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Photoreflectance study of $Al_{0.45}Ga_{0.55}As$/GaAs superlattice: optical transitions at the miniband Γ and Π points

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In this paper, we present the results of photoreflectance (PR) investigation of an $Al_{0.45}Ga_{0.55}As$/GaAs superlattice (SL). The modulation spectra have revealed a number of features at both room and low temperature (10 K) which could be associated with the optical transitions between the minibands of the superlattice. Based on calculations within the effective mass approximation they have been identified as transitions between the miniband edges, *i.e.*, the so-called Γ and Π points, respectively, including the high index transitions and those related to the light holes. Tuning the structure parameters around the nominal ones treated as semi-free in the theoretical considerations allowed the growth accuracy of such a complex system to be verified.

Keywords: superlattice, photoreflectance, modulation spectroscopy.

1. Introduction

Originally, at the end of the 1980s and in the 1990s, the superlattices (SLs) have attracted much attention due to their interesting properties related to strong quantum-mechanical coupling between the quantum wells (QWs) leading to spatially distributed eigenstates and an artificial and controlled formation of the so-called minibands [1–5]. Then, they appeared to be suitable for the realization of the infrared lasers based on the quantum cascade concept. The quantum cascade lasers (QCLs) [6] based on low dimensional semiconductor structures, *e.g.*, GaAs/AlGaAs multiple quantum wells or superlattices [7, 8] are considered as an important kind of light sources in the mid and far infrared region especially, which can be utilized in spectroscopy, medical, military and many other applications. One of the most important QCL applications is gas sensing, which is focused on detection of many harmful gases or substances like CO_2, NH_3, SO_x and others.

Fabrication of QCLs requires a very high precision with respect to multilayer structure of the entire device consisting of hundreds of layers of a a few nm in thickness. In particular, one has to provide procedures which allow control of the width, content [9] and carrier concentration [10] of all the barriers and quantum wells.

Modulation spectroscopy [11–16] has been proven to be a powerful tool for investigating optical properties of semiconductor structures due to a derivative spectra character and hence high sensitivity to even low intensity (oscillator strength) optical transitions. Combining the experimentally obtained information with the results of the band structure calculations allows such system quantities as the energy levels, effective masses, band gap discontinuities to be derived [17, 18]. Additionally, based on the spectra analysis such structure properties as built-in electric fields [19], the Fermi level at the surface or interfaces [20], or even the degree of strain relaxation can be determined [21].

In this work, we used photoreflectance spectroscopy to investigate optical transitions in GaAs/AlGaAs superlattice. The aim was to show that modulation spectroscopy is sensitive enough for studying the electronic structure details of such a complex quantum system and, on the other hand, can be used for verification of the growth accuracy with respect to the assumed design or the repeatability of the multilayer growth.

2. Experimental details

In order to measure the PR spectra the so-called bright configuration of the setup has been used [15]. Light from a halogen lamp was reflected off the sample and then came through a single-grating 0.55 m focal-length monochromator and was detected by a silicon photodiode. The pump beam was provided by an Ar ion laser (514.5 nm line) and mechanically chopped at a frequency of 275 Hz. Phase sensitive detection of the normalized reflectivity changes was performed using a lock-in amplifier.

The undoped test heterostructure was composed of the SL region placed on about 1 μm thick GaAs buffer layer, and capped by a 5.5 nm thick GaAs layer. The SL was built of the 100 periods of 1.1 nm $Al_{0.45}Ga_{0.55}As$/8.1 nm GaAs double layer. The sample was grown by molecular beam epitaxy (MBE) in the Riber Compact 21T machine. The solid elemental sources (SS) were used. The molecular beams of group III elements were generated from the standard ABN 80 DF (Double Filament) effusion cells, filled with the ultrapure metals: Al 6.5N, Ga 7N. Arsenic was emitted as As_4 molecules, from the valved cracking cell. Heterostructures were deposited on the nominally (100) oriented GaAs substrates, delivered by AXT Inc. Temperature of the crystalline surface (T_s) during the growth process was controlled by a pyrometer, and had a constant value of 580 °C. Processes of epitaxy were controlled automatically, by computer procedures, while the temperatures of effusion cells as well as the substrate were controlled by the system of thermocouples and the Eurotherm controllers.

The superlattice region was deposited continuously, *i.e.*, without any interruptions of epitaxy process, between the adjacent layers. The gallium molecular flux ensured a constant growth rate of $V_{\mathrm{GaAs}} = 0.5$ ML/s. The appropriate aluminum flux was adjusted to obtain the $Al_{0.45}Ga_{0.55}As$ composition of barrier layers. The *in situ* method of growth rate measurements of the binary materials was the reflection high energy electron diffractometry (RHEED). The beam equivalent pressure values of the molecular fluces were measured by the Bayard–Alpert gauge. The purity of the reactor's environment was controlled by the quadrupol mass spectrometer as well as by the appropriately placed Bayard–Alpert gauge.

3. Experimental results and discussion

Figure 1 shows a room temperature PR spectrum for the GaAs/$Al_{0.45}Ga_{0.55}As$ superlattice investigated. Besides the oscillatory feature in the form of Franz–Keldysh oscillations at 1.42 eV related to GaAs band gap transition a number of PR resonances can be observed on the high energy side. This part of the spectrum is very complex and seems to be composed of a number of superimposing features of different lineshape and intensity.

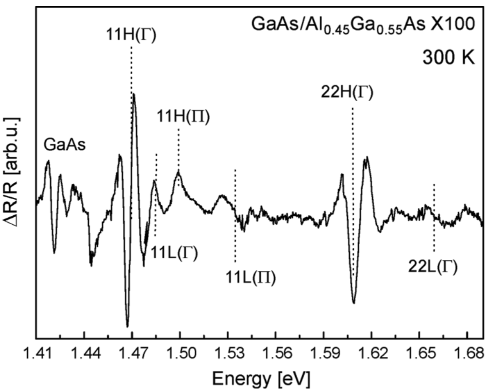

Fig. 1. Room temperature PR spectra of GaAs/AlGaAs SLs structures.

In order to resolve the possible individual spectral features the experiment has been repeated at low temperature (10 K). The corresponding spectrum is shown in Fig. 2. Due to the line narrowing and significantly improved signal to noise ratio well separated PR lines can be observed, which can be related to particular transitions in the superlattice (the feature at 1.51 eV corresponds to GaAs band gap). The spectrum has been analyzed using the third derivative functional form of the modulated spectra [11], which allowed extracting information on the transition energies. They have been labeled based on the calculations performed in the effective mass approximation formalisms and all necessary structural parameters were taken from Ref. [22]. The notation of *mn*H (*mn*L) means the transitions between the *m*-th electron state and the *n*-th heavy hole (light hole) state, symbols Γ and Π denote the transition at the respective points of the SL minibands.

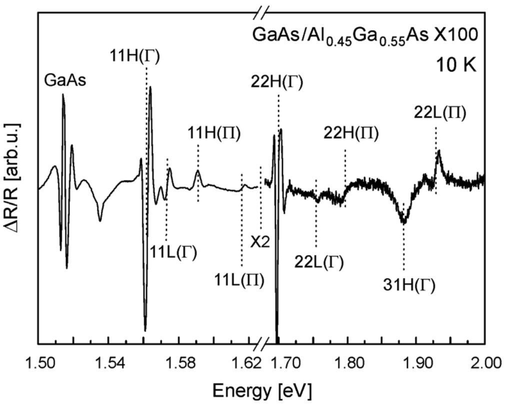

Fig. 2. The PR spectra (obtained at 10 K) of GaAs/AlGaAs SL structures.

In order to show how the calculated energies agree with the experimental ones and simultaneously verify the nominal structure parameters Fig. 3 shows the dependence of the transition energies versus the width of the separating $Al_{0.45}Ga_{0.55}As$ barrier (changed by 0.5 nm to 1.5 nm). The solid lines correspond to transitions involving heavy hole states, whereas the dashed lines to transitions associated with the light holes. The squared symbols represent the experimental data for the nominal barrier layer thickness of 1.1 nm (full symbols for the heavy hole related transitions and open ones for the light hole related transitions). Additionally, transitions between the bottom and top edges of the minibands are denoted by Γ and Π, respectively. As can be seen, a very good agreement between the theory and experiment has been achieved. This agreement made it possible to confirm the structural superlattice details (assumed in the growth process and measured X-ray diffraction). As the barrier thickness is

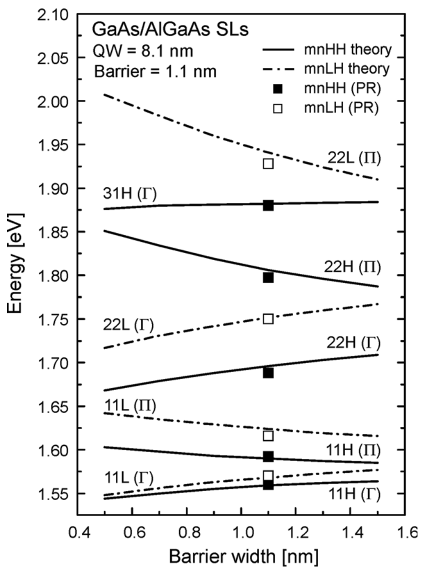

Fig. 3. The calculated energies of optical transitions for GaAs/AlGaAs SLs structures. The energies associated with heavy hole levels (solid black lines), the energies associated with light holes levels (black dashed lines). The energies taken from the analysis of PR spectra (black and white squares).

a parameter that most strongly affects the optical transition energies further tuning of other quantities such as QW width or barrier composition has not given any significant improvement with respect to the experimental values.

The results obtained not only prove the precision of design and growth calibration but show a high uniformity over the 100 SL periods. No fingerprints of the significant thicknesses or content dispersion could be observed in the PR spectra (for instance, the line broadening for the lower energy transitions is about 2–3 meV at low temperature).

4. Conclusions

A $GaAs/Al_{0.45}Ga_{0.55}As$ superlattice has been optically investigated by means of modulation spectroscopy. The PR spectra allowed detection of a number of transitions which based on the band structure calculations have been identified and proven to involve heavy and light hole states at both miniband edges. Based on these results the structural parameters could be verified and high superlattice uniformity confirmed between the periods. Such an analysis could be possible due to the enhanced sensitivity of the modulation technique in contrast to typically expected probing of the lowest energy transitions by common photoluminescence.

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