



One phonon resonant Raman scattering in semiconductor quantum wires: Magnetic field effect

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ABSTRACT

We have developed a theory of one phonon resonant Raman scattering in a semiconductor quantum wire of cylindrical geometry in the presence of an external magnetic field distribution, parallel to the cylinder axis. The effect of the magnetic field in the electron and hole states, and in the Raman scattering efficiency, is determinate. We consider the electron–phonon interaction using a Fröhlich-type Hamiltonian, deduced for the case of complete confinement phonon modes by Comas and his collaborators. We also assume $T=0$ K, a single parabolic conduction and valence bands. The spectra are discussed for different magnetic field values and the selection rules for the processes are also studied.

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1. Introduction

The magnetic field provides additional information and shows new proprieties of carriers in bulk and nanostructured materials [1–4]. Moreover, the nanometer-scale confinements of the electrons and holes in the semiconductor materials provide varieties of quantum phenomena, dramatically changing the dynamics of charge carriers. Thus, the presence of both the magnetic field as the confinement allows the study of new phenomena which cannot be seen when applied separately.

The electronic structure of nanostructures and other materials can be studied through Raman scattering processes, by considering different polarizations of incident and emitted radiation [5–10]. Thus, the analysis of the differential cross-section for a Raman scattering allows the determination of the sub-band structure of the system. This is done by a direct inspection of singularity positions in the spectra, considering the selection rules. The Raman scattering efficiency, in general, shows singularities related to inter-band and intra-band transitions. The Raman

spectra has multiple singularities that change position when the electron band structure changes due to the confinement regime or the presence of electric or magnetic fields. Recently, the electron Raman scattering by means of Fröhlich-type interaction has been investigated in semiconductor quantum wires with and without the presence of magnetic fields [11–15]. Resonant Raman scattering (RRS) has been investigated in semiconductor quantum wires, [16–18] and our interest is to analyze the effect of a magnetic field on one phonon resonant Raman scattering. The magnetic field chosen is parallel to the cylinder axis being constant with value zero outside and B_0 within, with a circular wire shape. The magnetic field effect is particularly noticeable in the electrons due to the unfolding of electronic bands, breaking the degeneracy existing in the electron sub-band system of a quantum wire; this could be studied with the Raman spectra.

In this paper, we present a model of RRS in a semiconductor quantum wire (QWW), where we assume that $T=0$ K, there is a single parabolic conduction and valence bands. Within the strong-confinement regime, and disregarding the exciton contribution, the electron intermediate states were considered as uncorrelated electron–hole pairs (EHP). Furthermore, we must consider the selection rules described in Ref. [19], considering the scattering configuration according to the electron–phonon interaction using a Fröhlich-type Hamiltonian (see Fig. 1 in Ref. [19]). These devices are fabricated from GaAs/AlAs using high-resolution electron-beam lithography techniques. The resonant Raman scattering processes can be qualitatively described in the following way: first, the EHP is created due to the absorption of a

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laser radiation photon of energy $\hbar\omega_l$, by inter-band transition. In the second step, the EHP carries out an intra-band intermediate transition with the emission of one longitudinal optical phonon of energy $\hbar\omega_q$, and in the last step the EHP is annihilated due to inter-band resonant transition, emitting a secondary radiation photon of energy $\hbar\omega_s$. For the electron–phonon interaction we used the same Fröhlich-type interaction Hamiltonian, developed in the reference, deduced for quantum wire by Comas and his collaborators [21–24].

2. Model and applied theory

The Raman scattering efficiency per unit solid angle is given in Refs. [18,20], and can be obtained as:

$$\frac{1}{V} \frac{d\sigma}{d\Omega} = \frac{V(\omega_l - \omega_q)^2 \eta(\omega_s) 2\pi}{8\pi^3 c^4 \eta(\omega_l)} \sum_f |M_{fi}(\omega_l - \omega_0, \hat{\mathbf{e}}_s, \varepsilon_l, \hat{\mathbf{e}}_l)|^2 \quad (1)$$

where

$$M_{fi} = \sum_{a,b} \frac{\langle f | \hat{H}_r^+ | b \rangle \langle b | \hat{H}_p | a \rangle \langle a | \hat{H}_r^- | i \rangle}{(\hbar\omega_l - E_a + i\Gamma_a)(\hbar\omega_s - E_b + i\Gamma_b)} \quad (2)$$

$\eta(\omega)$ is the refraction index as a function of the radiation frequency ω , $\hat{\mathbf{e}}_s$ ($\hat{\mathbf{e}}_l$) is the unit polarization vector for the emitted secondary (incident) radiation, and c is the light velocity in vacuum. M_{fi} is the scattering amplitude probability of the Raman process, considering only the resonant terms.

In this case we have a completely occupied valence band and unoccupied conduction band. Therefore, the initial state $|i\rangle$ of the system consists of an incident photon of frequency ω_l and polarization $\hat{\mathbf{e}}_l$ and the final state $|f\rangle$ consists of a photon of frequency ω_s and an excited phonon of frequency ω_q .

In Eq. (2), $|a\rangle$ and $|b\rangle$ represent the intermediate states with energies E_a and E_b . Γ_a and Γ_b are the corresponding lifetime broadening. $\hat{H}_r^\pm$ is the electron–photon interaction Hamiltonian; the sign $+$ ($-$) corresponds to the emission (absorption) of a photon. The operator $\hat{H}_r^\pm$ is of the form:

$$\hat{H}_r^- = \frac{|e|}{\mu_0} \sqrt{\frac{2\pi\hbar}{V\omega_l}} \hat{\mathbf{e}}_l \cdot \hat{\mathbf{p}} \quad \text{and} \quad \hat{H}_r^+ = \frac{|e|}{\mu_0} \sqrt{\frac{2\pi\hbar}{V\omega_s}} \hat{\mathbf{e}}_s \cdot \hat{\mathbf{p}} \quad (3)$$

where μ_0 is the free electron mass [20]. This operator describes the interaction with the incident radiation field in the dipole approximation. In this paper we propose to study the resonant Raman scattering which implies the existence of EHP.

The work referenced by endnote [15] considers only intra-band transitions due to absorption or emission of a photon and phonon-assisted transitions. For this reason, it is not possible in this case to consider the creation or annihilation of electron–hole pairs which are related to inter-band transitions.

Referring to endnote [21], the authors present the macroscopic continuum model, coupling the mechanical phonon displacement vector $\mathbf{u}$ with the electrostatic potential ϕ , the optical vibrational modes and the electron–phonon interaction Hamiltonian. The results are in close agreement with both experiments and microscopic calculation, for further details Refs. [21–24] should be consulted. The above theoretical treatment has been tested in GaAs/AlAs quantum well and wire structures where excellent agreement with microscopic *ab initio* calculations [24,25] and experimental results [26] were observed.

In the theory of long-wavelength polar optical modes in quantum wires, results show that the phonon modes are no longer purely longitudinal, transversal or interface modes but are coupled modes showing a mixed character due to discontinuities at the interface. This theory proves that the surface and interface phonon modes are a particular case of the general

dispersion relation when the mechanical matching boundary conditions do not play a significant role in the vibrational amplitude [27]. Therefore, no special considerations are required to consider the contribution of surface and interface phonon modes [28]. In this case, we will take a long wave approach, where $q_z = 0$ can be considered [21,22]. The electron–phonon interaction Hamiltonian can be written as [21]:

$$\hat{H}_p = \sum_{n,m} C_{n_p m_p} [F_{n_p m_p}^*(r) \exp[in_p \theta] \hat{b}_{n_p m_p} + \text{H.C.}] \quad (4)$$

where

$$C_{n_p m_p} = \sqrt{\frac{\pi\omega_L \rho}{\varepsilon_{n_p m_p}}} r_0^2 C_F \quad \text{and} \quad C_F = -e \sqrt{\frac{2\pi\hbar\omega_L}{V} (\varepsilon_{a\infty}^{-1} - \varepsilon_{a0}^{-1})}$$

$\omega_q = \omega_{n_p m_p}$ are the optical vibrational modes; $\varepsilon_{a\infty}$ and ε_{a0} are the high and static frequency dielectric constant in the interior of QWW; ω_L is the limiting (bulk) longitudinal optical frequency of the oscillations; ρ is the reduced mass density,

$$F_{0m_p}^* = \bar{B}_{0m_p} \begin{cases} x_q^{-1} J_0(\eta_{r_0}^+) - S_0(\eta) & r \leq r_0 \\ x_q^{-1} J_0(\eta) - S_0(\eta) & r > r_0 \end{cases},$$

the related expression, as $\omega_{n_p m_p}$, η , x_q and $\bar{B}_{0m_p}$, can be found in Refs. [18,21]. The presence of a constant magnetic field, B_0 value within and zero outside of the quantum wire does not change the conditions from which the Hamiltonian of electron–phonon interaction follows, in the phenomenological model Comas–Trallero [21,28]. This is because the contribution of the magnetic field can be neglected by calculating the phonon modes and electron–phonon interaction as less than 20T, so that the cyclotron frequency is too small for the ionic cores. For this reason we use magnetic fields smaller than 20T in the calculation of the Raman scattering cross section.

According to our calculations, the QWW geometry is cylindrical, with a circular cross-section of radius r_0 , and length L . The confinement potential, the magnetic field and the vector potential associated with this field distribution are:

$$V_c, \mathbf{B}, A = \begin{cases} 0 & B_0 \mathbf{e}_z, \quad \frac{1}{2} B_0 r \hat{\mathbf{e}}_\theta; & 0 \leq r \leq r_0 \\ V_0 & 0, \quad \frac{1}{2r} B_0 r_0^2 \hat{\mathbf{e}}_\theta; & r_0 \leq r < \infty \end{cases}$$

where $\hat{\mathbf{e}}_z$ ($\hat{\mathbf{e}}_\theta$) is the unit vector in the z -direction (θ -direction). Notice that $\nabla \mathbf{A} = B_0$ in $r \leq r_0$ and $\nabla \mathbf{A} = 0$ outside of the QWW [13–15], as required by the field distribution. Also notice that the symmetric choice $\nabla \mathbf{A} = 0$. Moreover, it is easy to prove that the magnetic field defined in this way fulfills the boundary conditions, when assuming no surface currents.

We assumed a parabolic band for the electron and the hole, which are split into a sub-band system due to the confinement and the magnetic field. This model is commonly used in II–VI and III–V semiconductors when the description is near to the center of the Brillouin zone in the reduced zone scheme. Under these dynamical conditions, and since the potential barriers do not imply inter-band transitions, or the complex valence band of III–V and II–VI semiconductor compounds, the contribution of band mixing is small under the confinement regime assumed in this work, and is consistent with previous treatments [20,29]. The electron–hole Coulomb interaction is not considered. To eliminate the possibility of the absorption of phonons in the electron–phonon interaction, we will assume that $T = 0$ K. The solution of the Schrödinger equation, in the envelope function approximation, leads to:

$$\Psi(\mathbf{r}) = \frac{\exp[i(m\theta - k_z z)]}{\sqrt{2\pi L}} u_0(\mathbf{r}) \begin{cases} A \exp(-\frac{\gamma}{2}) x^{\frac{|m|}{2}} {}_1F_1(\beta, 1 + |m|, x), & r \leq r_0 \\ B K_{|v|}(\frac{\gamma}{r_0} r), & r > r_0 \end{cases} \quad (5)$$

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