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Optical transitions in AlGaAs/GaAs quantum wires on GaAs(6 3 1) substrates studied by photoreflectance spectroscopy

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ABSTRACT

We present the synthesis and characterization of a system of self-assembling GaAs quantum wires (QWRs) embedded in $Al_x Ga_{1-x}$ As barriers grown by molecular beam epitaxy on GaAs(6 3 1)-oriented substrates. We studied the optical transitions in the QWRs as a function of temperature (T) by photoreflectance (PR) spectroscopy. The energy transitions were extracted from the PR spectra employing the third-derivative functional form, and they were compared with the transitions theoretically calculated from both, a model of QWRs with cylindrical geometry and a model of a conventional square quantum well. The results show a good agreement between experimental and theoretical data in the case of the QWR model, and from this comparison we were able to identify up to 12 different transitions in the PR spectra and to study their behavior dependent on temperature.

1. Introduction

Controllable production of nanometer-sized structures is currently an important field of research. In particular the synthesis of one-dimensional (1D) arrays, such as III–V semiconductor quantum wires (QWRs), is a rapidly expanding area triggered by various unique quantum effects predicted in 1D electronic systems and by the numerous potential applications of these nanostructures in electronic, optoelectronic and photonic devices [1,2].

At present, the fabrication of semiconductor QWRs with the necessary characteristics to allow the investigation of 1D quantum effects has proven to be a very challenging task [3,4]. Out of the various methods for nanostructure fabrication, self-assembled growth by molecular beam epitaxy (MBE) is quite reliable because it is not limited by the resolution of lithography, and does not need additional processing which may induce defects in the nanostructures [4]. In this sense, self-organization of QWRs grown on high index substrates by MBE is a promising approach because of their resulting high density, high optical quality, and easy fabrication [5,6].

High-index planes are energetically unstable and tend to break up into stable facets at the epitaxial growth temperatures to minimize their surface energies. We have used this process to produce periodic surface corrugations, oriented along the [−5,9,3] direction, composed of nanometer-sized microscopic facets on originally GaAs(6 3 1)A substrates. This ordered microscopic steps array has been employed as the template for QWRs formation.

In this work, we report on the use of photoreflectance (PR) spectroscopy as a function of temperature to study interband transitions in the QWR system. We use a rather wide GaAs active layer of thickness of 20 nm, to obtain a enough number of transitions to perform the photoreflectance study. PR is a contactless form of electromodulation spectroscopy which produces third derivative-like features in the optical dielectric function, in the vicinity of critical points [7]. Consequently, is possible to observe very sharp differential reflectance lines even at room temperature. In order to elucidate the 1D character in the optical transitions of our system, we carried out the comparison between the experimental data with the calculated transitions from the square quantum well (SQW) and the cylindrical QWR models.

2. Experimental

The samples studied in this work were grown using GaAs(6 3 1)A undoped wafers. The wafers were degreased and etched, and then loaded in a Riber C21 MBE system. Before the GaAs growth the surface oxide was desorbed in the MBE chamber by annealing the

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substrates at 580 °C under arsenic overpressure during 10 min. After that the growth temperature was set at 600 °C and a 80 nm-GaAs buffer layer was deposited just before the growth of the QWR structure, which consists of 40 nm-$Al_{0.23}Ga_{0.77}As$/20 nm-GaAs/40 nm-$Al_{0.23}Ga_{0.77}As$. Finally, in order to avoid oxidation, the upper $Al_{0.23}Ga_{0.77}As$ layer was covered with a 20-Å thick GaAs layer. A constant As_4/Ga beam flux ratio of 16 with a GaAs growth rate of 0.3 ML/s were employed, the sample surface was in situ monitored by reflection high-energy electron diffraction (RHEED).

Under these growth conditions, we are able to induce on the GaAs layers the self-assembling of high density and uniform nanogrooves oriented along the [−5,9,3] direction having at the top interface a lateral period of 12 nm and a vertical amplitude of 1.5 nm [8] while, a flat interface with the bottom AlGaAs barrier is conserved. This corrugated surface induces a periodical lateral modulation in the thickness of the GaAs active layer. Consequently, the narrower regions of this modulated layer act as lateral potential barriers confining electrons and holes in the thicker GaAs regions, thus producing the effective confined QWRs system.

The optical properties of the samples were studied by PR spectroscopy. The PR measurements were performed as a function of temperature from 300 to 8 K, employing a tungsten-halogen quartz lamp as probe beam and the photomodulation was accomplished by mechanically chopping at 150-Hz the $\lambda = 632.8$ nm emission line from a He–Ne laser. The PR spectra were analyzed with a Si photodetector using standard lock-in techniques.

3. Modeling and theory

In order to obtain reference values to identify the PR lines, we have carried out the calculation of the electronic transitions in a QWR system. For the calculation of electronic states in QWRs several schemes have been used with different levels of sophistication [3]. In this work, we have used the effective-mass approximation and a model of cylindrical GaAs-QWR with cross-section of radius r and length L surrounded by $Al_{0.23}Ga_{0.77}As$ as the barrier material.

We assume parabolic bands for electron and holes which, due to the confinement split into subbands. As the confinement potential is a slowly varying function on the scale of the lattice periodicity, we are allowed to work within the envelope function approximation in which the solution of Schrödinger's equation, neglecting electron–hole Coulomb interaction, leads to [9]:

$$\Psi_{l_j m_j} = (2\pi L)^{-1/2} \exp[-i(l_j\phi + k_{zj}z)]u_j \begin{cases} AJ_{l_j}\left(x_{l_j m_j}\dfrac{r}{r_0}\right), & r \le r_0, \\ BK_{l_j}\left(y_{l_j m_j}\dfrac{r}{r_0}\right), & r > r_0, \end{cases} \quad (1)$$

with

$$B = \frac{J_{l_j}(x_{l_j m_j})}{K_{l_j}(y_{l_j m_j})}A,$$

$$A = \left\{ |J_{l_j}(x_{l_j m_j})|^2 + \left[\frac{\mu_2 x_{l_j m_j}}{\mu_1 y_{l_j m_j}}\frac{J'_{l_j}(x_{l_j m_j})}{K'_{l_j}(y_{l_j m_j})}\right]^2 \times |K_{l_j}(y_{l_j m_j})|^2 \right\}^{-1/2}$$

and

$$y_{l_j m_j} = \sqrt{\frac{2\mu_2 r_0^2 V_j}{\hbar} - \frac{\mu_2}{\mu_1}x_{l_j m_j}^2},$$

where j=e(h) represents the electron (hole), V_j stands for the band offset, J_{l_j} and K_{l_j} are the Bessel and modified Bessel functions of order l_j; J'_{l_j} and K'_{l_j} are their corresponding derivatives; μ_1 and μ_2 are the effective electron masses in the interior and exterior media, respectively. The states are described by the quantum numbers $l_j = 0,1,\ldots$ and $m_j = 1,2,\ldots$; k_{z_j} is the wave number of the free motion of carriers along the wire axis. u_j is the Bloch function taken at $\mathbf{k}_0 = 0$ where, by assumption, the band extremum is located. After considering appropriate boundary conditions, we can obtain the energy levels via:

$$E_j(l_j.m_j,k_{zj}) = \frac{\hbar^2}{2\mu_1}\left[k_{zj}^2 + \left(\frac{x_{l_j m_j}}{r_0}\right)^2\right]. \quad (2)$$

In the following discussion we use the notation $L(l)(me–m'$ hh(lh)) to describe the transitions between electrons in the lm-th conduction subband to the lm'-th valence subband of heavy (hh) and light (lh) holes.

Additionally, in order to clarify the difference between the QWR system and a conventional two dimensional quantum well, we have also calculated the allowed heavy- and light-hole transitions corresponding to a square quantum well, of width L_W, under appropriate interfacial boundary conditions [10]. We use the usual notation $ne–n'$hh(lh) denoting the transitions between the n-th conduction subband to the n'-th valence subband of heavy (light) hole character.

For the calculation in both models, a conduction-band offset of 0.65 and the following effective mass values in the [6 3 1] direction [11] has been used: $0.0665m_0$, $0.4697m_0$ and $0.0828m_0$ in the GaAs-interior layer and $0.0857m_0$, $0.5041m_0$ and $0.1004m_0$ in the $Al_{0.23}Ga_{0.77}As$-barriers for the electron, heavy hole and light hole, respectively, where m_0 is the mass of the electron in the vacuum. The mass values of the heavy and light holes were calculated from an analytic expression obtained by a generalized $\mathbf{k}\cdot\mathbf{p}$ model on high-index crystal planes given in Ref. [11].

The PR spectra were analyzed by employing the third derivative functional form developed by Aspnes [7]:

$$\frac{\Delta R}{R} = \sum_k^m \mathrm{Re}[C_k e^{i\theta_k}(\hbar\omega - E_k + i\Gamma_k)^{-7/2}], \quad (3)$$

where m is the number of spectral features, in the region to be fitted, C_k is the amplitude, θ_k the phase, $\hbar\omega$ the incident photon energy, Γ_k is the broadening parameter and, E_k is the energy corresponding to the k-th QWR transition.

4. Results and discussion

In Fig. 1 we show, by dotted lines, the experimental PR spectra taken at the different temperatures. Also we plot, with continues lines, the resulting from the fitting of the spectra by means of the Aspnes function (Eq. (3)), where the E_k have been pointed by short lines.

We observe that as the measurement temperature is lowered, the features in the spectra at higher energies become weaker as a result of carriers freezing at the lower energy levels. Despite of this, we were able to identify, even at the lower temperature up to seven different transitions related to confined states.

We also note that the lower energy confined states have a much larger PR amplitude than the GaAs band-gap transition, reflecting the effective carrier trapping at the QWR. In order to compare the experimental data with the different calculations, we will fix the attention at this point on the set of transitions corresponding to $T = 300$ K, were all the spectra features can be fitted with the maximal accuracy.

In Table 1 we list the energy transition values for both; those obtained by means of the experimental data via Eq. (3) and, the calculated ones employing the cylindrical QWR model via Eq. (2). We also list the value of $\Delta E(E_{Exp} - E_{model})$ and the type of transition