Both the giant and zero g factors are dependent sensitively on temperature, magnetic field, and

magnetic-ion doping. There may be other ways to get giant and zero g factors, which are more stable in the variations of magnetic field or temperature and are more easy to control. The newly found band bowing effect via nitrogen (N) doping may be a candidate.

In this letter, we calculate the electronic structures and electron g factors of dilute nitride InSb and GaAs nanowires and bulk material. We represent the ten-band Hamiltonian in the absence of external fields at the Bloch function bases $|S_N\rangle \uparrow, |S\rangle \uparrow, |11\rangle \uparrow, |10\rangle \uparrow, |1-1\rangle \uparrow, |S_N\rangle \downarrow, |S\rangle \downarrow, |11\rangle \downarrow, |10\rangle \downarrow$, and $|1-1\rangle \downarrow$ as

$$H_{\text{ten}} = \begin{pmatrix} H_{\text{five}} & \\ & H_{\text{five}} \end{pmatrix} + H_{\text{so}}, \quad (1)$$

where $|S_N\rangle$ is the base of the N, and H_{so} is the valence band spin-orbit coupling Hamiltonian and is given before.¹⁴ H_{five} is written as

$$H_{\text{five}} = \begin{pmatrix} E_N & V_{\text{NC}}s^{1/2} & 0 & 0 & 0 \\ V_{\text{NC}}s^{1/2} & E_g & (i/\sqrt{2})p_0k_+ & ip_0k_z & (i/\sqrt{2})p_0k_- \\ 0 & -(i/\sqrt{2})p_0k_- & 0 & 0 & 0 \\ 0 & -ip_0k_z & 0 & 0 & 0 \\ 0 & -(i/\sqrt{2})p_0k_+ & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & H_{k2} \end{pmatrix}, \quad (2)$$

where $E_N=0.65$ eV, $V_{\text{NC}}=3.0$ eV,¹⁵ s is the composition of N, $E_g=0.2352$ eV, and H_{k2} is a 4×4 matrix¹⁴ which includes all the k -quadratic terms. We assume that the wire direction is along the z direction. The wave function for the

Hamiltonian [Eq. (1)] consists of ten components. As an approximation, we treat the lateral interface as an infinitely high potential barrier and expand each component of the wave function of the nanowires as $\Psi_{k_z} = \sum_{l,n} c_{l,n} A_{l,n} J_l(k_n^l r) e^{il\theta} e^{ik_z z}$,¹⁴ where $J_l(k_n^l r)$ is the Bessel function.

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FIG. 1. Electron g factors of $\text{InSb}_{1-x}\text{N}_x$ nanowires as functions of R and s . (a) g_z . (b) g_x .

When the external electric field and magnetic field are applied, the whole Hamiltonian can be written as

$$H = H_{\text{ten}} + H_{\text{asym}} + H_{\text{mm}} + H_{\text{Zeeman}} + V, \quad (3)$$

where H_{asym} , H_{mm} , and H_{Zeeman} are the magnetic-antisymmetric Hamiltonian, the magnetic-momentum Hamiltonian, and the spin-Zeeman-splitting Hamiltonian,¹⁶ respectively, and V is the electric field potential term.

For magnetic field ($\mathbf{B}$) applied along the z direction, we choose the symmetric gauge in which the vector potential is written as $\mathbf{A} = (-\frac{1}{2}B_z y, \frac{1}{2}B_z x, 0)$. When $\mathbf{B} \parallel x$, we choose the Landau gauge, and $\mathbf{A} = (0, 0, B_x y)$, when $\mathbf{B} \parallel y$, $\mathbf{A} = (0, 0, B_y x)$. In the presence of magnetic field, the momentum operator changes into $\mathbf{p} \Rightarrow \mathbf{P}$ ($\mathbf{P} = \mathbf{p} + e\mathbf{A}$), then we can deduce $H_{\text{ten}}|_{\mathbf{p} \Rightarrow \mathbf{P}} = H_{\text{ten}} + H_{\text{asym}} + H_{\text{mm}}$.¹⁶ For bulk material, we assume that $\mathbf{B} \parallel z$ and expand the wave function as $\Psi_{k_z} = \sum_n a_n u_n(x, y) e^{ik_z z}$, where $u_n(x, y)$ is the harmonic oscillator wave function and the index n indicates the Landau level. By using the Hamiltonian and wave function given above, we can calculate the electronic structure and the electron g factor $g = \Delta E / \mu_B B$, where ΔE is the spin splitting energy.

Taking into account the dielectric effect, the electric field in the nanowires is

$$\mathbf{F} = \frac{2\epsilon_0}{\epsilon_r + \epsilon_0} \mathbf{F}_{\text{ext}}, \quad (4)$$

where ϵ_r and ϵ_0 are the dielectric constants in and outside the nanowires. We assume that $\mathbf{F} \parallel x$, so $V = eFx = eFr(e^{i\theta} + e^{-i\theta})$.

Figure 1 shows the electron g factors of $\text{InSb}_{1-x}\text{N}_x$ nanowires as functions of R and s . We see that the variations of the g_z and g_x are similar. Actually, g_x is a little smaller than g_z .¹⁶ The g factors decrease as R increases, when $s=0$, the g factors both decrease to the g factor of bulk InSb which can be calculated out by

$$g = 2 - \frac{2E_P \Delta_{\text{so}}}{3E_g(E_g + \Delta_{\text{so}})}; \quad (5)$$

the value is -44.5 which is close to the experimental value of -47.8 .¹⁷ The absolute value of the bulk g factor is moder-

FIG. 2. (a) g_z of $\text{InSb}_{1-x}\text{N}_x$ nanowires as a function of s , $R=5$ nm. (b) Solid line: nanowires with $R=300$ nm. Dashed line: bulk material. (c) N-state proportion of the lowest electron state in $\text{InSb}_{1-x}\text{N}_x$ nanowires as a function of s , $R=5$ nm. (d) Similar to (c) but $R=300$ nm. (e) Band gap of $\text{InSb}_{1-x}\text{N}_x$ nanowires as a function of s , $R=5$ nm. (f) Similar to (e) but $R=300$ nm. (g) Lowest two electron states of $\text{InSb}_{1-x}\text{N}_x$ nanowires with $R=300$ nm and $s=0.016$ as functions of B .

ately large, while we can see from Fig. 1 that the N doping can even decrease the g factors to very large negative values. The decrease of g factors with increasing s is more obvious in larger R case.

For clarity, we show g_z (the case of g_x is similar) extracted from Fig. 1(a) for $R=5$ nm in Fig. 2(a) and for $R=300$ nm as well as bulk material in Fig. 2(b). We can see from Fig. 2(b) that the g factor can decrease to -912 for bulk material and -730 for nanowires with $R=300$ nm, whose absolute values are even larger than the g factor obtained in DMSs.^{11,12} This effect of giant g factor is more remarkable in bulk material than in nanowires. Compared to the giant g factor in DMSs, this giant g factor is more stable in the variation of magnetic field. It depends sensitively on temperature because the band gap is very small and depends on temperature. With this giant g factor, we can obtain huge spin splitting, and the transferring carriers feel smaller than the spin-dependent scattering compared to those in DMSs because there are no magnetic ions in $\text{InSb}_{1-x}\text{N}_x$. The numerically calculated g factor of bulk InSb is -44.5 [see Fig. 2(b)], which is in agreement with the formula calculation [see Eq. (5)]. It is interesting to see from Figs. 2(a) and 2(b) that the variation rules of the $R=5$ nm and $R=300$ nm cases are quite different. When $R=5$ nm, as s increases, the g factor increases firstly, then decreases. While in the $R=300$ nm case, the g factor always decreases. We can explain these by the two effects of N doping on the g factor, the direct and indirect effects. The direct effect is that as s increases, the N state which has a g factor of 2 mixes into the lowest electron state, as shown in Figs. 2(c) and 2(d), so the g factor increases towards 2. The indirect effect is that, as the band gap decreases with increasing s due to the band bowing [see Figs. 2(e) and 2(f)], the conduction band feels more coupling from the valence band, which contributes a larger negative part to the electron g factor [see Eq. (5)], so the g factor decreases. In the $R=5$ nm case, when s is small, the

FIG. 3. (a) g_z of GaAs nanowires as a function of R . (b) g_z of $\text{GaAs}_{1-s}\text{N}_s$ nanowires with $R=6.5$ nm as a function of s .

N -state proportion increases rapidly with increasing s , and the relative decrease of band gap is small, so the direct effect dominates. When s is large, the N -state proportion saturates, while the band gap still decreases, so the indirect effect dominates. In the $R=300$ nm case, the band gap at $s=0$ is small and the relative decrease of band gap is large, so the indirect effect always dominates. From Fig. 2(g) we see that the lowest two electron states consist of mainly the conduction ground states, so the definition of the g factor is valid.

From Fig. 3(a) we see that the g factor decreases with increasing R and is zero at $R=6.18$ nm. So the g factor can be tuned to be zero by the size of the nanostructures, which has been discussed before.^{14,16} The case in Fig. 3(b) is similar to the case in Fig. 2(a), as s increases, the g factor increases firstly, then decreases. We also see that the g factor is tuned to zero two times by N doping. Compared to the $\text{InSb}_{1-s}\text{N}_s$ nanowires, the energy gaps of $\text{GaAs}_{1-s}\text{N}_s$ nanowires are larger, so there is no effect of giant g factor. Thus, it is expected that the giant g factor will be existed in thick nanowires or bulk material of narrow energy gap semiconductors doped with N .

Figure 4 shows that the external transverse electric field can increase the g factors towards 2. The quantum confinement effect can quench the orbital momentum,⁸ thus increase the g factor towards 2 as R decreases [see Eq. (5)]. The electric field can also act as a confinement on the electron

FIG. 4. (a) Electron g factors of InSb nanowires with $R=10$ nm as functions of F . (b) Case of GaAs nanowires with $R=6.5$ nm.

movement, so increase the g factor.¹⁰ It is interesting to see from Fig. 4 that the electric field has obviously asymmetric effects on the g factors in different directions. The g_y is affected much more than the g_z and g_x . As $\mathbf{B} \parallel y$, the electron moves in the xz plane which moves very freely in the z direction as there is no confinement, and the electric field confines the electron in the x direction, so affects the g factor a lot. In the GaAs case [Fig. 4(b)], g_y can be tuned to zero by the electric field $F=8.3$ mV/nm. If the g factor is zero, the spin degenerate states do not split, so the electron spin is unpolarized under magnetic field. With a fixed magnetic field, we can use the electric field to tune the electron spin to be polarized, unpolarized, or antipolarized.

In summary, we studied the electronic structures and electron g factors of dilute nitride InSb and GaAs nanowires and bulk material under the magnetic and electric fields. It is found that $\text{InSb}_{1-s}\text{N}_s$ bulk material may have a giant negative g factor with absolute value larger than 900. There are two effects of the N doping on the g factor, the direct effect increases the g factor and the indirect effect decreases it. A transverse electric field can increase the g factors towards 2, which has obviously asymmetric effects on the g factors in different directions. In $\text{GaAs}_{1-s}\text{N}_s$ nanowires, a proper electric field can tune the g factor to zero.

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