Investigation of two-dimensional hole gases in Si/SiGe heterostructures

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Two-dimensional (2D) hole gases are investigated experimentally and theoretically in modulationdoped Si/SiGe/Si double heterostructures with both symmetric and asymmetric doping grown by the rapid thermal chemical-vapor deposition technique. Shubnikov-de Haas and quantum Hall effect measurements show unambiguously that the charge transfer is equivalent at the two interfaces in this system. The 2D hole gas effective mass parallel to the interfaces is determined by microwave photoresistivity experiments. A simple theoretical analysis of these data leads to the determination of the valence-band profile and quantitatively explains the charge transfer. The hole mobility limitation is discussed and it is shown that the alloy scattering in SiGe could be the dominant process at low temperature.

In recent years, two-dimensional (2D) hole gases in $Si/Si_{1-x}Ge_x$ heterostructures have attracted considerable attention in order to investigate the band structure, the doping profiles, and the interface quality in this technically important system. Transport measurements have been reported on high-quality p-type modulation-doped $Si/Si_{1-x}Ge_x$ heterostructures grown by molecular-beam epitaxy (MBE),¹⁻³ ultrahigh vacuum chemical-vapor deposition (UHVCVD),⁴⁻⁶ and rapid thermal chemical-vapor deposition (RTCVD).^{7,8} In this paper, we report transport, magnetotransport, as well as microwave photoresistivity measurements obtained on both symmetrically and asymmetrically modulation-doped Si/Si_{0.8}Ge_{0.2} heterostructures grown by RTCVD. Well-defined Shubnikov-de Haas oscillations and integral quantum Hall plateaus were observed for magnetic field as low as 1.5 T. In symmetric samples, the carrier concentration obtained from the Shubnikov-de Haas effect was always half the measured Hall concentration and the Hall plateaus at low magnetic field were only observed at filling factors that were multiples of 4. This clearly shows that two parallel highly equivalent channels contribute to the Hall effect in these structures and that the charge transfer is similar at the Si/SiGe and SiGe/Si interfaces. The 2D hole mass parallel to the interfaces was obtained from microwave photoresistivity experiments, which is a very sensitive method for 2D heavy-hole gases. A simple theoretical analysis of the data leads to the determination of the valence-band profile of the heterostructure and quantitatively explains the charge transfer as a function of the sample parameters. Finally, the hole mobility limitation is discussed and we show that the alloy scattering in SiGe could be the dominant limitation process at low temperature.

Our samples, which are listed in Table I, consisted of a $Si/Si_{0.8}Ge_{0.2}/Si$ double heterostructure grown on a (100) Si substrate using the RTCVD technique. Details of this growth technique have been described elsewhere.^{8,9} An 80-nm silicon buffer layer was first grown at 900 °C on the substrate and the temperature was then reduced to 610 °C

for the growth of the heterostructure. The 40-nm-thick SiGe layer was unintentionally doped. For the symmetrically doped samples (1-3), the two Si barriers contained a 16-nm boron-doped region with a concentration $N_a \approx 2.10^{18}$ cm⁻³. In the single side doped samples, only the last (sample 4) or the first (sample 5) grown barrier contained a similar doped region. Undoped Si spacer layers of thickness *d* separated the doped regions from the SiGe layer. Finally, a cap layer (undoped 40-nm Si layer followed by a doped 20-nm Si layer) was grown on all samples. The Ge content *x* was measured by x-ray diffraction. Ohmic contacts were obtained by evaporating and annealing Al on these samples.

The schematic valence-band diagram obtained by requiring that the Fermi level E_F remains constant throughout the structure, is shown in Fig. 1 for both symmetrically doped and single side doped samples. The heavy-hole valence-band discontinuity is $\Delta E_v \approx 160 \text{ meV}$ for $x \approx 0.2$.² The ground hole subband HH₁ is in the cusp of the self-consistent potential, so that two parallel hole gases occur in the symmetric samples. Because of the large 2D hole density of states, the separation E_F -HH₁ is a few meV's for hole densities $p < 10^{12} \text{ cm}^{-2}$ and only the ground subband HH₁ is populated at low tem-

TABLE I. Parameters of the symmetrically and asymmetrically doped samples and carrier concentrations measured at 1.6 K by Shubnikov-de Haas and quantum Hall effects.

Sample No.	Spacer d (nm)	$p_{\rm SdH} \ (10^{11} \ {\rm cm}^{-2})$	$p_{\rm QHE}~(10^{11}~{\rm cm}^{-2})$
	Symmetr	ically doped struct	ures
1	10	6.2	12.4
2	20	4.0	7.8
3	40	2.25	4.3
	Single	side doped structu	res
4	10	6.8	6.8
5	10	6.7	8.1



FIG. 1. Schematic valence-band diagram for (a) a symmetrically doped structure and (b) a single side doped structure as sample 4. The doped cap layer is not represented.

perature. Carrier concentrations measured by both the quantum Hall effect (p_{OHE}) and Shubnikov-de Haas oscillations periodicity (p_{SdH}) at 1.6 K are shown in Table I. For the symmetric structures (samples 1, 2, and 3), p_{SdH} is always half the measured Hall concentration p_{QHE} . This result, previously reported by several groups,^{4,7} indicates that the two interfaces are equivalent and that the wave functions of the two 2D hole gases are nearly independent. For instance, in sample 1 a wavefunction extension of ≈ 3 nm is calculated by using a simple triangular potential model, leading to a 34-nm distance between the two symmetric hole gases. As the SiGe band bending leads to a potential barrier of a few tens of meV's separating the two gases, tunneling processes between the two channels are negligible and no splitting of the HH_1 ground subband is evidenced. For the single side doped samples 4 and 5, the p_{SdH} values are very similar, showing that charge transfer is equivalent at Si/SiGe and SiGe/Si interfaces unlike the $Al_xGa_{1-x}As/GaAs$ system where the "normal" and "inverted" interfaces present significantly different properties. In particular, one must point out the absence of dopant segregation in these samples, the charge transfer being very sensitive to the real thickness of the undoped Si spacer layer. For sample 4, which corresponds to a "normal" modulation-doped Si/SiGe heterojunction, p_{SdH} and p_{OHE} are quite similar as expected if no parallel conduction exists. In sample 5, which corresponds to an "inverted" modulated-doped SiGe/Si heterojunction, there is a discrepancy of $\approx 1.4 \times 10^{11}$ cm⁻² between p_{SdH} and p_{QHE} . This difference is explained by an additional charge transfer from the boron-doped cap layer into the SiGe layer, which gives rise to a second 2D hole gas with a lower density at the higher Si/SiGe interface.

The analysis of the charge transfer can be made by using a simple electrostatic calculation. Taking into account that the Fermi level E_F remains constant throughout the structure, the following relation is obtained in the low-temperature regime:

$$\Delta E_v = \mathbf{H}\mathbf{H}_1 + \pi \hbar^2 (p_{\mathrm{SdH}}) / m_{\parallel} + e^2 dp_{\mathrm{SdH}} / \varepsilon$$
$$+ e^2 (p_{\mathrm{SdH}})^2 / 2\varepsilon N_a , \qquad (1)$$

where $m_{\parallel} \approx 0.4 m_0$ is the 2D hole mass parallel to the interfaces and $\varepsilon = 12\varepsilon_0$ is the SiGe dielectric constant. Here we have assumed that, at low temperature, E_F is near the valence-band edge of Si(p +) doped to $N_a \approx 2.10^{18}$ cm⁻³ because this value is close to the valence-band degeneracy doping. Using a triangular potential approximation to calculate HH₁ and the data given in Table I, one deduced $\Delta E_v = 165 \pm 10$ meV for the five investigated samples, both symmetrically and asymmetrically doped. This remarkable result is quite consistent with previous determinations and calculations of ΔE_v .² It shows that, for given values of N_a and x (Ge content), charge transfer is mainly governed by the thickness d of the undoped spacer layer and does not depend too much on the nature of the interfaces.

Figure 2 shows the Hall resistance as a function of the magnetic field obtained at 1.6 K for symmetric samples 1 and 2. These curves were found to depend on the angle θ between the magnetic field and the surface normal as $(\cos\theta)^{-1}$. Quantized plateaus of resistance h/e^2v with



FIG. 2. Hall resistance versus B at T=1.6 K for (a) sample 2 and (b) sample 1. The arrows indicate the position of the quantized plateaus with the corresponding filling factors. The inset shows the Hall resistance at low B in sample 4.

filling factor v as high as v=32 are clearly resolved for magnetic field $B \ge 1.5$ T [Fig. 2(b)], which demonstrates the high quality of the 2D hole gases in these samples. At low magnetic field (B < 4 T) when the Landau-level spin splitting is not resolved because of the level broadening, plateaus are observed only at v=4n, where n is an integer (v=12, 16, 20, 24, 28, and 32 in sample 1 and v=8, 12, 16, and 20 in sample 2). On the other hand, plateaus at v=2n are visible in the asymmetric samples. For instance, the inset of Fig. 2 shows the low B Hall resistance in sample 4 where plateaus are visible at $v=8, 10, 12, \ldots, 18$. Similar plateaus at v=2n are also observed in sample 5. These data show unambiguously that two parallel highly equivalent channels contribute to the Hall effect in the symmetrically doped structures. Indeed, between two consecutive plateaus, four Landau levels are crossing the Fermi level instead of two in a single 2D hole or electron gas. Similarly, for higher magnetic field when the spin splitting is resolved, plateaus are visible only at even filling factors in samples 1, 2, and 3, while plateaus at both odd and even v are observed in the asymmetric samples 4 and 5. As it was previously pointed out,⁶ the pronounced plateaus and magnetoresistance minima occurring at odd filling factors in the single side doped structures are probably due to the large spin splitting of the Landau levels, which can be comparable to or larger than the cyclotron energy in such 2D hole gases.

Figure 3 shows the Hall mobility versus temperature measured in samples 1 and 2 using a van der Pauw geometry. As the temperature is decreased, mobility enhancement is observed because of the spatial separation of the carriers and ionized impurities. A Hall mobility $\mu \approx 4000 \text{ cm}^2/\text{V}$ s is obtained at low temperature for an undoped spacer layer thickness $d \approx 10-20$ nm. Note that the condition for observing Shubnikov-de Haas oscillations or quantized Hall plateaus is $\mu B \ge 1$, where μ is expressed in m^2/V s. As noted in Figs. 2 and 4, the onset of oscillations or Hall plateaus occurs at $B \le 1.5$ T, and thus the 2D hole gas mobility should be > 6000 cm²/\text{V} s at 1.6 K. Such mobilities are comparable to the best results obtained in similar MBE or UHCVD grown structures.



FIG. 3. Hall mobility versus temperature measured in samples 1 and 2.



FIG. 4. (a) Magnetoresistance ρ and (b) photoresistivity signal $\Delta \rho$ as a function of *B* obtained at 1.6 K in sample 4.

The reasons for the mobility limitation at low temperature could be the background impurity concentration in the SiGe layer, the quality of the heterointerfaces, or the alloy scattering in SiGe. Magnetotransport experiments performed in a double heterostructure similar to sample 3 but with thicker undoped spacer layers (80 nm instead of 40 nm) and, therefore, a lower Hall concentration $(p \approx 2.3 \times 10^{11} \text{ cm}^{-2} \text{ instead of } 4.3 \times 10^{11} \text{ cm}^{-2} \text{ at low}$ B), show a pronounced magnetic freeze-out effect for B > 5 T. This indicates that the quality of the interfaces as well as the residual impurity concentration in the SiGe layer could certainly be improved in these samples. Nevertheless, the dominant mobility limitation could be the alloy scattering. Indeed, the 2D hole gases are essentially localized in the $Si_{1-x}Ge_x$ binary alloy which is a "virtual" crystal with a random distribution of the Ge atoms. Using a simple model (one band approximation, Fang and Howard wave function for the ground state of the 2D hole gas,¹⁰ short-range scatters), the following expression has been obtained for the alloy scattering mobility limitation μ_{all} :¹¹

$$\mu_{\text{all}} = 16e \hbar^3 \{ 3b(m_{\parallel})^2 x (1-x) (\delta V)^2 \Omega \}^{-1} .$$
 (2)

Here Ω is the volume of the unit cell and $b = \{4e^2m_vp/\hbar^2\epsilon\}^{1/3}$ is the inverse of the spatial extension of the Fang and Howard wave function, ${}^{10}m_v \approx 0.3m_0$ being the valence-band mass of Si_{1-x}Ge_x. The quantity δV is the spatial average of the fluctuating alloy potential over the alloy unit cell.^{11,12} δV is difficult to evaluate but is usually found to be a fraction of an eV in the III-V ternary alloys such as Al_xGa_{1-x}As or In_xGa_{1-x}As.^{11,12} For a 2D hole concentration $p = 4 \times 10^{11}$ cm⁻², which is the average concentration in our samples, one obtains $b \approx 5.10^8$ m⁻¹. Taking $\delta V = 0.5$ eV leads to $\mu_{all} \approx 5000$ cm²/Vs, in very satisfying agreement with the lowtemperature mobilities reported here and by many groups in the best modulation-doped (*p*)Si/SiGe heterostructures.^{3,4,7} Even if this model is rather oversimplified and the exact value of δV is uncertain, it is clear that the mobility limitation by the alloy scattering must be taken into account and could explain the relatively low mobility values $\mu \le 6000$ cm²/Vs reported in these modulationdoped heterostructures grown by MBE, UHCVD, or RTCVD.

Finally, we have measured the 2D hole mass parallel to the interfaces m_{\parallel} by photoresistivity measurements under microwave illumination. This technique, previously used to study electron cyclotron and spin resonances,13-15 turns out to be a worthwhile method for the determination of the cyclotron mass, more accurate than direct transmission measurements in the case of 2D hole gases with rather low mobilities and heavy effective masses. The microwave sources were carcinotrons with frequency ranging from 120 to 500 GHz. Using a dc bias current $I \approx 1 \ \mu A$, changes $\Delta \rho$ in sample magnetoresistivity due to the chopped microwave radiation (750 Hz) were detected by using a lock-in amplifier. Figure 4 shows typical traces of the magnetoresistance and its change $\Delta \rho$ due to microwave irradiation at 270 and 333 GHz measured in sample 4 at 1.6 K. $\Delta \rho$ presents magneto-oscillations which correspond to the Shubnikov-de Haas effect and arise from 2D carrier heating. A strong enhancement of the photosignal is observed around the magnetic field $B_r \approx 4$ T at 270 GHz and 4.5 T at 333 GHz, corresponding to the 2D hole cyclotron resonance (CR) when the carrier absorption of the microwave is maximum. The CR absorption correlates, at least only in a first approximation, with the envelope of the trace $\Delta \rho(B)$ as shown in Fig. 4 by the dashed line. The CR linewidth gives some information on the scattering time in the 2D hole gas. For instance, the half-width at half amplitude $\Delta B \approx 2$ T measured at 333 GHz would lead to a hole mobility $\mu \approx 5000 \text{ cm}^2/\text{V}$ s at low temperature in a classical CR description, and to $\mu \approx 4700 \text{ cm}^2/\text{V}$ s if one uses the relation $\Delta B = 0.65 B_{r,17}^{1/2} \mu^{-1/2}$ established in the case of 2D electron gases.^{16,17} Such values are consistent with the

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determinations obtained from both transport measurements and the onset of the Shubnikov-de Haas oscillations in this sample. The maximum of the dashed line leads to $m_{\parallel} = (0.42 \pm 0.02) m_0$ in sample 4 for photon energy ≈ 1 meV. Similar experiments performed in the symmetric samples give $m_{\parallel} = (0.45 \pm 0.02) m_0$ and m_{\parallel} = $(0.42\pm0.02)m_0$ for samples 1 and 2, respectively. Such masses are comparable to or larger than those previously deduced from the temperature dependence of the Shubnikov-de Haas oscillations in similar samples.^{1,4} Furthermore, we have also performed cyclotron resonance experiments by measuring the microwave transmission. The resonance line is broad ($\Delta B \ge 2$ T) and weak with a 2-3% peak absorption comparable to the microwave source fluctuations. The hole mass determination is therefore difficult and, in this case, the photoresistivity method is likely to be more sensitive.

In summary, we have studied the electronic properties of 2D hole gases in symmetrically and asymmetrically modulation-doped Si/SiGe double heterostructures grown by RTCVD. From the quantum Hall measurements, we have demonstrated that the charge transfer is equivalent at each interface and that two parallel equivalent hole gases exist in the symmetric samples, the interactions between the two channels being negligible. A simple theoretical model accounts quantitatively for the charge transfer which is only dependent on the thickness of the undoped spacer layer. The 2D hole masses parallel to the interface were determined by microwave photoresistivity experiments and are found to be weakly dependent on the carrier density of the 2D gas. A more detailed analysis of our results would require Landaulevel calculations, which is not a simple problem in 2D hole gases. Moreover, we have shown that the 2D hole mobility in these modulation-doped heterostructures is most probably limited by the alloy scattering in SiGe at low temperature.

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