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Electric field tunable electron g factor and high asymmetrical Stark effect in $\text{InAs}_{1-x}\text{N}_x$ quantum dots

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The electronic structure, electron g factor, and Stark effect of $\text{InAs}_{1-x}\text{N}_x$ quantum dots are studied by using the ten-band $k \cdot p$ model. It is found that the g factor can be tuned to be zero by the shape and size of quantum dots, nitrogen (N) doping, and the electric field. The N doping has two effects on the g factor: the direct effect increases the g factor and the indirect effect decreases it. The Stark effect in quantum ellipsoids is high asymmetrical and the asymmetry factor may be 319. © 2007 American Institute of Physics. [DOI: 10.1063/1.2721130]

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 $\text{InAs}_{1-x}\text{N}_x$ alloys.² Meanwhile, dilute nitride semiconductor quantum dots are synthesized in a large range of materials and radius by several methods,³ and the method to dope nitrogen in semiconductor quantum dots is archived.⁴

Nowadays, the electron g factors of semiconductor nanostructures are widely investigated.^{5,6} The g factors depend sensitively and asymmetrically on the dimensions of the nanostructures.⁶ The effect of the electric field on the g factors is also studied.⁷ The magnetic field tunable zero g factor was found in dilute magnetic semiconductor quantum dots,⁸ which is dependent sensitively on the temperature and magnetic field. Meanwhile, the Stark effect of semiconductor quantum dots was studied experimentally⁹ and theoretically.^{10–12} The electric field induced semiconductor-metal transition was found in semiconductor nanowires.¹³ We expect that N doping will affect the electron g factor of $\text{InAs}_{1-x}\text{N}_x$ quantum dots a lot, which has not been discussed before, and the semiconductor-metal transition will also happen in these quantum dots. The Stark effect in quantum ellipsoids is obviously asymmetrical as one axis is e times larger than the other axes, while the asymmetry factor may be quite larger than e .

In this letter, we calculate the electronic structure, electron g factor and Stark effect of $\text{InAs}_{1-x}\text{N}_x$ quantum dots using the ten-band $k \cdot p$ model. We represent the ten-band Hamiltonian without external fields in 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, H_{so} is the valence band spin-orbit coupling Hamiltonian given before,¹⁴ and H_{five} is written as

$$H_{\text{five}} = \frac{1}{2m_0} \begin{pmatrix} 2m_0E_N & 2m_0V_{\text{NC}}x^{1/2} & 0 & 0 & 0 \\ 2m_0V_{\text{NC}}x^{1/2} & 2m_0E_g + P_e & -ip_0P_1^{(1)} & ip_0P_0^{(1)} & ip_0P_{-1}^{(1)} \\ 0 & -ip_0P_{-1}^{(1)} & -P_1 & -S & -T \\ 0 & -ip_0P_0^{(1)} & -S^* & -P_3 & -S \\ 0 & ip_0P_1^{(1)} & -T^* & -S^* & -P_1 \end{pmatrix}, \quad (2)$$

where E_g is the band gap of the bulk material, $p_0 = \sqrt{2m_0E_p}$, E_p is the matrix element of Kane's theory, $E_N = 1.44$ eV is the nitrogen band (NB) energy relative to the valence band maximum, $V_{\text{NC}} = 2.0$ eV is the coupling strength between conduction band and NB,¹⁵ and x is the composition of the N. The other part of the Hamiltonian Eq. (2) and the parameters of InAs are given in Ref. 6 and Ref. 16.

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

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

where V is the electric field potential term, H_{asym} , H_{Zeeman} , and H_{mm} are the magnetic-antisymmetric Hamiltonian, the spin-Zeeman-splitting Hamiltonian, and the magnetic-momentum Hamiltonian induced by the magnetic field, respectively.⁶

For simplicity, we assume that the electric field is in the xz plane. In the case of quantum ellipsoids, taking into account the dielectric effect, the electric field in the ellipsoids is $\mathbf{F}' = (F'_x, 0, F'_z)$, where

$$F'_z = \frac{\epsilon_0}{n_z\epsilon_r + (1 - n_z)\epsilon_0} F_z, \quad (4)$$

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FIG. 1. (a) Electron g factors of $\text{InAs}_{1-x}\text{N}_x$ quantum spheres at $F=0$ as functions of R . (b) $R=3$ nm as a function of x . (c) $R=15$ nm and $R=30$ nm as functions of x .

$$F'_x = \frac{\epsilon_0}{n_x \epsilon_r + (1 - n_x) \epsilon_0} F_x, \quad (5)$$

where ϵ_r and ϵ_0 are the dielectric constants in and outside the ellipsoids, respectively, and in the air environment, $\epsilon_0=1$. For quantum spheres $n_z=n_x=1/3$, while for quantum ellipsoids, they equal

$$n_z = \frac{1 - e'^2}{2e'^2} \left(\ln \frac{1 + e'}{1 - e'} - 2e' \right), \quad (6)$$

$$e' = \sqrt{1 - \frac{1}{e^2}}, \quad (7)$$

$$n_x = \frac{1 - n_z}{2}, \quad (8)$$

where e is the aspect ratio of the length to diameter. We make a coordinate transformation to transform the ellipsoidal boundary to the spherical boundary and obtain the electric field potential V in the newly defined coordinate.¹²

We assume that the electrons and holes are confined in an infinitely high potential barrier. The envelope function including the nitrogen, electron, and hole states is ten components, expanded with the spherical Bessel functions and spherical harmonic functions, similar to that in Ref. 6.

Then we calculate the electronic structure of $\text{InAs}_{1-x}\text{N}_x$ quantum dots in the magnetic field. The electron g factor is calculated as $g = \Delta E / \mu_B B$, where B is the magnetic field strength and ΔE is the splitting energy of the electron ground state. The electron g factors of $\text{InAs}_{1-x}\text{N}_x$ quantum spheres in the absence of electric field ($F=0$) as functions of the radius (R) are shown in Fig. 1(a). We see that the g factors decrease as R increases, when $x=0$, the g factor decreases to the g factor of bulk InAs whose experimental value is -14.4 .¹⁷ It is interesting to notice that the g factor changes from positive values to negative values as R changes, i.e., it can be tuned to be zero by R . We show the g factor of the $R=3$ nm spheres as a function of x in Fig. 1(b). We see that when $R=3$ nm, as x increases, the g factor increases firstly, then decreases. While in the large radius case [see Fig. 1(c)], the g factor always decreases with increasing x . We can explain these by the two effects of nitrogen doping on the g factors: the direct effect and the indirect effect. The direct effect is that as x

FIG. 2. Electron g factors of $\text{InAs}_{1-x}\text{N}_x$ quantum ellipsoids with $R=3$ nm, and $x=0$ at $F=0$ as a function of e . (b) Electron g factors of $\text{InAs}_{1-x}\text{N}_x$ quantum ellipsoids with $R=3$ nm, $e=3$, and $x=0$ as functions of F .

increases, the N state mixes into the lowest electron state, i.e., the N-state proportion increases. Because the N state has a g factor of 2, the g factor increases towards 2. The indirect effect is that, as the band gap decreases with increasing x due to the band bowing, the conduction band feels more coupling from the valence band, which contributes a larger negative part to the electron g factor, so the g factor decreases. In the $R=3$ nm case, when x is small, the N-state proportion increases with increasing x , and the relative decrease of the band gap is small, so the direct effect dominates, and the g factor increases as x increases. When x is large, the N-state proportion saturates, while the band gap still decreases, so the indirect effect dominates, and the g factor decreases with increasing x . In the $R=30$ nm case, as the band gap at $x=0$ is small and the relative decrease of band gap is large, the indirect effect always dominates.

Figure 2(a) shows the g factors of $\text{InAs}_{1-x}\text{N}_x$ quantum ellipsoids with $R=3$ nm and $x=0$ at $F=0$ as functions of e . We see that the g factor decreases as e increases and can be tuned to be zero by $e=1.96$. We show the electron g factors of $\text{InAs}_{1-x}\text{N}_x$ quantum ellipsoids with $R=3$ nm, $e=3$, and $x=0$ as functions of F in Fig. 2(b). It is interesting to see that when $F \parallel x$, the g factor is almost not affected, while it is increased a lot by the electric field when $F \parallel z$. The g factor can be tuned from negative to zero by the electric field $F=12.3$ mV/nm and to positive under larger electric field. This electric field tunable g factor is independent of the temperature and magnetic field, which is different from the magnetic field tunable g factor.⁸ If the g factor is 0, the spin degenerate states do not split, so the electron spin is not polarized under magnetic field. Therefore, under a fixed magnetic field we can use the electric field or control the shape and size of quantum dots to tune the electron spin to be polarized, unpolarized, or antipolarized.

We show the electron and hole Stark shifts of $\text{InAs}_{1-x}\text{N}_x$ quantum ellipsoids with $R=3$ nm, $e=3$, and $x=0$ as functions of F in Figs. 3(a) and 3(b), respectively. We see that when $F \parallel x$, the Stark shifts are nearly zero even if F is very large, while in the $F \parallel z$ case, the Stark shifts is as large as tens of meV when F is large. This high asymmetrical Stark effect is due to the dielectric effect and the quantum confinement effect. Due to the dielectric effect, the electric field in

FIG. 3. Stark shifts of $\text{InAs}_{1-x}\text{N}_x$ quantum ellipsoids with $R=3$ nm, $e=3$, and $x=0$ as functions of F . (a) Electron and (b) hole.

the quantum dots is smaller than the external electric field. When $e=3$, $n_z=0.102$, and $n_x=0.449$, the inner field when $F||x$ is about three times smaller than that when $F||z$ [see Eqs. (4) and (5)]. As the quantum confinements of the quantum ellipsoid along the x axis are larger than those along the z axis, the Stark shift in the x axis is smaller than that in the z axis. Taking into account the dielectric effect and the quantum confinement effect simultaneously, when $F=20$ mV/nm, the asymmetry factor of electron Stark shift is 319 in Fig. 3(a), which is larger than the asymmetry factor of hole Stark shift of 40 in Fig. 3(b), because the electron has smaller effective mass. With this high asymmetrical Stark effect of the quantum ellipsoids with different orientations in the electric field can emit light with quite different wave lengths.

The energy levels as functions of F for $F||x$ and $F||z$ are shown in Figs. 4(a) and 4(b), respectively, where the high asymmetrical Stark effect is more obviously seen. It is interesting to see that an electric field along the z axis with strength larger than 11 mV/nm can make the conduction band and valence band overlapping, and the energy gap tuned to be zero, similar to the wire case.¹³ Figure 4(c) shows the energy levels at $F=15$ mV/nm as functions of the orientation of the ellipsoid in the electric field. Thus the wavelength of light emitted from the quantum ellipsoid can change in a large range periodically when it rotates in a strong electric field.

In summary, we studied the electronic structure, electron g factor, and Stark effect of $\text{InAs}_{1-x}\text{N}_x$ quantum dots under the magnetic and electric fields by using the ten-band $k \cdot p$ model. It is found that the g factor can be tuned to be zero by the shape and size of quantum dots, N doping, and the electric field. Especially, under a fixed magnetic field, we can use the electric field to tune the electron spin in a quantum dot to be polarized, unpolarized, or antipolarized. The N doping has two effects on the g factor: the direct effect increases the g factor and the indirect effect decreases it. The Stark effect in quantum ellipsoids is highly asymmetrical, and the asymmetry factor (for example, 319 with only $e=3$) is quite larger than the aspect ratio e of the ellipsoid due to the dielectric effect and the quantum confinement effect. The energy gap can be even tuned to zero for quantum ellipsoids with large aspect ratio and strong electric field.

FIG. 4. (a) Energy levels of $\text{InAs}_{1-x}\text{N}_x$ quantum ellipsoids with $R=8$ nm, $e=4$, and $x=0.05$ at $B=0$ as functions of F ($F||x$ axis). (b) ($F||z$ axis). (c) $F=15$ mV/nm as functions of the angle between the z axis and the electric field θ .

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