Energy-level structure of two-dimensional electrons confined at the $Al_xGa_{1-x}As/GaAs$ interface studied by photoluminescence excitation spectroscopy

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The electronic structure of one-sided modulation-doped n-channel $Al_xGa_{1-x}As/GaAs$ heterostructures has been studied by photoluminescence excitation spectroscopy in samples with a narrow (≈ 500 Å) active GaAs region. The excited two-dimensional (2D) electron states are observed optically at 2 K, and 2D hole quantization is also found to be important for the structure investigated. Theoretical calculations including exciton effects show good agreement with the experimental data.

I. INTRODUCTION

Recombination of confined carriers at an $Al_xGa_{1-x}As/GaAs$ heterostructure interface has recently been investigated by conventional photoluminescence (PL) spectroscopy.[1-12] The properties of the observed PL bands from single $Al_xGa_{1-x}As/GaAs$ heterojunctions, the so-called H bands,[1,12] are found to be very sensitive to the design of the sample and the experimental conditions. The variations of, e.g., the line shape, spectral position, and decay times of the H bands are considerable. Detailed studies from stationary and time-resolved PL measurements have proven that the two H bands observed for n-channel heterojunctions involve the recombination between confined two-dimensional (2D) electrons at the $Al_xGa_{1-x}As/GaAs$ interface and holes which are either in the valence band of the active GaAs layer or bound to acceptors in the active GaAs layer.[1,6,12] A recent study has explained that the observed large variation of the properties of the H bands is mainly due to the corresponding variation in the potential across the active GaAs layer.[12]

In this paper we present new results for the electronic structure of $Al_xGa_{1-x}As/GaAs$ heterojunctions from photoluminescence excitation (PLE) spectroscopy. In these measurements excited 2D electron states are clearly observed at 2 K. An interesting result is that the holes are also found to be quantized because the band bending across the ~ 500-Å-wide active GaAs layer reduces substantially the effective range for the hole confinement by the inverted interface. PLE data clearly show two strong excitonic transitions between the first excited 2D electron state in the potential notch and the first heavy-hole or light-hole (hh, lh) states. It appears that the general results reported here for the excited states are consistent with excitonic spectra reported earlier for much narrower modulation-doped quantum wells (QW's).[13-15] Theoretical calculations at the present sample structures show good agreement with the experimental data.

II. SAMPLES AND EXPERIMENTAL PROCEDURE

The samples used in this study are grown by molecular-beam epitaxy (MBE) on semi-insulating GaAs substrates, followed by a ten-period AlAs/GaAs superlattice (SL), an undoped GaAs layer with thickness d, a 20-nm undoped $Al_{0.35}Ga_{0.65}As$ spacer layer, an 80-nm Si-doped (10^{18} cm^{-3}) $Al_{0.35}Ga_{0.65}As$ layer, and finally a 5-nm GaAs cap layer. The 2D electrons are confined in the notch potential at the interface between the undoped GaAs ($p \approx 10^{15}$ cm^{-3}) and the $Al_{0.35}Ga_{0.65}As$ spacer layer. The results shown below are from three samples: sample 1 and sample 2 have $d=50$ nm, and sample 3 has $d=60$ nm. Other parameters are the same for all three samples.

A conventional PL setup was used. The samples were mounted in a liquid-He bath cryostat, in which the temperature could be regulated down to 1.5 K. A tunable Spectra Physics Sapphire: Ti solid-state laser, which covers the wavelength range from 700 to 1000 nm, was used as excitation source to measure the PLE spectra. A double-grating monochromator and a GaAs photomultiplier tube were used to disperse and detect the PL signals.

III. EXPERIMENTAL RESULTS

Figure 1 shows a typical PL spectrum from sample 1 measured with moderately low excitation intensity (3×10^{-2} W cm^{-2}). The PL spectrum is dominated by the GaAs emissions originating from the substrate, which are due to the free and bound excitons, free to bound (FB), and donor-acceptor (DA) pairs. The band between the excitons and the FB emission, the so-called H band 1 (HB1), is related to the recombination of the 2D electrons confined at the $Al_xGa_{1-x}As/GaAs$ interface,[1,6,12] more

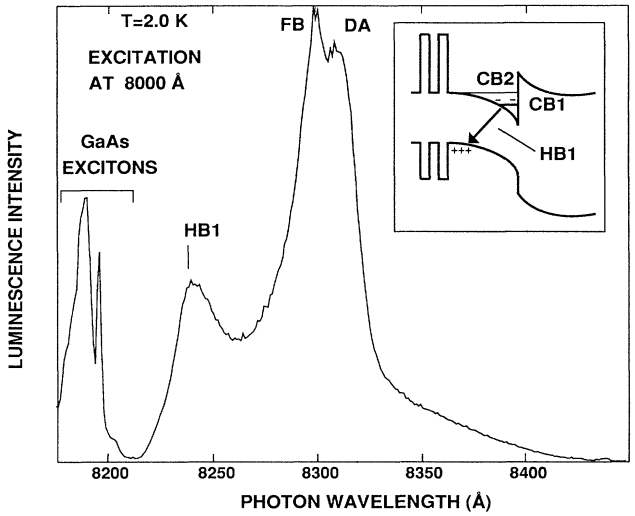

FIG. 1. PL spectrum of sample 1 measured at 2 K, with the laser excitation at 1.549 eV, and an excitation intensity of 3×10^{-2} W cm^{-2}. The peak HB1 at 1.504 eV originates from the recombination between confined electrons in the 2D potential and holes from the GaAs valence band in the active region (see inset).

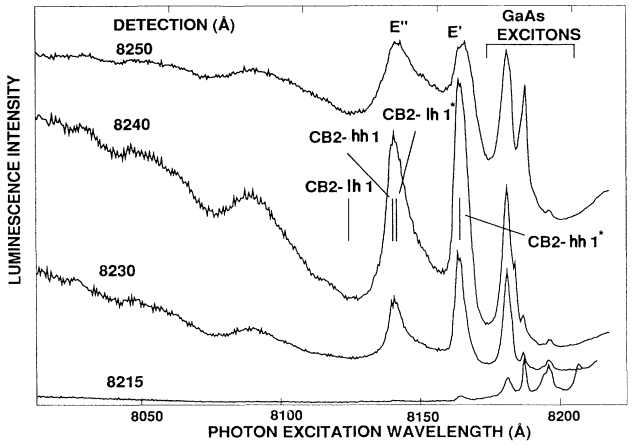

FIG. 2. PLE spectra of the same $Al_xGa_{1-x}As/GaAs$ heterojunction as shown in Fig. 1 measured at 2 K, with different detection energies resonant with and close to HB1. The vertical lines indicate theoretically calculated transition energies, which are described in the text.

specifically recombination between 2D electrons in the potential notch and holes in the GaAs valence band (see inset in Fig. 1). The intensity and energy position of HB1 are both dependent on the excitation intensity and excitation photon energy.[1,12]

Only the 2D electron ground state is populated at low temperature in these samples. Thus it is not possible to observe excited electron states confined in the interface potential in PL at low temperature. The higher states can only be observed at elevated temperatures, when they get thermally populated, but unfortunately PL spectra at elevated temperatures always show strong broadening effects. However, with PLE measurements, the empty 2D states can be detected even at temperatures as low as 2.0 K. Figure 2 shows typical PLE spectra of an *n*-channel $Al_xGa_{1-x}As/GaAs$ heterojunction from sample 1 at 2 K, for various detection photon energies. The excitation intensities are kept almost constant within the energy range of the scanning laser, and are about the same as used to measure the PL spectrum in Fig. 1. Two well-defined peaks, labeled E' and E'', are seen in the PLE spectra shown. These peaks (E' and E'') are related to the HB1 band in the PL spectrum, since they gradually disappear when the detection energy is shifted away from the peak position of HB1 (at 8240 Å) (see Fig. 2). This relation is clearly demonstrated in Fig. 3, where the peak intensities of the E' and E'' are plotted against the detection photon energy.

Additional structure is observed in the PLE spectra at higher energy (1.52–1.55-eV region in Fig. 2). We interpret these features as being higher excited states, i.e., confined states of the electrons and holes in the distorted potential across the 500-Å GaAs layer. For a detailed identification of these weaker features, further experimental investigations and theoretical work are needed.

Selective photoluminescence (SPL) spectra have also been measured to study the correlation between the E' and E'' peaks and the HB1 band. When the excitation energy is resonant with the E' and E'' peaks, an enhancement of the HB1 band emission is clearly seen, as expected from Fig. 3.

The emission HB1 (for convenience, in the following denoted as E^0) in *n*-channel heterojunction samples of the kind studied in this work has been suggested as originating from the recombination between 2D electrons in their ground state and holes in the active GaAs region.[1,6,12] Based on our established relation between the E' and E'' peaks and HB1, it is clear that the E' and E'' peaks are

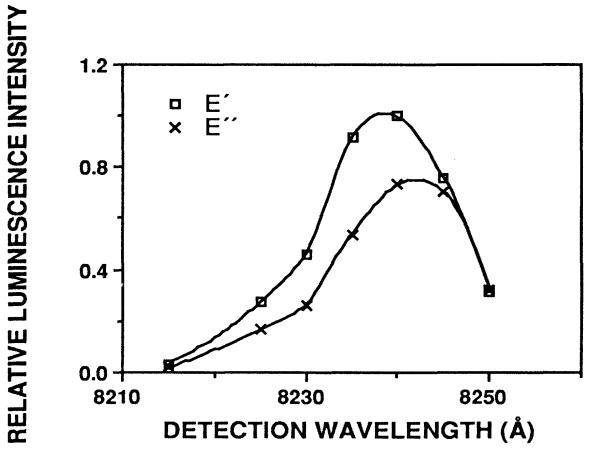

FIG. 3. The intensity of the peaks E' and E'' in the PLE spectrum as a function of detection energy.

the excited states of the HB1 emission. By combining the PLE and PL data, detailed information on the electronic energy levels in the interface potential can be obtained. The energy separation between the excited-state peak E' and the ground-state peak E^0 (HB1) is about 16 meV, while the distance between the two excited states E' and E'' is about 4.53 meV at an excitation intensity of 3×10^{-2} W cm^{-2} for sample 1. We found that those energy separations depend on the experimental conditions, e.g., excitation intensity. The energy separation between the E' peaks and the ground state E^0 ($E'-E^0$) depends more strongly on the excitation intensity, and is found to vary in the range from 12 to 18 meV, the corresponding separation between the E' and E'' peaks is found to vary in the range from 4.2 to 4.8 meV, when the excitation intensity is decreased about 1 order of magnitude. All peaks E^0, E', and E'' shift to higher energy with increasing excitation intensity, a behavior similar to the previous results for E^0 in narrower modulation-doped QW's.[16]

IV. DISCUSSION AND COMPARISON WITH THEORETICAL CALCULATIONS

To explain the origin of the PLE peaks of E' and E'', theoretical calculations have been done by using the effective-mass approximation and a realistic potential for the 500-Å active GaAs layer. The Schrödinger equation for the electron is

$$\left[\frac{-\hbar^2}{2m_e}\frac{\partial^2}{\partial z^2}+V_e(z)\right]\psi_{ie}(z)=E_{ie}\psi_{ie}(z)\ , \tag{1}$$

where

$$V_e(z)=E_c(z)-eU(z) \tag{2}$$

and

$$\nabla^2U(z)=-\frac{e}{\epsilon}\left[N(z)-\sum_i N_i|\psi_{ie}(z)|^2\right]\ . \tag{3}$$

Here m_e is the effective mass of the electron, $V_e(z)$ is the electron potential, $E_c(Z)$ is the conduction-band offset at the interface, and ϵ is the dielectric constant. $\psi_{ie}(z)$, E_{ie}, and $U(z)$ are determined by solving Eqs. (1), (2), and (3) self-consistently. The calculated results may be affected by the band-gap renormalization.[13,14,17] However, according to Ando,[18] in our case this effect is small and so has been ignored in the calculation. After the determination of $U(z)$, the Schrödinger equation for light or heavy holes can be written as

$$\left[\frac{-\hbar^2}{2m_h}\frac{\partial^2}{\partial z^2}+V_h(z)\right]\psi_{ih}(z)=E_{ih}\psi_{ih}(z)\ , \tag{4}$$

where

$$V_h(z)=E_v(z)+eU(z)\ . \tag{5}$$

Here $E_v(z)$ is the valence-band offset at the interface. Once these electron and hole Schrödinger equations have been solved, the optical transition energies and the energy reduction from exciton effects can be calculated.

The parameters used in the calculation are shown in Table I. $e\partial U/\partial z|_{Z=d}$ is an adjustable parameter to give the best fit to the transition energy from the first 2D electron state (CBn, $n=1$) to the first heavy-hole state (hh$n$, $n=1$) measured by PL. From the carrier concentration N_s, we find a very small Fermi circle around $k=0$ in the second 2D electron state (CB2). In this case the k-dependence of the exciton binding energy is very weak[19] and can be neglected. The so-obtained transition energies between different states are marked by vertical lines in Fig. 2. The CB2-lh1 (or CB2-hh1) line denotes the transition from the second 2D electron state to the first light-hole (or first heavy-hole) state, without exciton effects. When exciton effects are taken into account, the corresponding transitions are CB2-lh1* and CB2-hh1*. Our calculation also suggests that the E^0 PL peak is due to the transition from the first 2D electron state to the first (light and heavy) hole state, in agreement with the generally accepted interpretation. The calculation also shows that the separation of CB2-CB3 is about 10 meV, which is much larger than the separation of E''-E' (4.5 meV). Based on these results we believe that the peaks E'' and E' are both related to the second 2D electron state (CB2).

Sample 2 and sample 3 are fabricated under the same growth condition, but have different thickness of the active GaAs layer (500 and 600 Å, respectively). Hence, if the same experimental conditions are imposed on both samples, and the same parameter values are used to calculate the transition energies in both samples, then the

TABLE I. Parameters used to calculate the 2D optical transition energies.

		Sample 1	Sample 2	Sample 3
d (nm)		50	50	60
$e\frac{\partial U}{\partial z}\Big\|_{Z=d}$	(eV/Å)	1.65×10^{-5}	1.65×10^{-5}	1.65×10^{-5}
N_s (cm^{-2})		5×10^{11}	4.8×10^{1}	4.8×10^{11}
	Effective mass	$m_e=0.067+0.083x(m_0)$		
		$m_{hh}=0.353+0.05x(m_0)$		
		$m_{lh}=0.08+0.098x(m_0)$		
	Band gap	$E_g(Al_xGa_{1-x}As)=E_g(GaAs)+1.247x$ (eV)		
	Dielectric constant	$\epsilon=13.2\epsilon_0$		
	Band offset coefficient	$Q=0.65$		

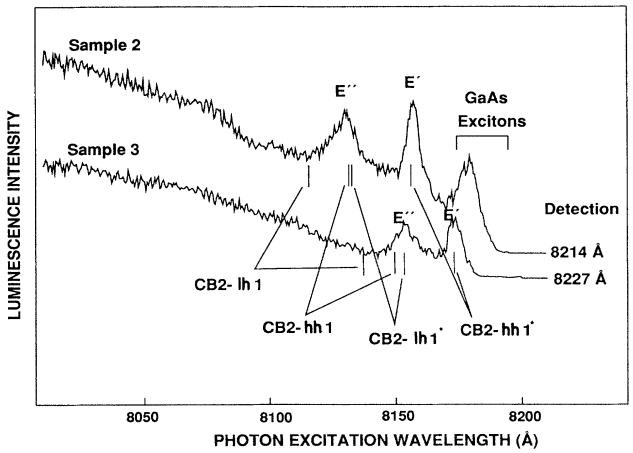

FIG. 4. PLE spectra of sample 2 and sample 3 measured at 2 K. The vertical lines indicate the transition energy positions from the theoretical calculations as described in the text.

degree of agreement between the measurement and the calculation should also be the same for both samples. This is indeed the case as shown in Fig. 4.

Theoretical calculations also show that the variation of the optical transition energy corresponding to the E^0 emission with the changes of 2D carrier concentration and potential across the active GaAs layer is much more sensitive than those corresponding to the E' and E'' peaks. This is consistent with the experimental results about the excitation intensity dependence of the energy separations E'-E^0 and E''-E', which was mentioned earlier.

An interesting result of this work is the observed importance of the electron-hole interaction (excitons) in excitations involving excited electron and hole states in a 500-Å modulation-doped heterojunction. From the experimental data in this work it is concluded that exciton effects are weak for the lowest *e-h* transition in the present sample structure which corresponds to a 500-Å one-side modulation-doped QW, while the transitions involving the first excited electron state in the notch show quite dominating exciton effects in the optical spectra. This is also in full agreement with the theoretical calculations of the exciton effects in different transitions performed in the present work.

V. SUMMARY AND CONCLUSIONS

In summary we have observed the 2D excited states in single modulation-doped $Al_xGa_{1-x}As$/GaAs heterojunctions with a thickness of the GaAs layer up to 600 Å at 2 K by using the PLE technique. The energy separations between the ground state and different excited states have been accurately obtained. Two distinct excitonic excited states are found, which are related to the transition between the first excited 2D electron sublevel and the first heavy-hole–light-hole level in the active GaAs layer. This is to our knowledge the largest spatial separation between electrons and holes for which excitonic states have been observed. Theoretical calculations show good agreement with experimental data when exciton effects are considered in the calculation of the optical transition to excited states. The so-determinated excited energy levels in a 2D potential provide a useful reference for more accurate theoretical calculations of the notch potential and electronic wave functions.

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