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$Ga_{1-x}In_xAs_ySb_{1-y}$/GaSb spherical quantum dot in a magnetic field

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Quaternary semiconductor alloys type-I are appropriated materials for heterostructure devices because they provide a natural form to tune the magnitude of the band gap so that it can operate in the mid-infrared (mid-IR) wavelength range. However electron spin degree of freedom and the electron spin splitting g-factor provide a new pathway to the development of a practical quantum communication systems, because the effective g-factor for electrons in III-V semiconductors vary as a function of the chemical concentration. We investigated theoretically electron g-factor in bulk $Ga_{1-x}In_xAs_ySb_{1-y}$ matched to GaSb and the Zeeman effect as well as the Landau levels in GaSb/$Ga_{1-x}In_xAs_ySb_{1-y}$/GaSb spherical quantum dot heterostructure under the framework of Kane eight-band effective-mass model, in which the mixing of the states in the lower conduction band and the highest valence bands is taken into account. Our calculations show that bulk electron g-factor values are in the range between the electron g-factor measured in bulk GaSb when $x \to 0$ (g =-9.25) and that measured in InAs when $x \to 1$ (g =-18.08), but there is a notable minimum in the g-factor value ($g \approx -23.14$) at $x \approx 0:67$. In GaSb/$Ga_{1-x}In_xAs_ySb_{1-y}$/GaSb spherical quantum dot our calculations show that the electron g-factor decreases as the radius increases reaching the value for the quaternary in bulk for a given In concentration, x, and increases when the radius decreases, approaching to the value in the barrier material, when $R \to 0$. Also for higher values of concentration of In, the g-factor as a function of R moves to the g-factor bulk limit.

Keywords: g-factor; heterostructures; Zeeman effect; Landau levels.

Las aleaciones cuaternarias tipo-I son materiales apropiados para dispositivos de heteroestructura, porque proveen una forma natural de ajustar la magnitud de la brecha de energía de modo que pueden operar en longitudes de onda en el rango del infrarrojo-medio (IR-m). Sin embargo, los grados de libertad del spin y el desdoblamiento de los estados electrónicos de spin a causa del factor g, permiten nuevas rutas para desarrollar sistemas prácticos de comunicación cuántica, lo anterior se debe a que el factor electrónico efectivo $g$en semiconductores III-V varía en función de la concentración química. Nosotros investigamos teóricamente el factor electrónico g en $Ga_{1-x}In_xAs_ySb_{1-y}$ sobre GaSb para el material en bloque, el efecto Zeeman y niveles de Landau en puntos cuánticos esféricos de GaSb/$Ga_{1-x}In_xAs_ySb_{1-y}$/GaSb bajo el modelo de ocho bandas con masa efectiva de Kane, en el cual la interacción de estados entre el fondo de la banda de conducción y el tope de la banda de valencia es considerado. Nuestros cálculos muestran que los valores del factor electrónico $g$para el material en bloque se encuentran en el rango entre el factor g medido en bloque de GaSb, cuando $x \to 0$ ($g = -9.25$) y el valor medido en bloque de InAs cuando $x \to 1$ (g =-18.08) con un notable mínimo del valor ($g \approx -23.14$) en $x \approx 0.67$. En el punto cuántico esférico GaSb/$Ga_{1-x}In_xAsySb_{1-y}$/GaSb, nuestros cálculos muestran que el factor electrónico $g$disminuye a medida que el radio aumenta, alcanzando el valor límite para el cuaternario en bloque, correspondiente a una concentración dada de In, x, y aumenta cuando el radio disminuye aproximándose al valor en el material de la barrera cuando $R \to 0$. Además para valores altos de concentración de In el factor g como función del radio se desplaza hacia el valor del factor g del bloque límite.

Descriptores: Factor g; hetereoestructuras; efecto Zeeman; niveles de Landau.

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1. Introduction

GaSb/$Ga_{x-1}In_xAs_ySb_{1-y}$/GaSb quaternary heterostructures have interesting characteristics over ternary alloys in regards to the possibility of tuning independently the energy band gap and lattice constant by adjusting the indium (In) concentration $0 \leq x \leq 1$ within the constraints of GaSb substrate, which covers the wavelength range from $1.7\mu m$ to 4.3 μm. There-fore, with the electron spin degree of freedom and the electron spin splitting g-factor in this semiconductors is possible the development of a practical quantum communication systems [1,2]. Type-I heterostructures can be fabricated using strained $Ga_{x-1}In_xAs_ySb_{1-y}$ alloys for the quantum dot and GaSb for the barriers, depending on the alloy concentration [3]. The values of conduction band-offset, band gap energy at a given point, spin-orbit splitting, Kane coupling matrix element value between the states of the lowest conduction band and the upper valence bands and electron g-factor in bulk are calculated by interpolation scheme. Calculations at room temperature of the electron g-factor in GaSb/$Ga_{x-1}In_xAs_ySb_{1-y}$/GaSb spherical quantum dots under eight-band effective-mass model and the energy states including the Zeeman effect on the electrons confined in quaternary heterostructure quantum dots, with a parabolic confining potential in the type-I band alignment as function of the quantum dot radius are performed.

2. Theoretical framework

Bulk material parameters of a quaternary alloy $Q(x, y)$ with composition of the form $Ga_{1-x}In_xAs_ySb_{1-y}$ lattice matched to GaSb can be estimated by interpolating scheme from the binary alloys parameters C_{ij} [4] as

$$Q(x,y)\sum_{i}^{2}\sum_{j}^{2}C_{ij}x^{i-1}y^{2-j}(1-x)^{2-i}(1-y)^{j-1}, \quad (1)$$

with lattice matched condition given by

$$y=\frac{0.384}{0.421+0.216(1-x)} \quad (2)$$

In a external magnetic field the Hamiltonian of a single electron in GaS/$Ga_{1-x}In_xAs_ySb_{1-y}$/GaSb type-I spherical quantum dot (SQD) system within the $\vec{k}\cdot\vec{p}$ eight-band effective-mass model is given by [5]

$$\widehat{H}(\hat{p},\mathbf{H})=\widehat{H}^0(\hat{p})+\mu_B\mathbf{H}(\widehat{D}+\widehat{D}^1), \quad (3)$$

where $\widehat{H}^0(\hat{p})$ describes the electron states in zero magnetic field and $\mu_B\mathbf{H}(\widehat{D}+\widehat{D}^1)$ describes the effects of external magnetic field, and are given by

$$\widehat{H}^0(\hat{p})=\begin{pmatrix} -\frac{1}{2m_0}\widehat{U}_2\hat{p}^2 & i\prod\widehat{U}_2\hat{p} \\ -i\prod\widehat{U}_2\hat{p} & \frac{1}{3}\Delta_{so}(\hat{I}\hat{\sigma})-(E_g+\frac{1}{3}\Delta_{so})\widehat{U}_2 \end{pmatrix}, \quad (4)$$

$$\widehat{D}=\begin{pmatrix} \frac{1}{2}g_0(\hat{\sigma}\hat{n}) & 0 \\ 0 & (\hat{I}\hat{n})\widehat{U}_2+\frac{1}{2}g_0(\hat{\sigma}\hat{n}) \end{pmatrix}, \quad (5)$$

$$\widehat{D}^1=\begin{pmatrix} -\widehat{L}\hat{n} & i\prod\frac{m_0}{\hbar}(\hat{n}\times\vec{r}) \\ -i\prod\frac{m_0}{\hbar}(\hat{n}\times\vec{r}) & 0 \end{pmatrix}\widehat{U}_2, \quad (6)$$

where $\hat{p}=i\hbar\nabla$ is the momentum operator with $\hat{k}=(1/h)(\hat{p}+(e/c)\mathbf{A})$, $A=(1/2)(\mathbf{H}\times\vec{r})$ is the vector potential of the magnetic field, $\widehat{U}_2$ is 2×2 unit matrix, $\hat{\sigma}=(\sigma_x,\sigma_x,\sigma_x)$ are the pauli matrices, $\Pi=-i(1/m_0)\langle S|p_x|X\rangle$ is the Kane matrix element coupling between the s-antibonding conduction and p-bonding valence-band states, $\hat{n}=\mathbf{H}/H$ is the unit vector in the magnetic field direction $\mathbf{H}$, $\widehat{L}=(1/\hbar)(\vec{r}\times\vec{p})$ is the angular momentum operator, $\widehat{I}=(I_x,I_y,I_z)$ is the vector operator and $g_0=+2$, m_0 are the free-electron mass and g-factor respectively. The total zero-order wave function in the $\vec{k}\cdot\vec{p}$ eight-band effective-mass model can be pre sented as the expansion [5,6]

$$\Phi(r)=\sum_j\sum_{v=\pm1/2}[\Psi_v^c(\mathbf{r})+\Psi_v^\nu(\mathbf{r})]\phi_{j,0}C_v, \quad (7)$$

here $\phi_{j,0}$ indicates the Bloch function at Γ point of the zinc blende structure [6], C_v are the eigenfunctions of the spin operator $\hat{S}=(1/2)\hat{\sigma}$, $\Psi_v^c(\mathbf{r})$ and Ψ_v^ν are the components of the envelope function for conduction-band and valence-band respectively. Under external magnetic field the envelope function $\Psi(\mathbf{r})=\{\Psi_v^c(\mathbf{r})+\Psi_v^\nu(\mathbf{r})\}$ is the solution of the Schrödinger equation

$$\widehat{H}\Psi(\mathbf{r})=E\Psi(\mathbf{r}), \quad (8)$$

where E is the energy measured from the bottom of the bulk $Ga_{x-1}In_xAsySb_{1-y}$ conduction band. Using $\widehat{H}^0\Psi(\mathbf{r})=E\Psi(\mathbf{r})$ one can express Ψ_v^ν by means of the gradient $\nabla\Psi_v^c$ as

$$\Psi_v^\nu=\frac{1}{\Pi}\Big\{-\frac{\hbar}{2m_t(E)}\nabla\Psi_v^c + i\frac{\hbar}{4m_o}[g_t(E)-g_0](\hat{\sigma}\times\nabla)\Big\}\Psi_v^c \quad (9)$$

Using Eq. (9) one can be derived the bulk Schrödinger equation describing the radial-component wave function $f(r)=\Psi_v^cC_v$ in a SQD for one spin state as.

$$-\frac{\hbar^2}{2m_t(E)}\nabla f(r)=Ef(r) \quad (10)$$

where electronic mass and electron g-factor energy- dependence, $m_0/m_t(E)$ and $g_t(E)$ are taken as in Ref. 8. Taking into account boundary conditions, the confinement potential $\Delta E_C(x)$ and spherical symmetry considerations in a SQD, the solution of Eq. (10) for the ground state level E has the form

$$f(r)=\begin{cases} \frac{A\sin k_1r}{r} & r\le R \\ \frac{A\sin k_1R}{r}e^{-k_2(r-R)}, & r\ge R, \end{cases} \quad (11)$$

where A is the normalization constant of the radial envelope wave function, R is the radius of the SQD and $i=1;2$ is defined as

$$k_i=\begin{cases} \left(\frac{2m_QE}{\hbar^2}\right)1/2, & i=1,\ r<R \\ \left(\frac{2m_B(\Delta E_C(x)-E)}{\hbar^2}\right)1/2 & i=2,\ r>R \end{cases}, \quad (12)$$

where m_Q denote the electron effective mass in the quaternary alloy and m_B denote the electron effective mass in the binary GaSb semiconductor, $\Delta E_C(x)$=0.6 $(E_{gB}-E_{gQ}(x))$ is the offset of the conduction band at the heterostructure and $E_{gQ}(x)$ is given by Eq. (1), the ground state energies E is determined solving numerically Eq. (9). The g-factor for GaSb/$Ga_{x-1}In_xAs_ySb_{1-y}$/GaSb heterostructure can be calculated from the second therm with **H**-dependence in Eq. (3) treated by first-order perturbation theory [5,9] with envelope radial wave function Eq.(11) and taking into account spherical symmetry and boundary conditions at $r=R$. Thus, in spherical coordinates system we obtain electron the g-factor as a function of both x and R as

$$g(x,R)=g_0+\frac{4}{3}\pi[g_B(E)-g_Q(E)]\frac{R}{\alpha_0}A^2\sin^2k_1R + [g_Q(E)-g_0]I_Q+[g_B(E)-g_0]I_B, \quad (13)$$

where $\alpha_0=1$ nm is a scale factor, I_Q, I_B and A are given by

$$I_Q=4\pi\int_0^R A^2\sin^2(k_1r)dr$$

$$I_B=4\pi\int_R^\infty A^2\sin^2(k_1R)e^{-2k_2(r-R)}dr, \quad (14)$$

$$I_Q=I_B+I_v=1 \quad (15)$$

where I_v is the valence-envelope wave function contribution with because $E \ll E_{gQ}$. Thus, we obtained $g(x,R)$ for GaSb/Ga$_{1-x}$In$_x$As$_y$Sb$_{1-y}$/GaSb SQD semiconductor heterostructure using the parameters obtained by Eqs. (1). Considering the conduction Γ_6 and valence Γ_7, Γ_8 bans and neglecting the higher bands the Hamiltonian Eq. (3) Lax *et al.* [8] obtained the bulk energy of the n-th Landau level of the conduction band in semiconductors III-V, showing that both the effective mass and the g factor are greatly modified by the band mixing with spin-orbit interaction effects and these are considered in energy Landau levels. Here we proposed a parabolic confining potential including the band mixing effects given by Eq. (13). Thus, when the magnetic field is applied parallel to z-direction, the quantum dot potential in the perpendicular plane is given by

$$V(r_\perp) = \frac{m_Q(\varepsilon)}{2}\omega_0^2 r_\perp^2 \tag{16}$$

where $m_Q(\varepsilon)$ is the energy-dependence mass for quaternary alloy, is the confining frequency and $r_\perp$ is the radius perpendicular to z-direction. The Hamiltonian in the presence of both magnetic field and confining potential $V(r_\perp)$ within the symmetric gauge $A = [-(1/2)H_y, (1/2)H_x, 0]$ can be written

$$\widehat{H} = \frac{p^2}{2m_Q(\varepsilon)} + \frac{1}{2}\hbar\omega_c L_z + \frac{m_Q(\varepsilon)}{2}\left[\left(\frac{\omega_c}{2}\right)^2 + \omega_0^2\right] r_\perp^2, \tag{17}$$

here $L_z = xp_y - yP_x$ is the z-component of the angular momentum **L** and $\omega_c = (eH/m)$ is the cyclotron frequency. In cylindrical coordinate (ρ, ϕ, z) the Schrödinger equation $\widehat{H}\psi(\rho) = \varepsilon\psi(\rho)$ has solutions given by

$$\varepsilon(n,m) = (2n + |M| - 1)\left[\left(\frac{\omega_c\hbar}{2}\right)^2 + (\omega_s)^2\right]^{1/2} \left(\frac{\hbar\omega_c}{2}\right) M \pm \frac{1}{2}\mu_B g_Q(\varepsilon), \tag{18}$$

with

$$\psi(\rho) = Ce^{i(M\phi + k_z z)}\rho^{|M|}e^{-\frac{\rho^2}{4l^2}} L_{n+|M|}^{|M|}\left(\frac{\rho^2}{2l^2}\right), \tag{19}$$

where

$$n = 1, 2, 3\ldots,\ M = 0, \pm 1, 2, \ldots,\ L_{n+|M|}^{|M|}\left(\frac{\rho^2}{2l^2}\right)$$

is the associated Laguerre function, $l = (\hbar/eH)^{1/2}$ is the magnetic length and $\mu_B = 9.274 \times 10^{-24}$ JT^{-1} is the Bohr magneton and $\omega_s = \hbar\omega_0$ is the effective confining energy defined as

$$\omega_s(x,R) = \frac{\hbar}{R}\left(\frac{2(\Delta E_C(x) - E)}{m_Q}\right)^{1/2} \tag{20}$$

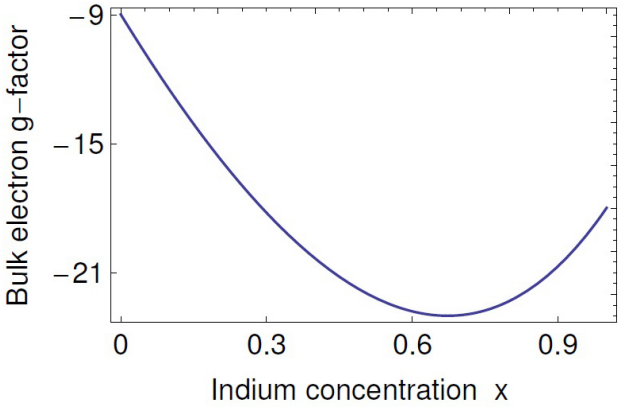

FIGURE 1. (Color online)Bulk electron g-factor as a function of x, for Ga$_{1-x}$In$_x$As$_y$Sb$_{1-y}$/GaSb quaternary alloys at T= 300 K.

3. Results and discussion

In this work, we show that the electron g-factor effects can not be ignored neither if a magnetic field is applied externally to the bulk material, nor to a quaternary alloy SQD, because bulk electron g-factor values are in the range -9.25 to -23.14. In Fig. 1 we display the variation of the bulk electron g-factor as a function of x. We observe that the bulk electron g-factor values fall in the range between the bulk electron g-factor measured for GaSb when $x \to 0$ ($g \cong -9.25$) and the bulk electron g-factor measured for InAs when $x \to 1$ ($g \cong -17.5$) but, there is a remarkable minimum at ($g \cong -23.14$) for $x \cong 0.67$. Also, we see that for $x$in the range $0.5 \leq x \leq 0.83$ the dependence of the electron g-factor on x is approximately parabolic. Experimental or theoretical bulk electron g-factor for Ga$_{1-x}$In$_x$As$_y$Sb$_{1-y}$/GaSb quaternary

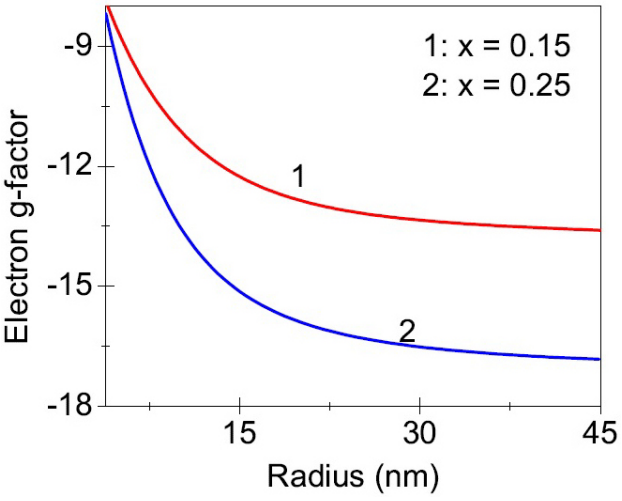

FIGURE 2. (Color online) Variation of the electron g-factor as a function of the radius in a GaSb/Ga$_{1-x}$In$_x$As$_y$Sb$_{1-y}$/GaSb SQD at T= 300 K. Lines 1 and 2 corresponds for x= 0.15 and x= 0.25 respectively.

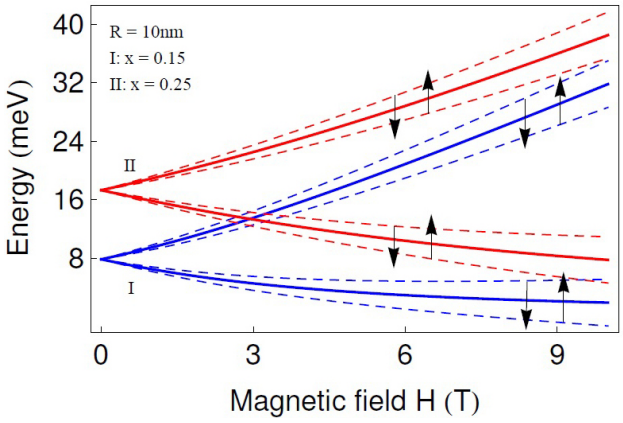

FIGURE 2. (Color online) Two Landau level splitting for the first energy confined state in GaSb/$Ga_{1-x}In_xAs_ySb_{1-y}$/GaSb SQD for R= 10 nm at room temperature. Curves I corresponds to x= 0.15, $g = -10.9$, $\omega_s = 8$ meV and Curves II corresponds to x= 0.25, $g = -11$, $\omega_s = 17$ meV. Neglecting the electron g-factor effect, full lines, and considering the electron g-factor effect dashed lines, to spin dow (up) state, $\downarrow$ ($\uparrow$).

alloy is not readily available. Thus, we make a prediction for bulk electron g-factor in quaternary alloy $g_Q(x)$ at T= 300 K based on the electron g-factor behavior of the binaries III-V and the interpolation proposed in Eqs. (1) and (2). Figure 2 displays the electron g-factor versus the radius of the SQD at room temperature. We see that the electron g-factor reaches the bulk values as the radius increases, $g = -14$ and $g = -17$ for x= 0.15 and x= 0.25 respectively. As the radius decreases, the electron g-factor in a GaSb/$Ga_{1-x}In_xAs_ySb_{1-y}$/GaSb SQD increases, approaching to $g = -9$ in the limit $R \to 0$, that is, to the barrier material g-factor value. Taking in mind that experimental and theoretical electron g-factor for $Ga_{1-x}In_xAs_ySb_{1-y}$ quaternary alloys are not avail able, we thus make a prediction of $g_Q(x, R)$ within the $\vec{k} \cdot \vec{p}$ eight-band effective-mass model using the parameters calculated in this work by means of Eqs. (1) and (2).

Figure 3 show two Landau levels splitting induced by the application of the external magnetic field in the range 0 - 10 T for the first excited energy confined state in a GaSb/$Ga_{1-x}In_xAs_ySb_{1-y}$/GaSb SQD for R= 10 nm at room temperature, curves I corresponds to x= 0.15, $g = -10.9$, $\omega_s = 8$ meV and Curves II corresponds to x=0.25, $g = -11$, $\omega_s = 17$ meV. We see that, as the magnetic field is increased the corresponding energies augment. Also, one notices that the difference between the energies corresponding to spin up($\uparrow$) and spin dow($\downarrow$) states is very apparent, 8 meV at H=10 T, for both type of curves, I and II, as well as for higher values of the applied magnetic field.

4. Conclusions

We have developed an interpolation method to calculate bulk electron g-factor $g(x)$ at T= 300 K, using a eight-band effective-mass model in order to calculate the electron g-factor as a function of both x and R and the Landau energy levels on the electrons confined in a SQD quaternary alloy. Our predictions show that bulk electron g-factor values are in the range between the electron g-factor measured in bulk GaSb when $x \to 0$ ($g = -9.25$) and that measured in InAs when $x \to 1$, ($g = -18.08$), but there is a remarkable minimum in the g-factor value $g \cong 23.14$ at $x \cong 0.67$. In a GaSb/$Ga_{1-x}In_xAs_ySb_{1-y}$/GaSbSQD our calculations show that the electron g-factor decreases as the radius increase, reaching the value of the bulk quaternary material, for a given value of x, and increases when the radius decreases, approaching to the value in the barrier material, that is, in the limit $R \to 0$. For x= 0:15 and $\omega_s = 8$ meV we notice that the energy levels increase with the applied magnetic field. Also, we have found that the difference between the energies corresponding to spin up($\uparrow$) and spin dow ($\downarrow$) states for both type of curves, I and II is notable, 8 meV at H= 10 T as well as for higher values of the applied magnetic field. We have found that the GaSb/$Ga_{1-x}In_xAs_ySb_{1-y}$/GaSb quaternary alloy is an appropriate material for spintronic applications due to its large response under the action of the magnetic field, H <10 T, when compared with other III-V semiconductors. We hope that these theoretical results will motivate experimental study that will confirm our predictions.

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