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Aluminum concentration and magnetic field effects on the Landé g factor in GaAs–(Ga,Al)As cylindrical quantum well wires

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ABSTRACT

We have performed a theoretical study of the Aluminum concentration and axis-parallel applied magnetic-field effects on the conduction-electron Landé *g* factor in GaAs–(Ga,Al)As cylindrical quantum well wires. Numerical calculations are performed by using the Ogg–McCombe effective Hamiltonian, which includes nonparabolicity and anisotropy effects for the conduction-band electrons. The quantum wire is assumed to consist of an infinite length cylinder of GaAs, surrounded by $Ga_{1-x}Al_xAs$ barrier. Theoretical results are given as functions of the Al concentration, radius and applied magnetic fields. We have studied the competition between the quantum-confinement (geometrical and barrier-potential confinements) and the magnetic field, finding that in this type of heterostructure the effects of the applied magnetic field are very small as compared with the Al concentration and geometrical-confinement effects. Present theoretical results are in very good agreement with previous theoretical findings for $x=0.35$.

1. Introduction

The study of the interaction between single-particle spins and the solid state environment has been the subject of a considerable amount of work in the last few years. In particular, studies of the properties of the conduction-electron *g* factor in semiconductor heterostructures have attracted the community attention both from the theoretical and experimental points of view, due to the possible use of the electronic spin as the architecture of a solid-state based quantum computer. The single qubit operation is essentially performed through the coupling with an external magnetic field and is of fundamental importance to have pure spin states in order to guarantee that no losses occur when the spins transport information. This may be achieved by manipulating the electron *g* factor in semiconductors heterostructures designing appropriate external gate control devices.

The *g* factor in zinc-blende type semiconductors heterostructures differs from the free electron *g* factor in vacuum, $g=2.0023$, due to the spin–orbit interaction, confinement and nonparabolicity effects. As a result, there has been a number of experimental and theoretical work devoted to the understanding of the properties of the electron effective *g* factor in semiconductor heterostructures [1–15]. Due to the potential applications in the design and fabrication of spintronic and optoelectronic devices [16], such studies have been focused in semiconductor-bulk materials [1,2], quantum wells (QWs) [3–8], quantum well wires (QWWs) [9,10], quantum dots (QDs) [11–14], and superlattices [15].

The investigations on the properties of the effective Landé *g* factor in QWWs have been mainly carried out without the consideration of the aluminum concentration effects. In III–V bulk materials, the properties of the electron Landé *g* factor may be investigated within the $\mathbf{k}\cdot\mathbf{p}$ framework [1,2]. According to this procedure, the behavior of the Landé *g* factor in each host material, as a function of the Al concentration, is determined by the dependence of the fundamental gaps [17–22] and interband matrix elements on the Al concentration [8]. In a semiconductor QWW with zinc-blende structure, the electron effective *g* factor must be studied by taking into account the anisotropy and nonparabolicity of the conduction band. In that respect, the effective Ogg–McCombe Hamiltonian [23] has been successfully used in order to obtain the electron effective Landé factor in GaAs–$Ga_{1-x}Al_xAs$ QWs [6,7].

The aim of the present work is to study the role of the quantum confinement determined by the geometrical parameters of the structure and by the Al concentration, as well as the effects of an on-axis applied magnetic field on the conduction-electron *g* factor in GaAs–$Ga_{1-x}Al_xAs$ cylindrical QWWs by taking into account the anisotropy and nonparabolicity of the conduction band. The present study is organized as follows. The theoretical procedure is given in Section 2. Results and discussion are in Section 3, and conclusions in Section 4.

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2. Theoretical framework

We consider a conduction electron in a cylindrical GaAs–$Ga_{1-x}Al_xAs$ QWW under an axis-parallel applied magnetic field, i. e., $\mathbf{B}=B\hat{\mathbf{z}}$. In the effective-mass approximation and taking into account the nonparabolicity and anisotropy effects on the conduction band, the Ogg–McCombe effective Hamiltonian [23] for a conduction-electron may be written as

$$\hat{H}=\frac{\hbar^2}{2}\hat{\mathbf{K}}\frac{1}{m^*(x,\rho)}\hat{\mathbf{K}}\hat{\mathbf{I}}+\frac{1}{2}g(x,\rho)\mu_B B\hat{\sigma}_z+a_1\hat{\mathbf{K}}^4\hat{\mathbf{I}}+\frac{a_2}{l_B^4}\hat{\mathbf{I}}+a_3[\{\hat{K}_\rho^2,\hat{K}_\varphi^2\}+\{\hat{K}_\rho^2,\hat{K}_z^2\}+\{\hat{K}_\varphi^2,\hat{K}_z^2\}]\hat{\mathbf{I}}+a_4B\hat{\mathbf{K}}^2\hat{\sigma}_z+a_5B\{\hat{\vec{\sigma}}\cdot\hat{\mathbf{K}},\hat{K}_z\hat{\mathbf{I}}\}+a_6B\hat{\sigma}_z\hat{K}_z^2+V(\rho)\hat{\mathbf{I}}, \tag{1}$$

where $\hat{\mathbf{K}}=-i\nabla+e/\hbar c\hat{\mathbf{A}}$, $\hat{\mathbf{I}}$ is the 2×2 unit matrix, μ_B is the Bohr magneton, $l_B=\sqrt{\hbar c/eB}$ is the Landau length, $\hat{\vec{\sigma}}$ is a vector for which the components are the Pauli matrices, $\{\hat{a},\hat{b}\}=\hat{a}\hat{b}+\hat{b}\hat{a}$ is the anticommutator between the $\hat{a}$ and $\hat{b}$ operators, and the coefficients a_i (i=1,…,6) are constants which depend, in principle, on the Al concentration x. Due to the absence of experimental measurements on the behavior of the a_i coefficients as functions of x, we have taken the a_i values corresponding to bulk GaAs and obtained by a fitting with magnetospectroscopic measurements [24]. The cubic Dresselhaus spin–orbit interaction [25] can be neglected because its contribution to the effective g factor in GaAs–$Ga_{1-x}Al_xAs$ heterostructures may be shown to be quite minor [26,27]. The conduction-band effective mass $m^*(x,\rho)$ and Landé factor $g(x,\rho)$ are considered to be position and Al concentration dependent. The confinement potential $V(x,\rho)$ is considered to corresponds to 60% of the gap difference between the two host materials [6], and the origin of energy is taken at the top of the GaAs valence band.

At low temperatures, we may consider that only the lowest electron states are populated and we can neglect the k_z terms. The Hamiltonian (1) then becomes diagonal and the ↑ spin-up and ↓ spin-down states are uncoupled. The Schrödinger equation is therefore given by

$$\begin{pmatrix}\hat{H}_\uparrow & 0\\ 0 & \hat{H}_\downarrow\end{pmatrix}\begin{pmatrix}\psi_\uparrow(\rho)\\ \psi_\downarrow(\rho)\end{pmatrix}=E\begin{pmatrix}\psi_\uparrow(\rho)\\ \psi_\downarrow(\rho)\end{pmatrix}, \tag{2}$$

where $\hat{H}_\uparrow$ and $\hat{H}_\downarrow$ correspond to the spin-up and spin-down electron states, respectively, and are obtained neglecting the k_z terms in the Hamiltonian (1).

Now, in order to tackle Eq.(1), it is well known [28] that the solutions should be the Kummer confluent F and U hypergeometric functions, and one should then solve the following transcendental equation, which may be obtained by assuming as valid the boundary condition for the solution for the parabolic [Eq. (1) with a_i=0] Hamiltonian, i.e.,

$$\frac{\frac{d}{d\varepsilon}(e^{-\varepsilon/2}\varepsilon^{l/2}F[-\alpha_W^{\uparrow,\downarrow};l+1;\varepsilon])}{e^{-\varepsilon/2}\varepsilon^{l/2}F[-\alpha_W^{\uparrow,\downarrow};l+1;\varepsilon]}=\frac{\frac{d}{d\varepsilon}(e^{-\varepsilon/2}\varepsilon^{l/2}U[-\alpha_B^{\uparrow,\downarrow};l+1;\varepsilon])}{U[-\alpha_B^{\uparrow,\downarrow};l+1;\varepsilon]}, \tag{3}$$

where

$$\alpha_{W,B}^{\pm}=-\frac{\chi_{W,B}^{\pm}l_B^2}{a_3+4a_1}-\sqrt{\left(\frac{\chi_{W,B}^{\pm}l_B^2}{a_3+4a_1}\right)^2+\frac{l_B^4(E_\rho^{\pm}-\xi_{W,B})}{a_3+4a_1}}-\frac{1}{2}, \tag{4}$$

$$\xi_{W,B}=\frac{a_2-0.75a_3}{l_B^4}\pm\frac{1}{2}g(x,\rho)\mu_B B+V(\rho), \tag{5}$$

$$\chi_{W,B}^{\pm}=\frac{\hbar^2}{2m^*(x,\rho)}\pm a_4B, \tag{6}$$

and the subindexes W and B denote the values of the magnitudes in the well and barriers, respectively. $\varepsilon=eB\rho^2/2\hbar c$ is evaluated at $\rho=R$, where R is the radius of the QWW.

The axis-parallel electron effective Landé g factor in GaAs–(Ga,Al)As heterostructures may, therefore, be defined as

$$g_\parallel^{(0)}=\frac{E_0^\uparrow-E_0^\downarrow}{\mu_B B}, \tag{7}$$

where $E_0^\uparrow$ and $E_0^\downarrow$ are the ground-state energies associated with the spin-up and spin-down, respectively. The electron effective $g_\parallel^{(0)}$ factor, obtained from Eq. (7), depends on the Al concentration in the $Ga_{1-x}Al_xAs$ barriers, applied magnetic field, and the radius of the cylindrical QWW.

To calculate the electron effective Landé g factor in the GaAs–$Ga_{1-x}Al_xAs$ QWW from Eq. (7) is needed to know the dependence of both Landé g factor and effective mass on the Al concentration in each host material. In that respect the five-band $\mathbf{k}\cdot\mathbf{p}$ theory fits with high precision the g factor and the effective mass of most common III–V compounds and alloys at low temperatures. The five-band $\mathbf{k}\cdot\mathbf{p}$ theory for the g-factor and effective mass may be written as follows:

$$\frac{g}{g_0}=1-\frac{\Pi^2}{3}\left(\frac{2}{E(\Gamma_6^c-\Gamma_8^v)}+\frac{1}{E(\Gamma_6^c-\Gamma_7^v)}\right)-\frac{\Pi'^2}{3}\left(\frac{1}{E(\Gamma_7^c-\Gamma_8^v)}+\frac{2}{E(\Gamma_8^c-\Gamma_8^v)}\right)-\tilde{\Delta}\left(\frac{2}{E(\Gamma_6^c-\Gamma_7^v)E(\Gamma_7^c-\Gamma_8^v)}+\frac{1}{E(\Gamma_6^c-\Gamma_8^v)E(\Gamma_8^c-\Gamma_8^v)}\right)-0.2051x-0.5074x^2+3.0089x^4+C'. \tag{8}$$

$$\frac{m_0}{m^*}=1+\frac{\Pi^2}{3}\left(\frac{2}{E(\Gamma_6^c-\Gamma_8^v)}+\frac{1}{E(\Gamma_6^c-\Gamma_7^v)}\right)-\frac{\Pi'^2}{3}\left(\frac{1}{E(\Gamma_7^c-\Gamma_8^v)}+\frac{2}{E(\Gamma_8^c-\Gamma_8^v)}\right)-\tilde{\Delta}\left(\frac{1}{E(\Gamma_6^c-\Gamma_7^v)E(\Gamma_7^c-\Gamma_8^v)}-\frac{1}{E(\Gamma_6^c-\Gamma_8^v)E(\Gamma_8^c-\Gamma_8^v)}\right)+0.6689x+6.0295x^2+C, \tag{9}$$

Here, g_0=2.0023 and m_0 are the free-electron Landé factor and effective mass, respectively, and $E(\Gamma_8^v,\Gamma_6^c,\Gamma_7^c,\Gamma_8^c)$ are the energy-gaps at the center of the Brillouin zone, $\tilde{\Delta}=\frac{4}{9}\Delta\sqrt{\Pi\cdot\Pi'}$ is the

Table 1
Parameters used in the present calculation.

$E(x)$	a (meV)	b (meV)	c (meV)
$E(\Gamma_6^c-\Gamma_8^v)$	1519 [a]	1360 [a]	220 [a]
$E(\Gamma_6^c-\Gamma_7^v)$	1849 [b]	1294 [b]	220 [b]
Π^2	28 900 [c,d]	−6290 [e]	0 [e]
Π'^2	6100 [f]	0 [g]	0 [g]
$E(\Gamma_7^c-\Gamma_8^v)$	4504 [h]	0 [i]	0 [i]
$E(\Gamma_8^c-\Gamma_8^v)$	4659 [h]	0 [i]	0 [i]

[a] From Ref. [19].
[b] From Ref. [22].
[c] From Ref. [1].
[d] From Ref. [8].
[e] Obtained from a linear fitting of the g factor values for bulk $Ga_{1-x}Al_xAs$, reported in Ref. [8].
[f] From Ref. [31].
[g] To our knowledge, there are no experimental measurements on the Al concentration dependence of the Π'^2 matrix element, so we have taken b=0 and c=0.
[h] From Ref. [32].
[i] The remote-band contributions to the electron Landé g factor and effective mass are taken into account in the Eqs. (8) and (9), respectively.