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Electric subbands in a both-side-modulation-doped $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As$ single quantum well

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Abstract. Shubnikov–de Haas and Van der Pauw Hall effect measurements on an $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As$ lattice-mismatched single quantum well grown by molecular beam epitaxy have been carried out to investigate the electrical properties of an electron gas and subband energies in a unique potential well. The measurements at 1.5 K have demonstrated clearly the existence of a quasi-two-dimensional electron gas in the quantum well. It is found that three subbands in the quantum well are occupied. Electron energy subbands in the quantum well were calculated by a self-consistent method taking into account exchange–correlation effects and making use of the experimentally determined carrier density.

The $In_yAl_{1-y}As/In_xGa_{1-x}As$ heterojunction has attracted increasing interest as a high-speed transistor material because of its high electron mobility at room temperature [1]. Even if a two-dimensional electron gas (2DEG) has led to very significant enhancement in mobility at low temperatures in $Al_xGa_{1-x}As/GaAs$ heterostructures [2], the modulation-doped $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ structures grown by molecular beam epitaxy (MBE) [3] have made it possible to apply this material to a high-electron-mobility transistor (HEMT) for room-temperature operation as a consequence of the small energy gap and effective mass of $In_xGa_{1-x}As$.

Recently, hereterojunctions using $In_xGa_{1-x}As$ and $In_yAl_{1-y}As$ almost lattice matched to InP have become very important not only as optoelectric and high-speed electronic devices [4] but also for the investigation of basic physics at heterointerfaces [5, 6]. So far, although the electrical transport properties characterizing device performance such as saturation velocity [5] have been reported, most investigations were carried out on samples of $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ [7–9]. However, to our best knowledge, no results on the magnetotransport measurements of a strained $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As$ single quantum well with three electric subbands have been reported yet [7, 10]. Hong *et al* [10] published details of the growth and characterization of pseudomorphic $In_{0.52}Al_{0.48}As/In_xGa_{1-x}As$ ($x > 0.53$) modulation-doped heterostructures, but clear subband energy calculations were not performed. Thus, in this study, Shubnikov–de Haas (SDH) and Van der

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Pauw Hall effect measurements at 1.5 K were performed on a both-side-modulation-Si-doped $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As$ single quantum well to investigate the properties of a 2DEG, and a self-consistent calculation of the subband structure in the well using these experimental results was carried out.

The MBE-grown sample used in this work had the following layer sequence: an Si-doped $In_{0.52}Al_{0.48}As$ capping layer ($t = 200$ Å, $n = 3 \times 10^{18}$ cm^{-3}); an undoped $In_{0.52}Al_{0.48}As$ layer ($t = 400$ Å); a Si-doped $In_{0.52}Al_{0.48}As$ layer ($t = 200$ Å, $n = 3 \times 10^{18}$ cm^{-3}); an undoped $In_{0.52}Al_{0.48}As$ spacer layer ($t = 150$ Å); an undoped $In_{0.65}Ga_{0.35}As$ layer ($t = 300$ Å); an undoped $In_{0.52}Al_{0.48}As$ spacer layer ($t = 100$ Å); an Si-doped $In_{0.52}Al_{0.48}As$ layer ($t = 100$ Å, $n = 3 \times 10^{18}$ cm^{-3}); an undoped $In_{0.52}Al_{0.48}As$ buffer layer ($t = 0.3$ μm); 30 periods of $[In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As]$ superlattice buffer layers; and an Fe-doped semi-insulating InP (100) substrate. All the layers were grown at 450 °C. A 2DEG is confined in the $In_{0.65}Ga_{0.35}As$ which is separated by the two spacer layers from the nearest ionized donors in the $In_{0.52}Al_{0.48}As$. Ohmic contacts to the samples were made by diffusing a small amount of indium through several layers. The SDH and Hall effect measurements were carried out at 1.5 K using a Keithley 224 constant-current source, a Keithley 181 nanovoltmeter and an Oxford superconducting magnet with a maximum magnetic field of 12 T.

Results of the SDH measurements on the $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As/In_{0.52}Al_{0.48}As$ single quantum well are shown in figure 1. These SDH measurements clearly show multiple oscillation periods, indicative of the occupation of several subbands by a 2DEG in the quantum well. The SDH results vary dramatically with the angle between the magnetic field and the surface normal. Since the oscillation patterns were too complicated to plot the slope of the reciprocal magnetic fields versus the oscillation peak number, the oscillation frequencies of the various subbands were obtained by digitizing the data linearly with the inverse of the magnetic field and fast Fourier transformation (FFT) of the SDH data by the computer. After the FFT had been carried out, the resulting data were expressed as a curve of arbitrary amplitude versus frequency as shown in figure 2. Peaks were observed at 12.5 T, 25 T and 30.5 T corresponding to 6.05×10^{11} cm^{-2}, 1.21×10^{12} cm^{-2} and 1.48×10^{12} cm^{-2} for the second, first and zeroth subbands, respectively, giving a total electron density of $(3.3 \pm 0.2) \times 10^{12}$ cm^{-2}. Van der Pauw Hall effect measurements at 1.5 K at a magnetic field of 0.5 T yield an electron density of $(3.5 \pm 0.2) \times 10^{12}$ cm^{-2}. Considering the combined uncertainties in the non-ideal geometry of the sample contacts, finite size contacts and determination of the SDH oscillation frequencies from the complex pattern, this is reasonably good agreement.

Using these experimental results, a possible schematic band diagram of the distribution of carriers in an $In_yAl_{1-y}As/In_xGa_{1-x}As$ single quantum well including energy eigenvalues and eigenfunctions was self-consistently calculated as shown in figure 3. A model structure used in the calculation is considered to have the following properties.

(1) The donor impurities are uniformly doped in semi-infinite $In_yAl_{1-y}As$ layers except in the region of the spacer layer, and electrons are released from the donor impurities to the quantum well.

(2) Any residual impurities in the spacer and the well are not taken into account, so that the number of electrons in the subbands is assumed to be equal to the number of ionized donors.

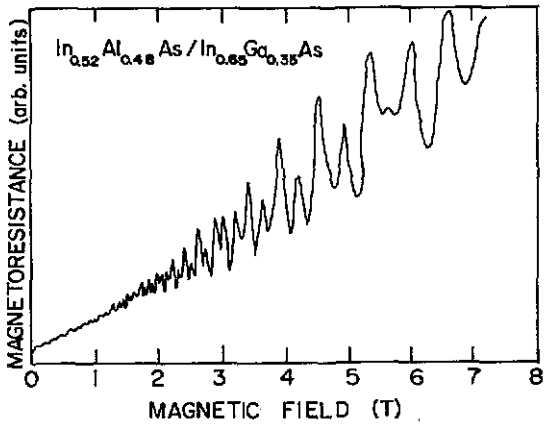

Figure 1. SDH measurements on $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As$ at 1.5 K.

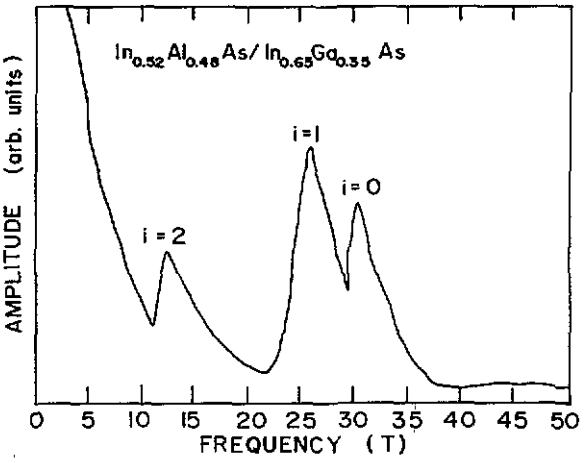

Figure 2. FFT analyses of the SDH measurements for $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As$. i is the subband index.

(3) The calculated results of the subband energy levels and the Fermi level are sensitive to the number of charges transferred from donors in the $In_yAl_{1-y}As$ to the $In_xGa_{1-x}As$ well. All the donor states with energies above the Fermi level are assumed to be ionized. Hence, the number of electrons transferred from the donor impurities to the quantum well can be determined in a self-consistent manner by the condition that the Fermi level is equal to the energy of an electron bound to a donor in the barrier layer where the effective potential profile is flat. Since the areal electron density is known experimentally, the energy difference between the conduction band edge of the barrier and the Fermi level can be calculated.

(4) The electron density is high enough that the effect of the electron screening reduces the exciton binding energy to zero, and conduction subband energies can be considered separately from those of the valence subbands.

(5) Non-parabolicity in the conduction band is not taken into account in the calculation.

In the effective-mass approximation, the envelope function of confined states in

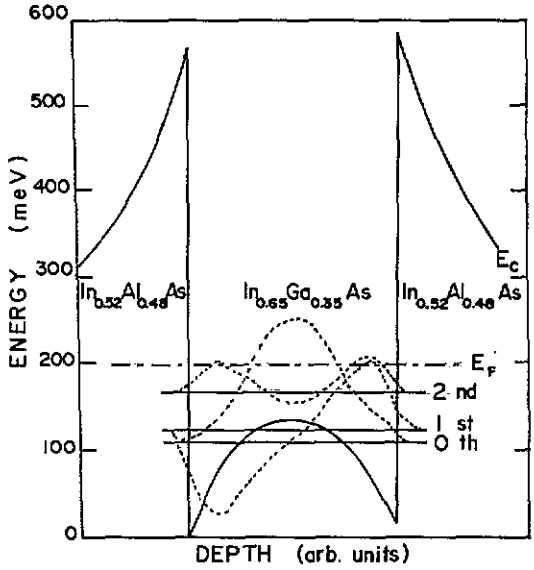

Figure 3. Subband structure of $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As$ determined by a self-consistent method: ——, electric subband energy; – – –, energy eigenfunctions. The quantum well width is 300 Å.

quantum well structures may be represented by single-particle wavefunctions that are solutions of the Schrödinger equation. In the calculation, the band edges and the effective electron mass are assumed to change abruptly at the interfaces between two different materials. In a single quantum structure, an electron moves in a potential $V(z)$ which can be represented by

$$V(z) = V_b(z) + V_H(z) + V_{xc}(z) \tag{1}$$

where $V_b(z)$ is the potential energy associated with the band-gap mismatch at the heterointerfaces, $V_H(z)$ is the electrostatic (Hartree) potential due to a donor deposited in the barrier material and to other conduction electrons, and $V_{xc}(z)$ is the exchange–correlation potential energy which is due to the many-body effects not included in the Hartree potential. The electrostatic potential V_H satisfies the Poisson equation. The dielectric constant is assumed to have the same value in both the barrier and the well. The exchange–correlation potential energy V_{xc} calculated in the local-density approximation, has been parametrized in several ways [11, 12]. In this calculation, an analytic form introduced by Hedin and Lundqvist [13] is used for V_{xc}:

$$V_{xc} = -[1 + 0.7734\chi \ln(1 + \chi^{-1})](2/\pi\alpha\gamma_s)Ry^* \tag{2}$$

where $\alpha = (4/9\pi)^{1/3}$, $\chi \equiv \chi(z) = \gamma_s/21$, and the effective Rydberg constant is given as $Ry^* = e^2/8\pi\epsilon_0\epsilon a^*$. The parameter r_s is defined in three dimensions as the radius of a sphere containing an electron, in units of the effective Bohr radius a^*:

$$r_s \equiv r_s(z) = [4/3\pi a^{*3} n(z)]^{-1/3} \tag{3}$$

where $a^* = 4\pi\epsilon_0\epsilon\hbar^2/m_e^{*2}$, and m_e^* is the effective mass of an electron in the $In_xGa_{1-x}As$ layer. The dielectric constant ($\epsilon = 13.7$) is assumed to be the same in

both the barrier and the well, while the band edges and the effective electron mass are considered to change abruptly at the interfaces. The potential barrier between $In_{0.52}Al_{0.48}As$ and $In_{0.65}Ga_{0.35}As$ is assumed to be 0.586 eV [14]. The values of the effective masses are taken as m_e^* ($In_yAl_{1-y}As$) = $[0.15(1-y)+0.023y]m_e$ and m_e^* ($In_xGa_{1-x}As$) = $[0.0665(1-\chi)+0.023\chi]m_e$ [14]. In the numerical procedure, iterative calculations of the subband energies, wavefunctions, subband electron densities, Fermi level and new potential are performed until self-consistency between these quantities is achieved. Since calculated subband energy levels and carrier densities in the potential well are sensitive to various parameters such as barrier height, effective mass and dielectric constant, the exchange–correlation effects are significantly affected when determining the energy levels and carrier concentrations. As a criterion of self-consistency, the mean deviation between the new calculated potential energy from the old potential energy is chosen to be less than 0.1 meV.

In the modulation-doped $In_yAl_{1-y}As/In_xGa_{1-x}As$ quantum well sample, three subbands are found to be occupied at $T = 0$ K when 3.3×10^{12} electrons cm^{-2} are assumed to fill the $In_xGa_{1-x}As$ channel. On the assumption also that all the donor impurities ($N_d = 3.0 \times 10^{18}$ cm^{-3}) with energies above the Fermi level are ionized and transfer electrons to a quantum well, a doping layer of only 55 Å width in each side is depleted and the self-consistent potential is still symmetric. Consequently, subband wavefunctions are either symmetric or antisymmetric. In this case, one half of the quantum well domain is sufficient for the numerical calculation. The calculated subband energies from the band edge potential in the centre of the quantum well are −23 meV, −17 meV and 35 meV and the corresponding electron densities are 1.44×10^{12} cm^{-2}, 1.35×10^{12} cm^{-2} and 0.51×10^{12} cm^{-2} for the zeroth, first and second subbands, respectively. It is also noted that the Fermi level is located 67 meV above the reference energy, and the potential energy at the interface of the $In_xGa_{1-x}As$ layer is −129 meV. The comparison between the experimental and theoretical data of subband electron densities shows good agreement, within 10%. The small deviation may be due to effects including residual impurities which are not considered in the calculation. The potential profile, the wavefunctions of two subbands from the bottom, their energies and the Fermi level are also plotted in figure 3.

In summary, SDH and Hall effect measurements at 1.5 K have demonstrated clearly the existence of the 2DEG in an $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As/In_{0.52}Al_{0.48}As$ single quantum well. From the FFT of the SDH data, three electron densities were identified which indicated the occupation of three subbands in the well. Using the experimental results, the electric energies and energy wavefunctions in the well with three subbands were determined by a numerical self-consistent method. Although some details including optical studies on the well remain to be carried out, these observations have possibly interesting device implications such as an $In_yAl_{1-y}As/In_xGa_{1-x}As$ FET.

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