Electric subbands in an $In_{0.65}Ga_{0.35}As$ quantum well between $In_{0.52}Al_{0.48}As$ and $In_{0.53}Ga_{0.47}As$ potential barriers

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Shubnikov–de Haas and Van der Pauw Hall-effect measurements on $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As/In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ quantum wells grown by molecular-beam epitaxy have been carried out to investigate the electrical properties of an electron gas and to determine the subband energies and wave functions in a potential well. Shubnikov–de Haas measurements have demonstrated the existence of a quasi-two-dimensional electron gas in the $In_{0.65}Ga_{0.35}As$ potential well between the $In_{0.52}Al_{0.48}As$ and $In_{0.53}Ga_{0.47}As$ barriers. With use of these experimental results and a self-consistent numerical method, the electric subband energies and energy eigenfunctions were determined.

I. INTRODUCTION

Recently, with rapid advances in epitaxial-growth technologies in molecular-beam epitaxy (MBE) and metalorganic chemical vapor deposition, it has become possible to fabricate complicated structures with high-quality epitaxial films.[1–3] Many investigations have been performed on field-effect transistor[4,5] (FET) and semiconductor lasers[6] using lattice-matched and strained quantum wells of $In_xGa_{1-x}As$, but very few studies on basic physical properties have been carried out. Although the basic physical principles for such structures have already appeared in graduate-level texts for many years,[7] the corresponding experimental results have not yet been performed because of problems encountered in the growth techniques. However, rapid advancements in epitaxial-film-growth technology have made possible studies of the two-dimensional electron gas (2DEG) of variable density and relatively high mobility in quantum wells.

Recently, $In_yGa_{1-y}As/In_xAl_{1-x}As$ systems have been used not only as optoelectric and high-mobility electronic devices,[8] but also for the investigation of fundamental physics at heterointerfaces.[9,10] Since $In_{0.53}Ga_{0.47}As$ is closely lattice matched to $In_{0.52}Al_{0.48}As$ and InP, high-quality strain-free $In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ layers can be grown in semi-insulating Fe-doped InP substrates. Although several groups[4,5,11] have investigated and sought to improve device performance in FET's fabricated with lattice-mismatched modulation-doped heterostructures, to our best knowledge, a clear experimental determination of subband energies and energy eigenfunctions in such a complex structure as $In_{0.52}Al_{0.48}As/In_{0.65}Ga_{0.35}As/In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As$ has not been reported to date. Thus, in this paper, Shubnikov–de Haas (SdH) and Van der Pauw Hall-effect measurements were carried out to investigate the electrical transport properties in a MBE-grown pseudomorphic lattice-mismatched and lattice-matched modulation-doped $In_xAl_{1-x}As/In_yGa_{1-y}As$ quantum well. Furthermore, with these experimental results, the electric subband energies and energy wave functions have been determined by a self-consistent numerical method.

II. EXPERIMENTAL DETAILS

The $In_xAl_{1-x}As/In_yGa_{1-y}As$ samples used in this study were grown on Fe-doped semi-insulating (100) InP substrates by MBE in the following layer structure: a Si-doped $In_yGa_{1-y}As$ capping layer ($y=0.53$, $t=200$ Å, $n=3\times10^{18}$ cm^{-3}), an undoped $In_xAl_{1-x}As$ layer ($x=0.52$, $t=400$ Å), a Si-doped $In_xAl_{1-x}As$ layer ($x=0.52$, $t=200$ Å, $n=3\times10^{18}$ cm^{-3}), an undoped $In_xAl_{1-x}As$ spacer layer ($x=0.52$, $t=100$ Å), an undoped $In_yGa_{1-y}As$ layer ($y=0.65$, $t=150$ Å), an undoped $In_yGa_{1-y}As$ layer ($y=0.53$, $t=400$ Å), an undoped $In_xAl_{1-x}As$ layer ($x=0.52$, $t=0.3$ μm), and a 30-period $[In_xAl_{1-x}As$ $(x=0.53)]/[In_yGa_{1-y}As$ $(y=0.53)]$ superlattice buffer layer. The SdH and Hall-effect measurements were carried out at the temperature of 1.5 K in magnetic fields up to 12 T in an Oxford Super-

conducting magnet system using a dc technique in conjunction with a Keithley 224 current source and a Keithley 181 nanovoltmeter.

III. RESULTS AND DISCUSSION

Results of the SdH measurements on the $In_xAl_{1-x}As/In_yGa_{1-y}As$ samples are shown in Fig. 1. Figure 1 shows the magnetoresistance as a function of the magnetic field applied perpendicular to the sample surface. These SdH results show complicated patterns, indicative of the occupation of several subbands by a 2DEG. The 2DEG concentrations were obtained by carrying out a fast Fourier transform (FFT) of the SdH data on a computer. The resulting data points can be expressed as a curve of amplitude versus frequency (T) as shown in Fig. 2. Peaks were observed at 7.6 and 30.8 T corresponding to electron densities of 3.68×10^{11} and 1.49×10^{12} cm^{-2} for the first and zeroth subbands, respectively, giving a total electron density of $(1.86\pm0.3)\times10^{12}$ cm^{-2}. Van der Pauw Hall-effect measurements at 1.5 K in a magnetic field of 0.5 T yield a sheet electron density of $(2.0\pm0.3)\times10^{12}$ cm^{-2}. In view of the combined uncertainties in determining the electron density from the nonideal geometry of the sample contacts, finite-size contacts, and the complex pattern of the SdH oscillations, the agreement between those two results is good.

Although the electrons may contribute to the conduction layer with a complicated confinement potential well and the shapes of the potential well may be quite complicated, a quantitative measure of the energy eigenvalues and eigenfunctions can be obtained by considering the experimental results together with a self-consistent numerical calculation. In a modulation-doped $In_xAl_{1-x}As/In_yGa_{1-y}As$ quantum well, electrons are transferred from donors deposited in the $In_xAl_{1-x}As$ layer to the $In_yGa_{1-y}As$ layer. Band bending due to electrostatic and many-body effects, the energy levels of the confined states and areal densities of electrons in the subband can be calculated numerically in a self-consistent manner.

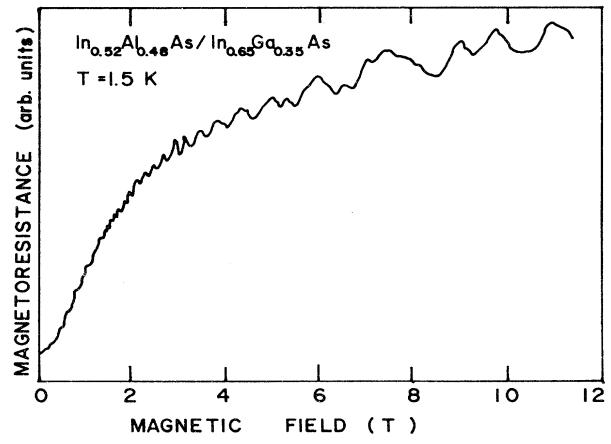

FIG. 1. Shubnikov–de Haas measurements on $In_xAl_{1-x}As/In_yGa_{1-y}As$ at 1.5 K.

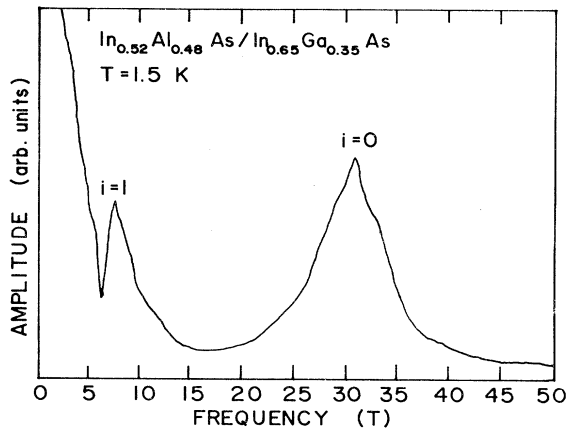

FIG. 2. FFT analysis of Shubnikov–de Haas measurements for $In_xAl_{1-x}As/In_yGa_{1-y}As$. i is the subband index.

However, the results of the calculation are quite sensitive to some less well-known quantities, such as the ionization energies of donor and other impurities. Hence, the total electron density determined experimentally is used as an input parameter to calculate subband structures of a given sample. It is also noted that the ionization energy of a donor can be calculated if the ionized-donor density in the depletion layer of $In_xAl_{1-x}As$ is known. In this calculation, all the Si donor states with energies above the Fermi level are assumed to be ionized and to release electrons to the quantum well. Other effects due to residual impurities and nonparabolicity in the conduction band are not taken into account.

In the envelope-function approximation, a 2DEG moves in a potential $V(z)$ which can be represented by $V(z)=V_b(z)+V_H(z)+V_{xc}(z)$, where $V_b(z)$ is a potential energy associated with the band-gap discontinuity at the heterointerfaces, and $V_H(z)$ is an electrostatic (Hartree) potential due to both the donors deposited in the barrier material and other conduction electrons, and $V_{xc}(z)$ is an exchange-correlation potential energy originating from many-body effects not included in the Hartree potential. The electrostatic potential $V_H(z)$ satisfies Poisson's equation. For the exchange-correlation potential energy $V_{xc}(z)$, the analytic form introduced by Hedin and Lundqvist[12] was used,

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

where $\alpha=(4/9\pi)^{1/3}$, $\chi=\chi(z)=r_s/21$, and the effective Rydberg constant is given as $\mathrm{Ry}^*=e^2/8\pi\epsilon_0\epsilon a^*$. 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^*. Both the Schrödinger equation and Poisson's equation are calculated numerically over the domain of equally spaced abscissas. When the areal electron densities in a quantum well are known, the eigenenergies and the wave functions can be solved initially with the potential $V_b(z)$. Subsequently, the Fermi energy, the Hartree potential, and the exchange-correlation potential energy due to conduction electrons are calculated with the given electron density. A new potential energy can be constructed by a mixture of the calculated potential and

the nominal old potential in appropriate proportions to avoid any nonphysical potential. With use of the new potential energy, the eigenenergies and wave functions are calculated again. This process is repeated until self-consistency in the potential energy is achieved. As a criterion of self-consistency, the mean deviation of the calculated potential energy from the nominal old potential energy was chosen to be less than 0.1 meV.

Results of numerical calculations for the conduction subbands in a $In_xAl_{1-x}As/In_yGa_{1-y}As$ structure are shown in Fig. 3. The dielectric constant ($\epsilon=13.5$) is assumed to be the same in both the barrier and the well, while the band edges and the electron effective mass are considered to change abruptly at the interfaces. Even though the band offsets are not yet well established, the height of the potential at the $In_{0.52}Al_{0.48}As/In_{0.53}Ga_{0.47}As$ interface is supposed to be 0.520 eV,[10] which is given by the conduction-band discontinuity; and 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.[13] The values of the effective masses are taken as $m_e^*(In_xAl_{1-x}As)=[0.15(1-x)+0.023x]m_e$ and $m_e^*(In_yGa_{1-y}As)=[0.0665(1-y)+0.023y]m_e$.[13] For the given electron density, the subband energies and the effective binding energy (ionization energy) of a donor impurity doped in $In_xAl_{1-x}As$ can be calculated in a self-consistent manner. Calculated subband electron densities were 3.2×10^{11} and 1.58×10^{12} cm^{-2} corresponding to the first and zeroth subbands, respectively. These values are in reasonable agreement with experiment. The small deviation may originate from effects (including residual impurities and nonparabolicity in the conduction band) not considered in this calculation. In this case, calculated values of two eigenenergies and the Fermi level from the potential bottom in the well are 119, 199, and 219 meV, respectively. The energy eigenfunctions are indicated by the dashed lines in Fig. 3.

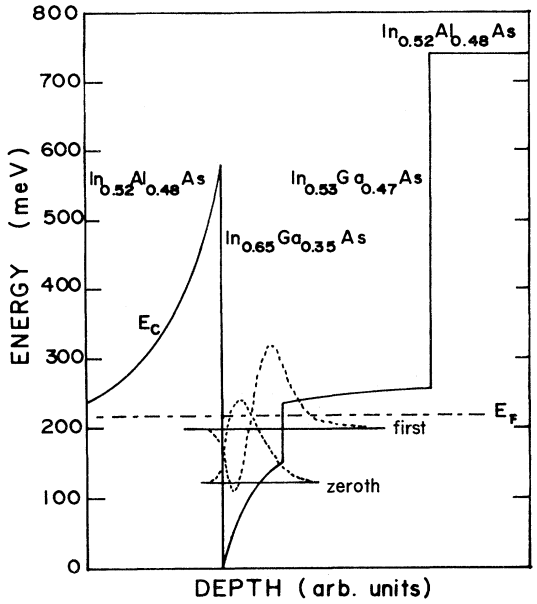

FIG. 3. Subband energy structure of $In_xAl_{1-x}As/In_yGa_{1-y}As$ determined by a self-consistent method. Solid lines indicate the electric subband energy; dashed lines, the energy eigenfunctions.

IV. SUMMARY AND CONCLUSIONS

The results of SdH and Van der Pauw Hall-effect measurement at 1.5 K demonstrate clearly the existence of a 2DEG in a $In_{0.65}Ga_{0.35}As$ potential well between $In_{0.52}Al_{0.48}As$ and $In_{0.53}Ga_{0.47}As$ barriers, and the FFT of the data shows two oscillation frequencies, indicating the occupation of two subbands in the well. Self-consistent numerical calculations show the subband energy structures in this complex potential well. Although more detailed studies on basic physical properties, including optical measurements, remain to be carried out, the present observations can help improve our understanding of these complex quantum-well structures.

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