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Spectroscopic Characterization of GaAs and $Al_xGa_{1-x}As$ / $Al_yGa_{1-y}As$ Quantum Well Heterostructures

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This work presents the results of the characterization of GaAs and $Al_xGa_{1-x}As$ / $Al_yGa_{1-y}As$ quantum well hetero-structures growth by MOVPE system. The main goal is to explore the ability of characterization techniques for multilayer structures like quantum wells. The characterization was performed using photoreflectance spectroscopy, surface photovoltaic spectroscopy and X-ray diffraction. The experimental results are verified by numerical simulation.

Keywords: Photoreflectance spectroscopy, Surface photovoltaic spectroscopy, HRXRD, Heterostructures.

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1. INTRODUCTION

Due to vast application of semiconductors heterostructures in lasers and detectors etc., electrical and optical properties of many semiconductor heterostructures are became a very important for technological development [1, 2]. To explore various physical properties of these materials and structures, a lot of techniques are in fashion [3, 4]. However, most of the methods require special experimental conditions such as low temperatures and special sample preparation number, which makes these techniques quite expensive and time taking for results. Spectroscopic techniques, such as; photo-reflectance spectroscopy [5], surface photovoltaic spectroscopy [6] have been applied for its advantageous to use, which are simple and at the same time provide a lot of valuable information. Expect it, these techniques can used at room temperature, without the need for cryogenics as is often necessary with photoluminescence measurements. Moreover, Spectroscopic techniques found important techniques, which play a crucial role in the development of advanced semiconductor heterostructures based devices, where an accurate knowledge of all QW transitions, as well as the barrier band gap energy can be obtained without any complicacy. Modulation spectroscopic techniques and SPS are essentially contactless techniques measure the absorption spectra of incident light source even at room temperature, without any sample damage or contamination [7, 8].

In this paper, we focus our attention on the photoreflectance spectroscopy and surface photovoltaic spectroscopy for investigations of low-dimensional semiconductor structures because of extreme sensitivity to interband electronic transitions, which provides the better understanding of the optical processes in semiconductor device structures. We have identified the QW transitions by solving the Schrödinger equation using finite difference method (FDM) for a finite square potential well [9] and from high-resolution x-ray diffraction (HRXRD) measurements and include a brief introduction to line shape formulas associated with photoreflectance.

2. EXPERIMENTAL DETAILS

GaAs and AlGaAs / AlGaAs QW samples were grown in a metal organic vapor phase epitaxy (MOVPE) system with a rotating substrate holder on GaAs (001) substrates at 770 °C with 5 nm GaAs cap layer and about 250 nm barrier. Arsine (AsH_3), trimethyl compound of gallium (TMGa) and trimethyl aluminum (TMAl) was used as precursors. Spectroscopic measurements were carried out by at room temperature (RT). PR measurement [10] is performed with 100 W quartz-tungsten-halogen (QTH) lamp, 1/4 m monochromator as the light source. The band pass of monochromator is adjusted at 3 nm. A chopped beam of He-Ne laser is used as a pump to modulate the built-in surface electric field. The probe beam from the monochromator is incident on the sample and the reflected beam is focused at the detector. The change in reflectivity of the sample (ΔR) due to the modulation as a function of wavelength of the probe beam is measured. The chopping frequency of the pump beam is fixed at 330 Hz. The dc part of the signal from the detector is extracted, which is proportional to the reflectivity (R). The final spectrum $\Delta R / R$ is obtained by dividing the dc signal to the ac signal.

SPS is performed with the chopped light source used in PR and lock-in amplifier with same chopper frequency and instrumental band pass. Periodic excess carrier generation and subsequent redistribution changes the surface potential; which is measured as a function of wavelength in a range by lock-in amplifier. The modulated SPV signal was measured in soft contact method, where a front electrode is made with the help of transparent conducting glass coated with indium tin-oxide put on the front surface of sample and flat copper sheet is used as a back electrode on which sample is attach with conducting silver paste. The SPV signals were corrected later for the system response.

HRXRD single scans were performed by using a PANalytical X'Pert Pro MRD diffractometer, equipped with a Ge (220) monochromator, with a beam divergence of 12 arc-second in the scattering plane for CuK_{α} 1 X-rays ($\lambda = 1.5406$ Å). QW parameters such as; thick-

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ness and composition (Al content) were measured from the HRXRD measurements by matching the measured diffraction pattern with simulated ones using the Takaji-Taupin equation implemented in the commercial software: X'pert epitaxy [11].

3. ANALYSIS TECHNIQUES

The measured PR spectra were fitted with the well-known Aspnes function, which represents the PR spectrum of excitonic transitions theoretically, given by [12],

$$\frac{\Delta R}{R} = \sum_{j=1}^{n} \mathrm{Re}\left[A_j e^{i\theta_j} / (E - E_{0j} + i\Gamma_j)^{m_j}\right] \qquad (1)$$

where, A_j is an amplitude, θ_j phase angle, E_{0j} critical point energy, Γ_j broadening parameter and m_j exponent which depends on the nature of the j-th critical point transition, and n is the number of critical point transitions. $m = 2$ is used for QWs, which represent the first derivative of a Lorentzian peak.

SPV measurements are basically depending on absorption of the sample and that can approximate peaks near the electronic transitions energy [13]. For analyzing the SPS data, we have followed the methodology used by Arora et al. [14]. According to it, SPV was multiplied by the photon energy and then differentiated with respect to energy. Now, the transition energy may be calculated by fitting with Eq. (1). The obtained transition energies from the PR and SPV were compared by solving the Schrödinger equation for particles in a square well potential. The material parameters for the structures were taken initially from recommended data of Vurgaftman et al. [15].

4. RESULTS AND DISCUSSION

Three QW samples (A-C) were studied during this work and the layer structure details obtained from the HRXRD measurements are shown in Table 1. Fig. 1a and b shows the RT PR and SPS spectrum of transitions in QW. The feature at about 1.76 eV is from the AlGaAs barrier layer. But at the time of growth the Al composition in barrier is plan 0.3. Corresponding to this composition the transition should be at 1.84 eV. So we can say that the transition of barrier is shifted towards the lower energy due to the photon assisted tunneling, also known as Franz Keldysh effect [16]. The actual composition of Al in barrier is listed in Table 1. To determine the transition energies of the QW, we fit the experimental PR spectrum by using Aspens line shape function as defined in Eq. (1) and after differentiation the SPS data, we fitted by the same function. All transitions observed in the PR and SPS spectrum with their energy positions are listed in the Table 2. Different effective masses of electron, heavy hole (hh) and light hole (lh) are used in the QW and barrier regions. The band offset value for this QW structure is taken to be 58 % [17].

Thus we are able to identify all the experimentally observed transitions in the PR data which is nicely matching with the planned thickness of the QW. The RT PR and SPS spectrum of sample B is shown in Fig. 2. Feature at about 1.77 eV is from AlGaAs barrier layer. The two sharp features observed at about 1.65 eV and 1.73 eV are from the QW. At the time of growth the Al

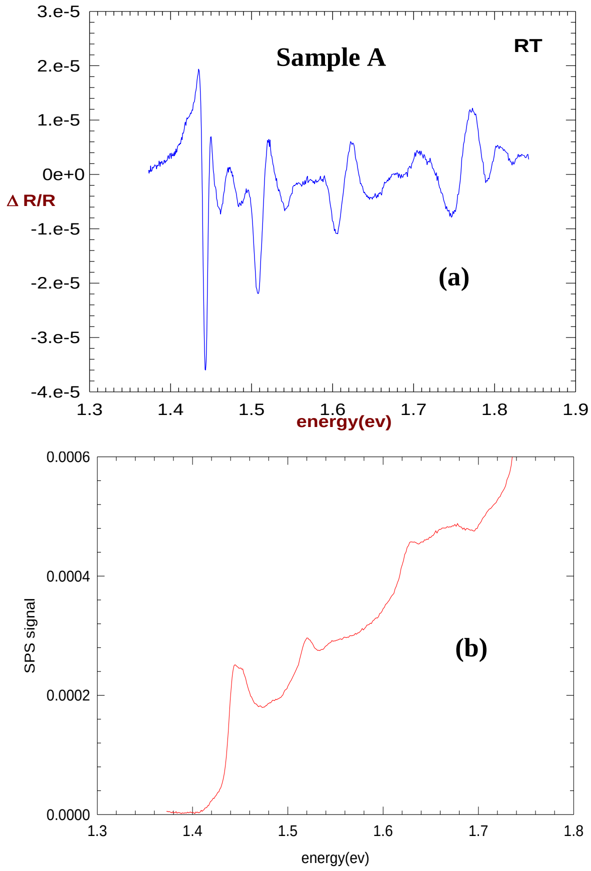

Fig. 1 – RT (a) and PR (b) SPS spectra of sample A

Table 1 – QW structures details of all samples obtained from the HRXRD measurement

Sample No.	QW parameters obtained from the HRXRD data		
	Al Content in QW for sample B and C (x)	QW thickness (nm)	Al Content in Barrier (y)
Sample A (GaAs / $Al_yGa_{1-y}As$)	—	12.3	29.2
Sample B ($Al_xGa_{1-x}As$ / $Al_yGa_{1-y}As$)	13.2	12	29.3
Sample C ($Al_xGa_{1-x}As$ / $Al_yGa_{1-y}As$)	14.2	12	29.2

Table 2 – Experimentally obtained and simulated transition energies for sample A

	e1-h11, (eV)	e1-h12,(eV)	e1-h13, (eV)	e1-h14, (eV)	e1-h23, (eV)	e1-h25, (eV)
PR	1.450	1.466	1.488	1.518	1.547	1.616
SPS	1.450	1.466	—	1.520	1.546	1.620
Simulated Transition energy with XRD QW parameters	1.450	1.466	1.492	1.528	1.556	1.634

composition in barrier is plan 0.3. In this sample, similar sample A, the transition of barrier is found shifted towards the lower energy due to the photon assisted tunneling. The SPS curve shows the only one QW transition and the first or last sharp increase in the surface potential is related to the GaAs substrate and barrier respectively. The similar analysis methodology has been employed to analyze the Sample B. The experimentally obtained transition energies from PR and SPS along with simulated one are listed in the table 3.

Figure 3 shows the RT PR and SPS spectrum of Sample C. Feature at about 1.77 eV is from the AlGaAs barrier layer. In addition to the barrier layer feature, two sharp features are also observed at about 1.65 eV and 1.72 eV, which are related to the QW. It should be noticed that In SPS curve, the first rise is related to the GaAs substrate and only one QW transition is observed. After this the sharp increase in the curve relates to the barrier. Sample C has been analyzed with same methodology used above for PR and SPS data. The all analysis of simulation and experimental transition energies from PR and SPS are presented in the Table 4.

Fig. 4a, b and c shows the measured and simulated X-ray diffraction pattern for sample A, B and C respectively. The highest diffracted pick at zero scale is related to thick GaAs substrate and left shifted pick represents the AlGaAs barrier. We have fitted these HRXRD data by

Table 3 – Experimentally obtained and simulated transition energies for sample B

	e1-h11 (eV)	e1-h22 (eV)
PR	1.650	1.725
SPS	1.650	–
Simulated Transition energy with XRD QW parameters	1.650	1.720

Table 4 – Experimentally obtained and simulated transition energies for sample C

	e1-h11 (eV)	e1-h22 (eV)
PR	1.664	1.727
SPS	1.664	–
Simulated Transition energy with XRD QW parameters	1.664	1.731

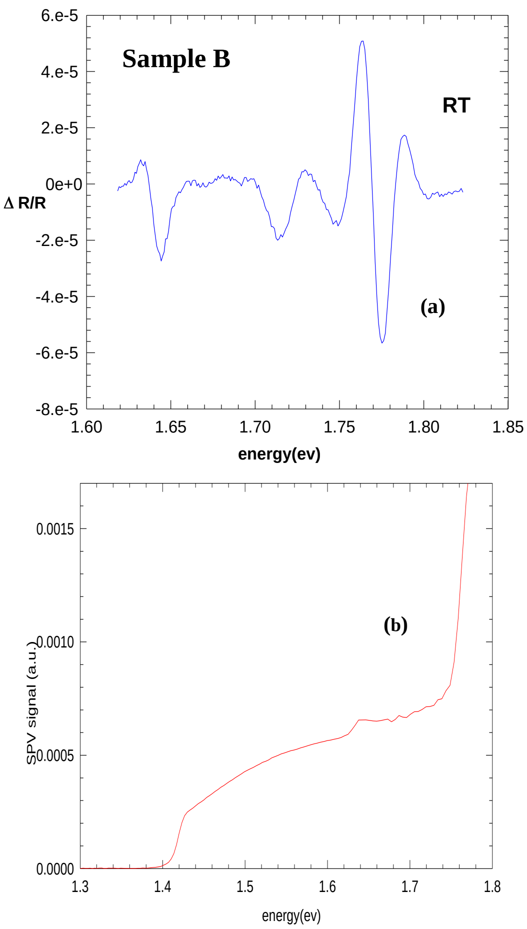

Fig. 2 – RT (a) PR (b) SPS spectra of sample B

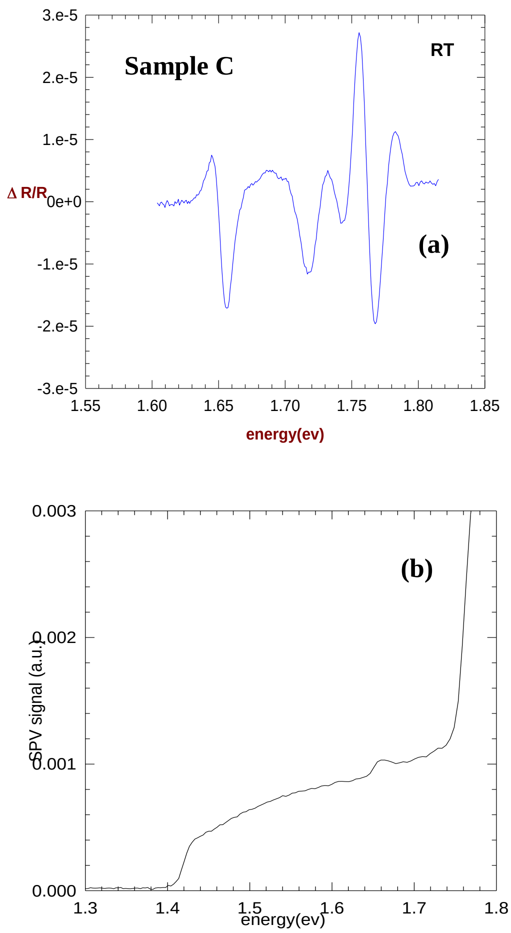

Fig. 3 – RT (a) PR (b) SPS spectra of sample C

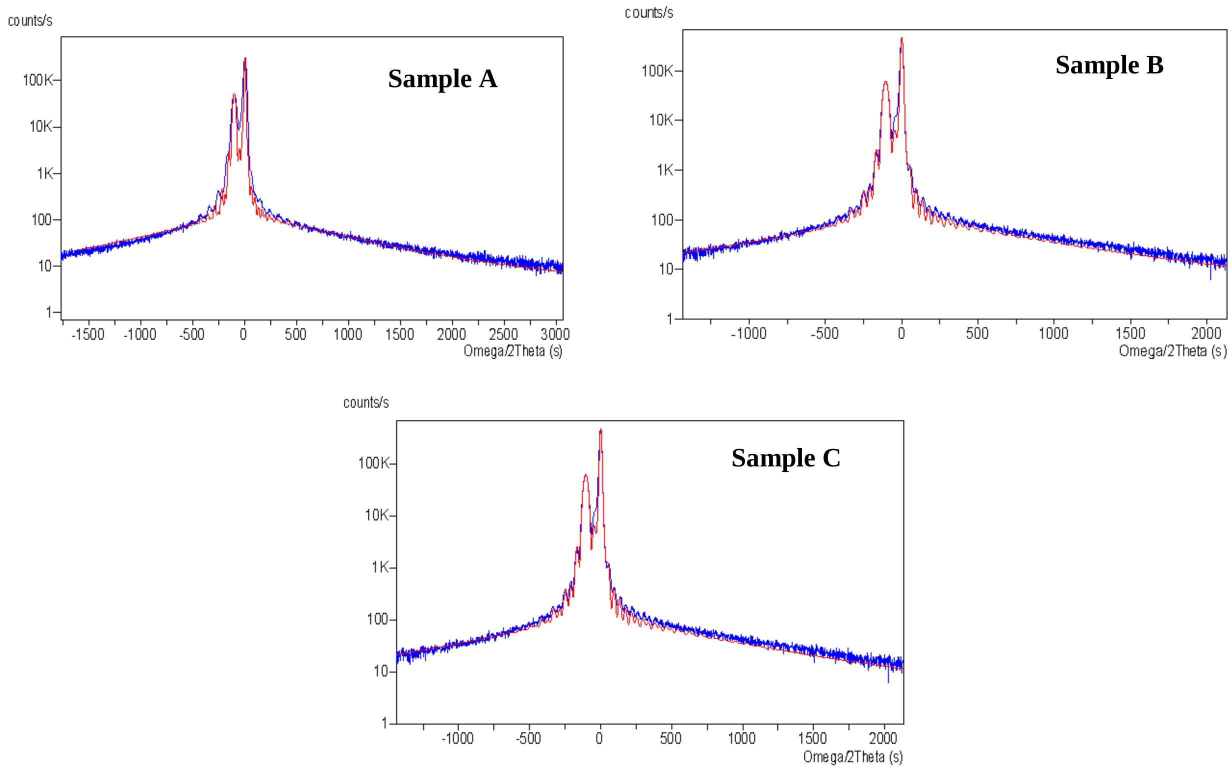

Fig. 4 – HRXRD rocking curve (a) Sample A (b) Sample B (c) Sample C; Blue shows the experimental measurement data and red line shows the simulation

varying different QW parameters by x'pert epitaxy software. The best fitted curve corresponding to experimental measurement is also shown in Figures, from where, we have taken idea about the Al composition and quantum well width. The best combination of QW parameters, from the XRD simulation, is listed in Table 1.

5. CONCLUSION

Modulated reflectance and surface photovoltage spectra have been measured at room temperature for all QW hetero-structures and compared with the simulation with QW parameters obtained from HRXRD measurement. The PR measurement shows the more transitions in comparison of SPS, that represents the PR is more sensitive spectroscopic technique for higher energy transitions. The SPV spectra found to be agreeing with the measured QW transition energies obtained in the PR. From all three samples, it should be noticed that as the Al content increases in the QW, the transition energy is shifted to higher value (lower lambda). The experimentally determined transition energies were well matched to those theoretically predicted by the Schrödinger equation solved by using FDM.

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